UNIVERSITÀ DELLA CALABRIA
Dipartimento di FISICA

ANNUAL REPORT 2010

ACADEMIC YEAR 2009-2010

Scientific publications in 2010

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GENERAL INFORMATION

RESEARCH ACTIVITY

DEPARTMENTAL ADMINISTRATION

Head of Department:
Pierluigi VELTRI

Executive Board:
Riccardo BARBERI, Rosina BARTUCCI, Assunta BONANNO, Vincenzo FORMOSO, Alessandro PAPA , Nicola SCARAMUZZA, Giancarlo SUSINNO, Pierluigi VELTRI

Department Council:
12 Full Professors
18 Associate Professors
23 Senior Researchers
11 Representatives of Post-Doctoral Research Fellows
10 Representatives of PhD students
6 Representatives of the Technical and Administrative Staff

Administrative Secretary:
Giocondo PERRI

RESEARCH PERMANENT STAFF

Full Professors

1. Riccardo BARBERI *FIS/07*
2. Roberto BARTOLINO *FIS/07*
3. Vincenzo CARBONE *FIS/07*
4. Elio COLAVITA *FIS/07*
5. Giovanni FALCONE *FIS/01*
6. Roberto FIORE *FIS/02*
7. Ignazio GUERRA *GEO/10*
8. Antonino OLIVA *FIS/01*
9. Luigi SPORTELLI *FIS/07*
10. Giancarlo SUSINNO *FIS/01*
11. Cesare UMETON *FIS/01*
12. Pierluigi VELTRI *FIS/03*

Associate Professors

1. Raffaele AGOSTINO *FIS/01*
2. Rosina BARTUCCI *FIS/07*
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5. Enzo CAZZANELLI *FIS/03*
6. Gabriella CIPPARRONE *FIS/03*
7. Gennaro CHIARELLO *FIS/07*
8. Giovanni CROSETTI *FIS/01*
9. Laura LA ROTONDA *FIS/01*
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11. Alessandro PAPA *FIS/02*
12. Francesco PIPERNO *FIS/03*
13. Nicola SCARAMUZZA *FIS/07*
14. Marco SCHIOPPA *FIS/01*
15. Enrico TASSI *FIS/01*
16. Carlo VERSACE *FIS/01*
17. Fang XU *FIS/01*
18. Gaetano ZIMBARDO *FIS/06*

Senior Researchers

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2. Michele CAMARCA *FIS/01*
3. Marcella CAPUA *FIS/01*
4. Roberto CAPUTO *FIS/03*
5. Tommaso CARUSO *FIS/07*
6. Anna CUPOLILLO *FIS/01*
7. Antonio DE LUCA *FIS/07*
8. Maria DE SANTO *FIS/07*
9. Vincenzo FORMOSO *FIS/01*
10. Domenico GIULIANO *FIS/02*
11. Antonella GRECO *FIS/07*
12. Rita GUZZI *FIS/07*
13. Fabio LEPRETI *FIS/03*
14. Anna MASTOBERARDINO *FIS/01*
15. Daniela PACILE' *FIS/01*
16. Pasquale PAGLIUSI *FIS/07*
17. Francesco PLASTINA *FIS/01*
18. Leonardo PRIMAVERA *FIS/05*
19. Pierfrancesco RICCARDI *FIS/01*
20. Marco ROSSI *FIS/02*
21. Antonello SINDONA *FIS/01*
22. Giuseppe STRANGI *FIS/07*
23. Francesco VALENTINI *FIS/03*

Post-Doctoral Research Fellows

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2. Marco CASTRIOTA
3. Enrico MACCALLINI
4. Giuseppina NIGRO
5. Marco ONOFRI
6. Barbara ORECCHIO
7. Valentino PINGITORE
8. Alfonso POLICICCHIO
9. Daniela SALVATORE
10. Sergio SERVIDIO
11. Tommaso VENTURELLI

Phd Students in Physics and Quantum Technology

1. Gennaro CORTESE (*XXIV Cycle*)
2. Salvatore LORENZO (*XXIV Cycle*)
3. Silvio PIERRO (*XXIV Cycle*)
4. Giacinto CIAPPETTA (*XXV Cycle*)
5. Vincenzo LAVORINI (*XXV Cycle*)
6. Beatrice MURDACA (*XXV Cycle*)
7. Amedeo PERRI (*XXV Cycle*)
8. Michele PISARRA (*XXV Cycle*)

Phd School "Science and Thecnique": Curriculum "Physics of Complex Systems"

1. Serena DALENA (*XXIV Cycle*)
2. Antonio Raimondo MARINO (*XXIV Cycle*)
3. Antoniou MYRSINI KYRIAKI (*XXIV Cycle*)
4. Giuseppe NISTICO' (*XXIV Cycle*)
5. Fabio COSENZA (*XXIV Cycle*)
6. Giuseppe PUCCI (*XXIV Cycle*)
7. Silvia SALSONE (*XXIV Cycle*)
8. Vincenzo CAPPARELLI (*XXV Cycle*)
9. Denise PERRONE (*XXV Cycle*)
10. Enrico Maria TROTTA (*XXV Cycle*)
11. Angela FASANELLA (*XXV Cycle*)
12. Raul Josuè HERNANDEZ (*XXV Cycle*)
13. Lucia MARINO (*XXV Cycle*)

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2. Gaspare PECORA (*Vice-Administrative Secretary*)
3. Lidia MAIDA
4. Anna Eduardina PASTORE

Secretary

5. Luigina DE ROSE
6. Luigi PARISE

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7. Mario LOMBARDI

Computer Staff

8. Nicola GUARRACINO (*Person in charge*)
9. Fedele STABILE

Research Laboratories

Ion-Matter Interaction and Surface Electronic Spectroscopy

10. Eugenio LI PRETI (*Person in charge*)
11. Vito FABIO

Elementary Particles

12. Francesco SCIOMMARELLA
13. Francesco PELLEGRINO
14. Paola TURCO

Geophysics

15.Gerolamo LATORRE

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Antonio BOZZARELLO (*Administrative Collaborator*)

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BOZZARELLO Antonio	6008
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CARBONE Vincenzo	6131-6033
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Dr. Pietro Giudice *(Trinity College, Dublino)*
The resonance width determination from lattice field theory

Feb 2, 2010
Dr. Tony J.G. Apollaro, (*Dip. Fisica-Polo Scientifico Sesto Fiorentino, Universita' di Firenze*)
Dynamics of entanglement in the presence of spin environment

Feb 12, 2010
Prof. Nico Sanna **(***CASPUR*)
Utilizzo di nuove tecnologie (GPU) nel calcolo ad alte prestazioni

Feb 12, 2010
Dr. Luca Serafini (*INFN)*
Sorgenti Thomson back-scattering (TBS) e sorgenti al THzetopause

Feb 12, 2010
Dr Stefano Lagomarsino (*CNR-INF***)**
Applicazioni di sorgenti TBS e THz, con particolare riguardo al campo bio medico

Feb 16, 2010
Dr. Sabrina Maniscalco (*University of Turku*)
Quantum discord

Feb 17, 2010
Dr. Gabriele Campagnano (*Weizmann Institute, Rehovot, Israel*)
Decoherence and Entanglement Dynamics of Coupled Qubits

Mar 3, 2010
Dr. K. Cosentino (*Dipartimento di Chimica, Università della Calabria*)
Physico-chemical properties of sub-micro and cell-sized unilamellar vesicles affected by millimeter wave radiations

Mar 25, 2010
Prof. A. Andrianov (*Black Holes on Branes: their creation on colliders*)
Gestione delle emergenze, test ed esercitazione

Mar 25, 2010
Prof. Domenec Espriu
The emergence of gravity: a two-dimensional toy model

Apr 22, 2010
Prof. Giuseppe Marmo, (*Università di Napoli "Federico II")*
Formulazione geometrica della Meccanica Quantistica: Separabilità ed Entanglement

Apr 27, 2010
Prof. Gaetano Zimbardo (*Dipartimento di Fisica, UNICAL*)
Galileo Galilei e l'Anno Internazionale dell'Astronomia

May 8, 2010
Prof. Pasquale Sodano (*Università di Perugia*)
Long Range Distance Independent Entanglement in the Kondo regime of the Kondo Spin Chain

May 10, 2010
Prof. C. De Renzis (*Universita' di Messina*)
Prospettive per nuove applicazioni dosimetriche

Jun 25, 2010
Prof. Derek Marsh (*Max-Planck Institut für biophysikalische chemie)*
Packing of lipids in membranes: densitometry and diffraction

Jun 10, 2009
Pasquale Sodano *(Università di Perugia)*
Teorie di Campo di Modelli di Spin (II)

Sep 17, 2010
Prof. William Matthaeus *(University of Dilaware, USA)*
Magnetic Reconnection I, II: Properties of the magnetic field, flux tubes, field lines and conservation laws, and early theoretical ideas

Sep 17, 2010
Prof. William Matthaeus (*(University of Dilaware, USA)*)
Magnetic Reconnection III: Fundamental ideas in reconnection theory

Sep 17, 2010
Prof. William Matthaeus (*(University of Dilaware, USA)*)
Magnetic Reconnection IV: Reconnection with Hall Effect and Turbulence, the influence of additional plasma effects

Sep 17, 2010
Prof. William Matthaeus ((*University of Dilaware, USA*))
Physical issues in coronal heating and origin of the solar wind

Sep 30, 2010
Prof. Massimo Robberto (*Space Telescope Science Institute, NASA, USA*)
Metodi Osservativi per Comprendere la Natura della Dark Energy

Oct 8, 2010
Prof. Dimitrios Gournis, (*Department of Materials Science & Engineering University of Ioannina Greece*)
Top-down and bottom-up approaches for the synthesis of novel layered hybrid materials

Oct 26, 2010
Prof. Abraham C.-L. Chian*(National Institute for Space Research (INPE), Brazil & California Institute of Technology (Caltech), USA*
Amplitude-phase synchronization and intermittent turbulence in the earth-ocean-space environment

LAUREA THESIS' in 2010

1st LEVEL DEGREE THESIS' IN 2010

July 20
Daniel Francesco FILICE
Emissione di elettroni secondari da grafene su Ni (111)
Relatore: Pierfrancesco RICCARDI

Laura ZINNO
Estinzioni di massa e raggi cosmici extragalattici: un modello basato sulla legge di Fick frazionaria
Relatore: Gaetano ZIMBARDO

Oct 6
Francesco LA RUFFA
Problemi dell'approccio delle storie consistenti alla teoria quantistica
Relatore: Giuseppe Antonio NISTICO'

Francesca CUTERI
La doppia buca di potenziale e gli istantoni
Relatore: Alessandro PAPA

Andrea NAVA
Meccanismo di Kibble-Zurek: difetti nei cristalli liquidi
Relatore: Domenico GIULIANO

Saverio Mirko VIOLA
Plasma diagnostic data analysis for the characterization of the ionosferic plasma environment reproduced in the INAF-IFSI Large Plasma Chamber facility
Relatore: Vincenzo CARBONE

Francesco PUCCI
Onde di Alfvén in mezzi disomogenei
Relatore: Francesco MALARA

Dec 13
Giovandomenico CARDUCCI
Prestazioni dello Spettrometro per Muoni dell'Esperimento ATLAS
Relatore: Enrico TASSI

Antonio GIUSEPPE
I Primi Risultati di Fisica dell'esperimento ATLAS
Relatore: Enrico TASSI

Domenico ALJ
Apparato f-PcT di tipo Sievert per la caratterizzazione di processi di fisisorbimento di idrogeno su materiali ad alta superficie specifica
Relatore: Alfonzo POLICICCHIO

Giuseppe BAGNATO
Studio delle proprietà elettroniche e di geometria locale di superfici di grafite mediante tecniche di assorbimento di raggi x o elettroni di alta energia
Relatore: Raffaele Giuseppe AGOSTINO

Michela DEL GAUDIO
Bubble domains in cristalli liquidi colesterici
Relatore: Riccardo BARBERI

Arianna APRILE
Sum frequency generation vibrational spectroscopy for molecular recognition at interface
Relatore: Pasquale PAGLIUSI

2st LEVEL DEGREE THESIS' IN 2010

May 11
Domenico MEDURI
The Solar Dinamo dilemma
Relatore: Vincenzo CARBONE

July 21
Aldo BRUNETTI
Stati legati e funzioni di correlazioni in teorie bosoniche su grafi a stella
Relatore: Domenico GIULIANO

Angelica RANIA
Dosimetria di un acceleratore lineare per radioterapia conformazionale 3D
Relatore: Luigi SPORTELLI

Oct. 21
Gaetano DE VITA
Studio delle proprietà topologiche del camppo magnetico solare nelle regioni attive
Relatore: Pierluigi VELTRI

Loris D'ALESSI
Modulazione quasi-biennale del flusso di neutrini solari e correlazioni con il ciclo di attività magnetica del sole
Relatore: Vincenzo CARBONE

Christian Natale GENCARELLI
Analisi e modellizzazione della qualità dell'aria nel Mediterraneo: impatto del traffico marittimo sulla produzione di ozono troposferico.
Relatore: Vincenzo CARBONE

Emanuele MANCINI
Adsorbimento di propano e propilene all'interno di zeoliti 13X
Relatore: Raffaele Giuseppe AGOSTINO

Dec. 6
LucantonioMUSTICA
Fattori naturali e antropogenici nei cambiamenti climatici su scale secolari: analisi della piovosità negli USA
Relatore: Vincenzo CARBONE

Mario CARDACI
Studio dei tubi flusso cromometrico nella teoria di gauge SU (3) su reticolo
Relatore: Alessandro PAPA

Caterina TONE
Studio di membrane di copolimeri a blocco con tecniche di microscopie a forza atomica
Relatore: Maria Penelope DE SANTO

Domenica CARLOMAGNO
Misura della sezione d'urto (e+ e- 3p) con l'esperimento KLOE all'acceleratore DAFNE di L.N.F.
Relatore: Marco SCHIOPPA

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(*22° Cycle*)
Massimo VENTURELLI
Study of Z0 and Higgs production at ATLAS & Dream calorimetry
Supervisore: Laura LA ROTONDA

(*23° Cycle*)
Roberta VASTA
Adsorption properties of carbon nanotubes and application of Thermal Desoprtion Spectroscopy to ammonia and methane ices and zoisite
Supervisore: Assunta BONANNO

Davide Remo GROSSO
Studi di superficie per migliorare le prestazioni degli acceleratori di particelle
Supervisore: Assunta BONANNO

Gianfranco MORELLO
Search of light U boson in e+e- --> mu mu gamma channel with KLOE experiment at DAFNE collider at LNF and application of GEM technology for the KLOE-2 Inner Tracker
Supervisore: Marco SCHIOPPA

Melissa INFUSINO
Periodic and a-periodic structures realized by innovative experimental techniques
Supervisore: Cesare UMETON, Raffaele AGOSTINO

1. ASTROPHYSICS

Professors and Researchers

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Gaetano Zimbardo
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Enrico Maria Trotta
Loris D'Alessi
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S. C. Solomon *(Department of Terrestrial Magnetism, Carnegie Institution of Washington, Washington DC, USA)*
R. B. Dahlburg *(Naval Research Laboratory, Washington DC, USA)*
P. Dmitruk *(Departemento de Fisica, Universitad de Buenos Aires, Argentina)*

Introduction

The research in Astrophysics in the Physics Department of University of Calabria is mainly devoted to study plasma physics. Most of interplanetary matter and of the solar atmosphere is actually formed by plasma. For that reason, most of data obtained in space missions, or by solar observatories, can be interpreted within the framework of plasma physics. Such data have allowed for the construction of models describing astrophysical phenomena, and they have represented a powerful tool of investigation which has often given new perspectives for the comprehension of phenomena in fundamental physics. This has allowed to use the space as a huge laboratory where measurements not accessible in a terrestrial laboratory can be performed. On the other hand, using analogue techniques both on space and on laboratory measures allows for a comparison of the basic physical phenomena that take place on completely different scales, and for a comprehension of such phenomena which are relevant both in the domain of controlled thermonuclear fusion and in the perspective of industrial applications.

The group of Astrophysical Plasmas of Calabria University has been involved in such kind of problems, in collaboration with other groups of Italian universities (Pisa; Milano) and with Italian Institutions (IFSI - CNR of Frascati;

Osservatorio Astrofisico di Arcetri; Consorzio RFX of Padova; INFN Milano) and foreign Institutions (Observatoire de Paris-Meudon, France; Observatoire de la Cote d'Azur, Nice, France; Université de Bordeaux, I/CNRS, Pessac, France; Goettingen University, Germany; International Space Science Institute, Bern, Switzerland; Swedish Institute of Space Physics, Uppsala, Sweden; Universitat Politecnica de Calalunya, Barcelona, Spain; Universidad Complutense de Madrid, Spain; University of Innsbruck, Austria; University of Ioannina, Greece; Tbilisi University, Georgia; Space Research Institute, Mosca, Russia; Bartol Research Institute, Newark, Delaware, USA; University of Delaware, Newark, USA; NASA Goddard Space Flight Center, Greenbelt, MD, USA; West Virginia University, USA; The John Hopkins University, Laurel, MD, USA; University of Colorado, Boulder, CO, USA; University of Michigan, Ann Harbor, MI, USA; Carnegie Institution of Washington, Washington DC, USA; Naval Research Laboratory, Washington DC, USA; Universitad de Buenos Aires, Argentina).

The specific research themes under study during the year 2010 are described in the following.

1.1 MAGNETOHYDRODYNAMIC TURBULENCE AND KINETIC EFFECTS IN THE INTERPLANETARY SPACE

Third-order law for Magnetohydrodynamic with constant velocity shear

The Yaglom-law for magnetohydrodynamic (MHD) turbulence relates the statistics of the third-order mixed momenta of velocity and magnetic field fluctuations to the characteristic scale of fluctuations through the transfer rate of turbulent energy to small scales. This theory for third-order structure functions, valid only in homogeneous and incompressible systems, has been extended to the case in which a constant velocity shear is present. A generalization is found of the usual relation between third-order structure functions and the dissipation rate in steady inertial range turbulence, in which the shear plays a crucial role. In particular, the presence of shear leads to a third-order law which is not simply proportional to the relative separation. Using direct numerical simulations of two-dimensional (2D) MHD turbulence with shear, this new generalization of the theory has been confirmed. The presence of the shear effect broadens the circumstances in which the law can be applied. This extension of the Yaglom-law may have possible implications for laboratory and space plasmas.

Local processes in MHD turbulence and non-Gaussian statistics

Two central features of magnetohydrodynamic (MHD) turbulence are generally studied independently: the production of intermittency and the appearance of distinctive states associated with turbulent relaxation. It is, for example, well known that the random phase approximation fails as a turbulence description in that it cannot produce non-Gaussian statistics, such as high kurtosis of vorticity and current, multifractal scaling of moments, and other signatures of intermittency. On the other hand, MHD relaxation theory has led to notable successes associated with Taylor relaxation, selective decay, global dynamic alignment, and helical dynamo action.

Direct numerical simulations show that undriven MHD turbulence spontaneously generates coherent spatial correlations of several types, associated with local Beltrami fields, directional alignment of velocity and magnetic fields, and anti-alignment of magnetic and fluid acceleration components. These correlations suppress nonlinearity to levels lower than what is obtained from Gaussian fields, and occur in spatial patches. We suggest that this rapid relaxation leads to non-Gaussian statistics and spatial intermittency. To further confirm this scenario, we have performed spectral method simulations of ideal MHD, investigating the production of coherent small scale structures. The near-identical growth (in the initial stage) of non-Gaussianity in ideal and non-ideal cases suggests that generation of coherent structures and breaking of self-similarity are essentially ideal processes. This has important implications for understanding the origin of intermittency in turbulence.

Magnetic reconnection in turbulence

Magnetic reconnection is a nonlinear process that occurs in many space, astrophysical, and laboratory systems. The underlying common feature for these systems is the presence of an inhomogeneous magnetic field that changes rapidly across a very narrow region. Generally, a strong peak in the electric current density is present. Reconnection implies the presence of a magnetic X-type neutral point in two-dimensions (2D), and more generally a change in magnetic topology resulting in the conversion of magnetic into kinetic energy. Since it might occur in any region separating topologically distinct magnetic flux structures, reconnection might be expected to be of importance in more general circumstances, including magnetohydrodynamic (MHD) turbulence (Fig. 1.1). Very high resolution numerical simulations of 2D MHD turbulence reveal the presence of a large number of X-type neutral points where magnetic reconnection occurs. In this scenario, reconnection is spontaneous, but locally driven by the fields and boundary conditions provided by turbulence

itself. Because of the complex magnetic topology, turbulence leads to different kinds of reconnecting patches. In contrast with laminar reconnection models that provide a single predicted reconnection rate for the system, turbulent resistive MHD gives rise to a broad range of reconnection rates that depend on local turbulence parameters. Many potential reconnection sites are present, but only a few are selected by the turbulence, at a given time, to display robust reconnection electric fields. In this way, the present problem differs greatly from studies of reconnection that assume that it occurs in isolation. In turbulence the associated reconnection rates are distributed over a wide range of values and scales with the geometry of the diffusion region. Locally, these events can be described through a variant of the Sweet-Parker model, in which the parameters are externally controlled by turbulence. This new perspective on reconnection is relevant in space and astrophysical contexts, where plasma is generally in a fully turbulent regime.

Study on the Turbulent Magnetic Dynamo: A Self-consistent Nonlinear Model

Magnetic fields are ubiquitous in our Universe: planets, stars, entire galaxies, black holes etc. all having associated magnetic fields. The most accredited mechanism which explains the generation and self-sustaining of a magnetic field is the so-called dynamo effect, i.e. the maintaining of a magnetic field against diffusive effects by the motion of electrically conducting fluids. One of the examples of dynamo effect closest of our experience is the presence of the Earth's magnetic field. Paleomagnetic measurements showed that the Earth's magnetic dipole reverses stochastically in time, with intervals ranging from 10^4 to 10^7 years. Many researchers have dealt with this problem using direct numerical simulations (DNS), even if realistic parameter regimes are beyond the power of actual supercomputers. Difficulties arise from the realistic description of both large-scales and small-scale (high Reynolds numbers) turbulence, which is responsible of dynamo effect. Actual DNS are able to simulate only some few polarity reversals of the magnetic field. To overcome these difficulties we have built a self-consistent nonlinear dynamo model, which can describe turbulent fluctuations at very large Reynolds numbers. In particular, our model couples the evolution of the large-scale magnetic field with turbulent dynamics of the plasma at small scales by electromotive force. We solve the induction equation, describing the time evolution of the large-scale magnetic field, in local approximation; while the turbulent dynamics at small scales is described by using a low-dimensional model (shell model). Turbulent fluctuations at small scales generate a dynamical situation in which the large–scale magnetic field randomly jumps between two states which represent the opposite polarity of the magnetic field. An important result of this research is related to the critical role that the turbulence plays in the dynamo effect. The model allows us to reproduce very long time series of reversals. The statistical study of these polarity reversals reveals, together with paleomagnetic data, the presence of long-time hidden correlations in the chaotic dynamo process, bringing to light some degree of memory in the history of the Earth's magnetic field.

Intermittent structures and magnetic discontinuities in MHD turbulence and solar wind

We re-examine the statistics of rapid spatial variations of the magnetic field in simulations of Hall magnetohydrodynamic (HMHD) turbulence, using analysis of intermittency properties of the turbulence, and also using methods often employed to identify discontinuities in the solar wind (as in the earlier work of Tsurutani & Smith 1979). The hypothesis is that the statistics of intermittent events might be related to the statistics of classical MHD discontinuities. Indeed, those methods give similar distributions of events, often identifying the same structures. This suggests that observed discontinuities might not be static solutions to the MHD equations, but instead may be related to the intermittent structures that appear spontaneously in MHD turbulence. Then, we further examine the link between intermittency and MHD discontinuities, directly comparing statistical analysis from solar wind data and 3D and 2D simulations of MHD turbulence. The comparison between ACE solar wind data and simulations of magnetohydrodynamic turbulence shows a good agreement in the Waiting-Time analysis of magnetic field discontinuities. This result adds to evidence that solar wind magnetic structures may emerge fast and locally from nonlinear dynamics that can be properly described in the framework of MHD theory.

Using high Reynolds number simulations of two-dimensional magnetohydrodynamic (2D MHD) turbulence as a test case, a statistical association between tangential discontinuities and magnetic reconnection is demonstrated. Methods employed in previous studies on discontinuities and reconnection in turbulence are used to identify sets of possible reconnection events along a one-dimensional path through the turbulent field, emulating experimental sampling by single detector in a high speed flow. The goal is to develop numerical algorithms for identifying candidate reconnection events in space physics applications. We find that sets of strong discontinuities, identified using the normalized partial variance of vector increments (PVI), include an increasing fraction of reconnection events as the threshold for identification grows. Magnetic discontinuities become almost purely reconnection events for high thresholds, with values generally higher than six standard deviations.

Inhomogeneous heating in the solar wind

Solar wind observations and magnetohydrodynamic (MHD) simulations are used to probe the nature of turbulence heating. In particular, the electron heat flux, electron temperature, and ion temperature in the solar wind are studied using ACE and Wind data. These heating diagnostics are also compared with MHD simulation estimates of the local dissipation density. Coherent structures, which are sources of inhomogeneity and intermittency in MHD turbulence, are found to be associated with enhancements in every heating-related diagnostic. This supports the hypothesis that significant inhomogeneous heating occurs in the solar wind, connected with current sheets that are dynamically generated by MHD turbulence. Indeed, a subset of these coherent current sheets might be candidates for magnetic reconnection. However, the specific kinetic mechanisms that heat and accelerate particles within these structures require further study.

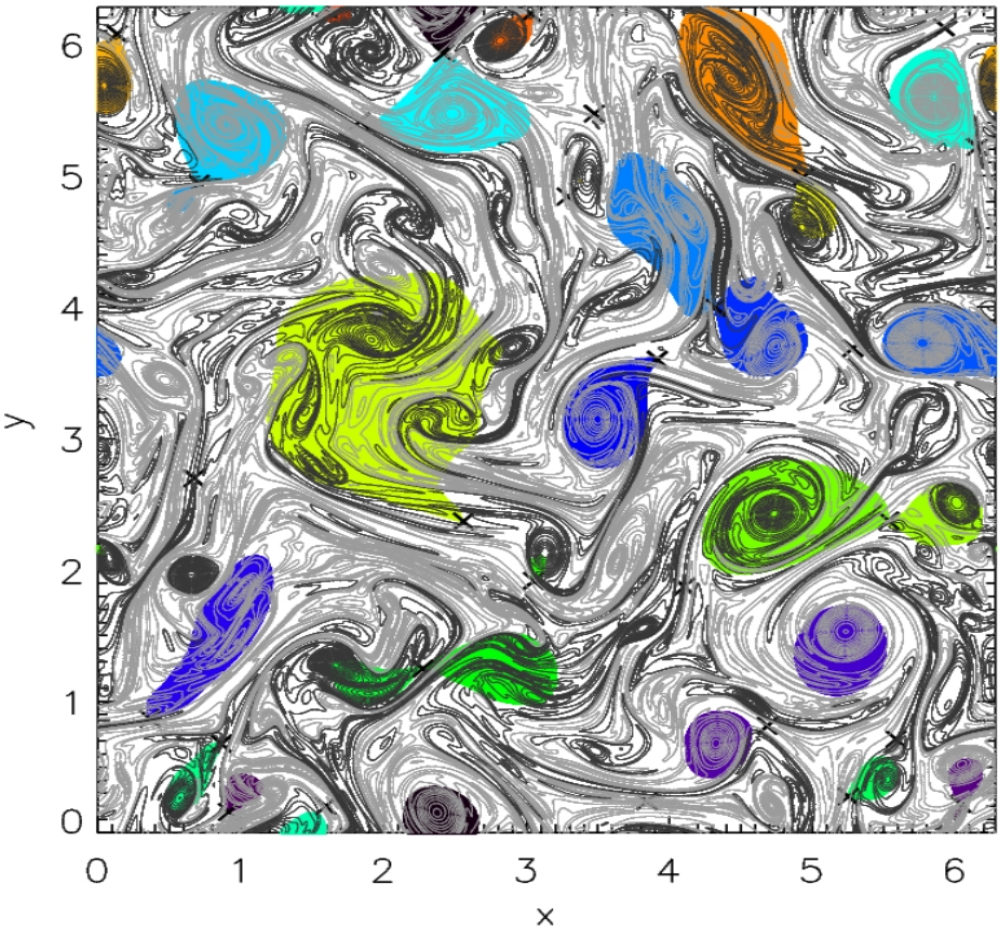

Fig 1.1: *Level contour of the vorticity in two-dimensional turbulence. Colored (shaded) surfaces indicates regions of quasi-equilibrium, where strong vortices persist in time.*

Kinetic driven turbulence: Structure in space and time

The structure in space and time of a driven turbulent magnetoplasma is analyzed using kinetic simulations. For a two dimensional case with a strong uniform out-of-plane magnetic field, large scale driving produces a turbulent state that spans fluid scales to kinetic proton scales. There are fluid electrons in this hybrid representation. In near steady conditions, spectral analysis shows an almost complete absence of discrete point spectral features that would be associated with a dispersion relation and wave activity. While there is indication of a low level of wave activity, the results show that the dynamics are dominated by nonlinear activity. Implications for understanding plasma cascade, dissipation, and heating are discussed.

Local relaxation and maximum entropy in two-dimensional turbulence

The phenomenon of vortex merging in two-dimensional hydrodynamics has been investigated through direct numerical simulations. The fast and local processes that occur during the turbulent relaxation of a randomly initialized system in periodic geometry have been examined. The analysis reveals that many of the coherent structures can be described by a local principle of maximization of entropy. The validity of this entropy principle has been further confirmed by time-dependent statistics using a contour-tracking technique. Implications for the description of persistent coherent vortices (Fig. 1.1) commonly observed in nature are suggested, including growing evidence for the wide applicability of maximum entropy-based relaxation principles.

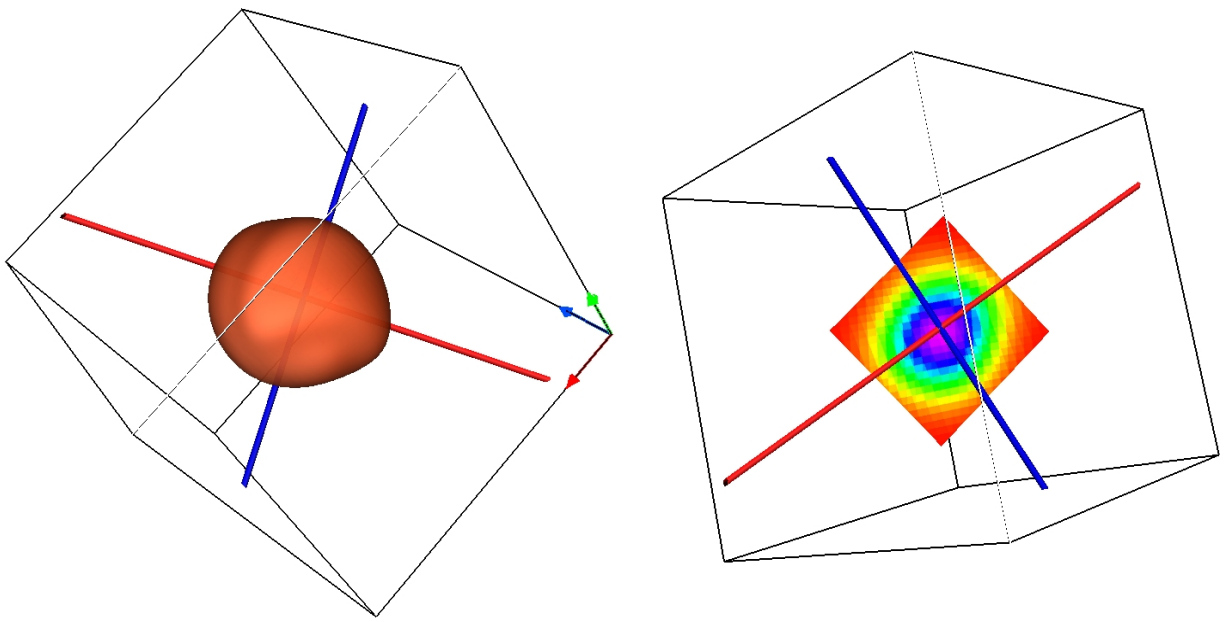

Fig 1.2*: Left: Isosurfaces of the velocity distribution function at a given spatial position in turbulence. Right: two dimensional cut of the distribution function in the minimum variance reference frame. The red (blue) axis indicate the maximum (minimum) variance direction. The distribution function is elongated along the direction of the local magnetic field.*

Kinetic processes in Vlasov Turbulence

Strong turbulence, a difficult problem in fluid regimes, is an even more challenging subject in a kinetic, low collisionality, plasma. Plasma turbulence additionally involves wave-particle interactions that are responsible for crucial effects such as plasma dissipation, acceleration mechanisms, heating, temperature anisotropy and so on. We study these local kinetic processes using a hybrid-Vlasov numerical code, in a fully turbulent regime (Fig. 1.2). Nearby regions of strong magnetic activity, evident kinetic effects manifest through a deformation of the distribution function. These departures from a equilibrium Maxewllian configuration may be responsible for the production of heating and anisotropy (Fig. 1.3), commonly observed in many astrophysical turbulent systems.

Short-scale termination of solar wind turbulence

In interplanetary plasmas, due to the absence of collisional viscosity, fundamental questions about how energy is transfered from large to small scales and how it is eventually dissipated are still open. Since astrophysical plasmas are known to be highly turbulent, the understanding of the role of turbulence in such collisionless systems would be of key relevance for the explanation of the energy transport and heating problem in space. The fast technological development of supercomputers gives nowadays the possibility of using kinetic Eulerian Vlasov codes that solve the Vlasov-Maxwell equations in multi-dimensional phase space. The use of these "zero-noise" codes is crucial in the analysis of the

development of turbulent spectra at typical kinetic scales, where the energy level of the fluctuations is typically very low. To study the system dynamics at frequencies of the order of the ion cyclotron frequency, we built up a hybrid-Vlasov model, in collaboration with Prof. A. Mangeney (Observatory of Paris-Meudon) and Prof. F. Califano (Università di Pisa). Within this model, the ion dynamics is described through the Vlasov equation and the electrons are treated as a fluid. A generalized Ohm equation, that retains Hall effect and electron inertia terms, is considered. Faraday equation, Ampere equation (the displacement current is neglected) and an equation of state for the electron pressure close the system. Quasi-neutrality is assumed. The above equations are solved through a numerical hybrid-Vlasov code in a multi-dimensional phase space (typically 1-D or 2-D in physical space and 3-D in velocity space), discretized on a uniform Cartesian grid. Our numerical analysis showed that the electrostatic turbulence in space plasmas with plasma beta of the order of unity (typical value for the solar wind) consists of longitudinal waves with dispersion relations of the acoustic form and it is associated with the generation of ion-beam distributions. Beside the ion-acoustic branch, which is in agreement with solar wind data from Helios 1 and 2 spacecraft, the kappa-omega spectrum of the numerical signals indicates the presence of a new branch of kinetic waves propagating at velocity close to the ion thermal speed. These waves are driven by kinetic effects of particle trapping and are stable against Landau damping due to the formation of trapping plateaus in the ion velocity distributions. We found that these novel kinetic fluctuations are nonlinear Bernstein-Green-Kruskal-like (BGK) solutions of the hybrid Vlasov-Maxwell equations, driven by particle trapping phenomena. In fact, taking into account particle trapping allows for the existence of fluctuations with phase speed in the bulk of the ion velocity distribution, which represent a privileged way for electrostatic turbulence to develop towards short scales.

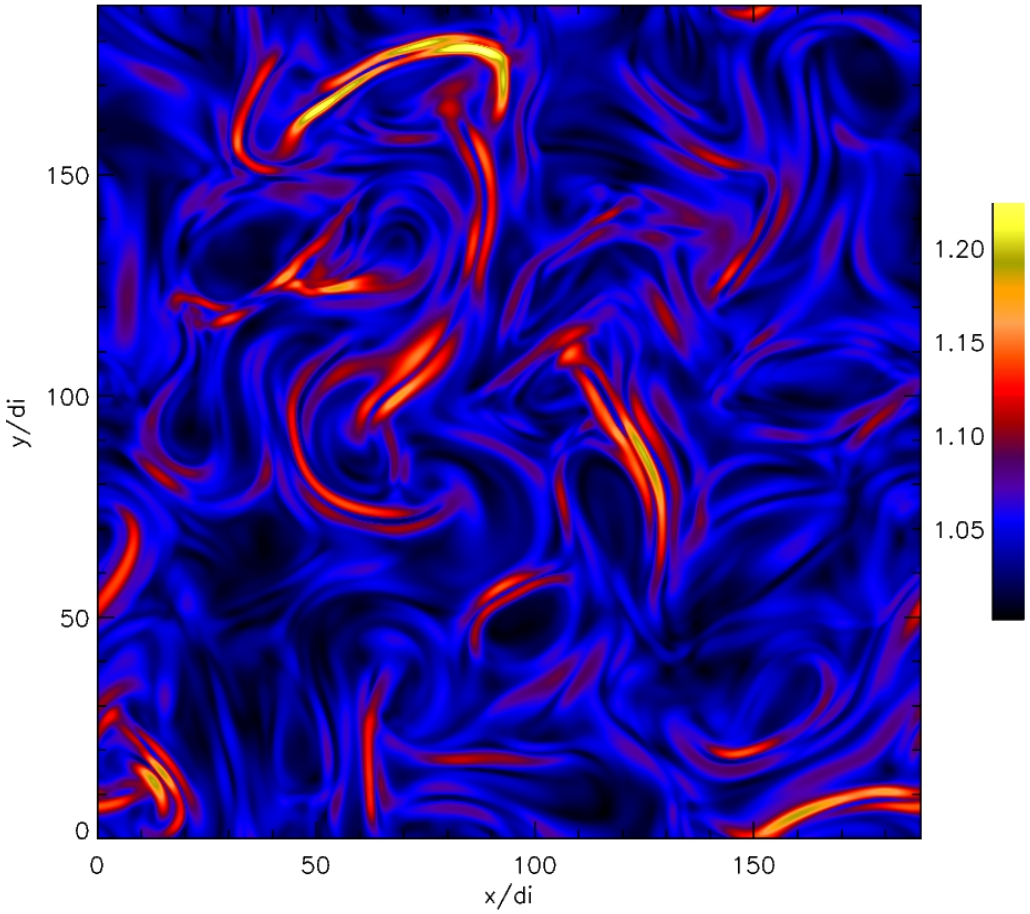

Fig 1.3: *Color contour of the temperature anisotropy in two-dimensional plasma turbulence. Sites of strong anisotropy appear intermittently in space, nearby regions of strong magnetic stress.*

A massive parallelizzation process on the numerical algorithm through which the hybrid – Vlasov equations are solved, performed in collaboration with Dr. Carlo Cavazzoni (CINECA), allowed for the first time simulations of turbulence at short wavelengths in the solar wind in a 2D-3V phase space(2D in physical space and 3D in velocity space) with significant numerical resolution. The results of these simulations open a new scenario in the study of kinetic effects in the dynamics of space plasmas. In fact, through our numerical analysis we give evidence that in presence of a background magnetic field the longitudinal direction can be a preferential channel to transfer the energy injected at large wavelengths towards short kinetic scales. We found that this channel consists of electrostatic fluctuations driven by particle trapping effect. The analysis of the numerical signals showed that this dynamics favors the generation of longitudinal anisotropy in the energy spectra. It is worth noting that previous MHD or PIC simulations in regime of large wavelengths predicted the generation of perpendicular anisotropy, then our results point out that the inclusion of kinetic effects is crucial in the description of the solar wind dynamics at short scales.

Recently, a new version of the hybrid Vlasov-Maxwell code has been developed to include the kinetic dynamics of heavy ions (alpha particles) in the solar wind. The inclusion of an additional kinetic species required to modify the generalized Ohm's law for the electric field and caused a significant increase in the computational time needed to run a typical simulation. On the other hand, the new hybrid Vlasov code gives for the first time the possibility to analyze the role of the heavy minor ions in the development of the solar wind turbulent cascade. In situ measurements from spacecraft in the solar wind have clearly shown that the heavy minor ions are heated and accelerated preferentially as compared to protons and electrons. The physical mechanisms responsible for this phenomenology are not yet identified and their explanation could provide relevant insights into the nature of the turbulent heating process in space plasmas.

Kinetic acoustic-like fluctuations driven by particle trapping effects

The novel kinetic electrostatic fluctuations recovered in the hybrid-Vlasov simulations of turbulence in solar wind plasmas turn out to be analogous (at low frequency) to the so-called electron acoustic waves (EAWs), which are acoustic-like fluctuations at phase speed close to the electron thermal speed. An EAW is a nonlinear wave with a carefully tailored trapped particle velocity distribution. Within linear theory an EAW would be heavily Landau damped, since the wave phase velocity is comparable to the thermal speed. However, the EAW is a Bernstein-Greene-Kruskal (BGK) nonlinear mode with electrons trapped in the wave troughs. Because of the trapped electrons, the velocity distribution is effectively flattened at the wave phase speed, and this turns off Landau damping. We proved the existence of these kinetic oscillations, predicted within kinetic theory, both numerically through PIC and Vlasov simulations and experimentally in a pure ion plasma apparatus, in collaboration with the nonneutral plasma laboratory at University of California at San Diego, lead by Prof. T. O'Neil. These kind of machines (Penning-Malmberg traps) are extremely useful for the study of fundamental physics in the kinetic regime, since the confining time of the nonneutral plasmas is of the order of several days. For example, it is possible to investigate the energy exchange between waves and particles in Landau damping phenomena both in linear and nonlinear regimes or the nature of the instabilities driven by nonthermal distributions of particle velocities as well as plasma heating processes. This kind of analysis is relevant in the interpretation of physical phenomena also observed in space plasmas.

1.2 OBSERVATIONS AND TURBULENCE MODELS IN THE SOLAR ATMOSPHERE

Nonlinear development of current sheet instability for a solar coronal loop

We investigated the dynamics of the coronal plasma in order to understand the physical mechanism responsible for nanoflares. Studying the dynamical behaviour of a current sheet in a plasma system with line-tied boundary conditions, we can relate the explosive plasma instability, which takes place in this framework, to the impulsive energy release thought to take place in a solar coronal loop. Within this interpretation, we want to investigate a basic situation in which the instability develops in a specific magnetic topology driven by a shearing velocity at the boundaries of the simulation box (top and bottom). Imposing a velocity shear at boundary, we expect the formation of current sheets which undergo a fragmentation after the saturation of the tearing modes and the secondary instability. In this case we expect also the formation of energy spectra (kinetic and magnetic energy spectra) with a power-law range with slope around two. The line-tied boundary condition however strongly restricts the plasma dynamics. We want to study closely this situation in order to understand how the energy which heats the corona is derived from stresses that have built up in the magnetic field. We solve the cold plasma MHD equations with a background homogeneous magnetic field neglecting loop curvature by using a new parallelized viscoresistive three-dimensional code. The code employs a Fourier collocation-finite difference spatial discretization, and uses a third-order Runge-Kutta temporal discretization.

Dynamics of the solar chromosphere

The exact nature of the quiet solar chromosphere and especially its temporal variation, are still subjects of intense debate. One of the contentious issues is the possible role of the magnetic field in structuring the quieter solar regions. This is the motivation that has led our research group, in collaboration with the Osservatorio Astrofisico di Arcetri, to concentrate on multiwavelength observations and interpretation of small scale phenomena, both in the quiet and active Sun. In particular, we characterize the dynamics of the quiet inter-network chromosphere by studying the occurrence of acoustic shocks and their relation with the concomitant photospheric structure and dynamics, including small scale magnetic structures. For this scope we use the Interferometric Bidimensional Spectrometer (IBIS) which has been built at Arcetri and is presently installed at the Dunn Solar Telescope of the US National Solar Observatory. By analyzing a comprehensive data set that includes high-resolution chromospheric (Ca II 854.2 nm) and photospheric (Fe I 709.0 nm) spectra we have identified the spatio-temporal occurrence of the acoustic shocks and compared it with the photospheric dynamics by means of both Fourier and wavelet analysis and study the influence of magnetic structures on the phenomenon. Mid-chromospheric shocks occur within the general chromospheric dynamics pattern of acoustic waves propagating from the photosphere. In particular, they appear as a response to underlying powerful photospheric motions at periodicities nearing the acoustic cut-off, consistent with 1-D hydrodynamical modeling. However, their spatial distribution is highly dependent on the local magnetic topology. We find that large portions of the fields of view undergo very few shocks, since they are "shadowed" by the horizontal component of the magnetic field. The latter is betrayed by the presence of chromospheric fibrils, namely slanted structures with distinct dynamical properties.

Our results indicate that the magnetic field might play a larger role in structuring the quiet solar chromosphere than normally assumed. The presence of fibrils highlights a clear disconnection between the photospheric dynamics and the response of the geometrically overlaying chromosphere. As these results hold for a mid-chromospheric indicator such as the Ca II 854.2 line, it is expected that diagnostics formed in higher layers, such as UV lines and continua, will be affected to a greater extent by the presence of magnetic fields, even in quiet regions. This is relevant for the chromospheric models that make use of such diagnostics.

Turbulence in the solar chromosphere

Convective and oscillatory motions occurring in the Sun interior continuously inject energy in the solar atmosphere and perturb its magnetic structure, giving rise to several non-linear dynamical processes and turbulence phenomena. The behaviour of the outer layers of the solar atmosphere (chromosphere and corona) at small spatial and time scales still presents many open questions and is an ongoing subject of study. In particular, the nature of the solar chromosphere and the source of its heating remains one of the main open problems of solar physics. In this framework, the role played by turbulence has not yet been investigated in sufficient detail. We have studied the acoustic properties of the solar chromosphere in the high-frequency regime using a time sequence of velocity measurements in the chromospheric Ca ii 854.2 nm line taken with the Interferometric Bidimensional Spectrometer (IBIS). By using the Yaglom law for third order moments of velocity increments we have estimated the energy dissipation rate of acoustic turbulence in regions of the solar chromosphere with different magnetic properties. The results of this analysis suggests that the turbulent dissipation could give a significant contribution to the heating of the chromosphere.

Energy balance and cascade in MHD turbulence in the solar corona.

The dynamics of fluctuations in a closed coronal structure is regulated by two phenomena: the resonance excited by motions at the loop basis, that stores energy within the loop; nonlinear couplings, that move energy towards smaller scales. We extended a previous work that had been carried out considering a uniform background to the case of a nonuniform density, in order to include possible effects due to the longitudinal stratification in a loop. In fact, density inhomogeneities affect the properties of resonant eigenmodes (frequencies and spatial profiles) which, in turn, could modify the nonlinear couplings among eigenmodes thus affecting the energy balance. Results shows that the basic aspects of phenomenology, namely: the input energy flux, the nonlinear flux and the level of velocity fluctuations are non substantially modified by the presence of a longitudinal density inhomogeneity, the spatial average of density profile playing the major role in determining the above quantities..

Coronal heavy ion reflection and heating by quasi-perpendicular collisionless shocks.

We propose a new model for explaining the observations of preferential heating of heavy ions in the polar solar corona. We consider that a large number of small scale shock waves can be present in the solar corona, as suggested by recent observations of polar coronal jets by the Hinode and STEREO spacecraft. The heavy ion energization mechanism is,

essentially, the ion reflection off supercritical quasi-perpendicular collisionless shocks in the corona and the subsequent acceleration by the motional electric field E = - V x B. The acceleration due to the electric field is perpendicular to the magnetic field, giving rise to large temperature anisotropy with perpendicular temperature much larger than the parallel one, which can excite ion cyclotron waves. Also, heating is more than mass proportional with respect to protons, because the heavy ion orbit is mostly upstream of the quasi-perpendicular shock foot. The observed temperature ratios between O(5+) ions and protons in the polar corona, and between alpha particles and protons in the solar wind are easily recovered. We also identify the mechanism of heavy ion reflection, which is based on ion gyration in the magnetic overshoot of the shock. A test particle numerical simulation has been developed which allows to study the process of heavy ion reflection, showing that under typical conditions the rate of reflection of heavy ions is comparable to that of protons.

Plasma jets in the solar corona.

We have started a new research activity based on the analysis of UV data from the STEREO dual spacecraft. Preliminary analysis has led to the identification of about 80 plasma jets in the polar corona, which have been organized in a catalogue. This jets show that a substantial activity is going on even in the quiet regions. An assessment of the energetic of jets is under way. Analysis of the STEREO data has allowed to publish two catalogues of coronal hole jets, one related to polar corona jets and the other to equatorial coronal jets. The main morphological featuers of these jets have been determined, and a classification in terms of Eiffel-Tower jets, lambda-type jets, and helical structures has been proposed. We also developed a technique for obtaining the temperature maps from the ultraviolet observations. This is based on the filter ratio method and on the background subtraction. First results show good agreement with existing methods.

Solar activity cycle and solar neutrinos

The investigation of the main features of the solar cycle are essential in order to set parameters for theoretical dynamo models. The magnetic solar cycle consists of two components: the well-known main cycle with period around 22 yr, and a high-frequency component with period close to 2 yr, known as Quasi Biennial Oscillations (QBO). The spatio-temporal dynamics of the solar magnetic field has been investigated by using NSO/Kitt Peak synoptic magnetic maps covering the period August 1976-September 2003. Results obtained for the <22 yr cycle, mainly related to the polarity inversions of the large-scale dipolar field, show an antisymmetric behavior with respect to the equator and a marked poleward flux migration in the radial and meridional components. Our findings suggest a deep seated alpha-effect and support alpha-omega dynamo models which also include meridional circulation. The quasi biennial oscillations are also identified as a fundamental periodicity of the magnetic field and linked to a dynamo action which possibly causes magnetic flux migration at < 2 yr rate both polewards and equatorwards from low latitudes (-25◦ and +25◦ in the Southern and Northern hemisphere, respectively). In particular, the equatorwards drift is clearly found in the toroidal component and shows antisimmetry with respect to the equator. The reproducibility of these features represents a validation test of the theoretical dynamo models, developed to understand the spatio-temporal evolution of the solar magnetic field. The QBO origin is still unknown even if it seems to be related to the dynamo action in the inner solar layers, being also detected in phenomena directly connected with the solar interior. In fact, the equatorial rotation rate close to the tachocline varies with a 1.3 yr period, as detected from GONG and MDI observations as well as the solar angular momentum; a < 2 yr signal has been detected for the natural p-mode frequencies of the Sun. In this field our studies provide evidence for the quasi-biennial modulation of the solar neutrino flux, generated in the solar core. We found that, at the QBO time scale, the neutrino flux results significantly correlated with solar activity indicators. These findings support the hypothesis of a connection between solar neutrinos and solar magnetic fields, probably through direct interaction with the neutrino magnetic moment.

Sun-Earth interactions

The presence of long-term persistence in climate system is already debated. It is commonly investigated through the estimate of the detrended fluctuation analysis (DFA) scaling exponent δ, representing a statistical index related to the dynamics of fluctuations of a stochastic process. Some Earth's temperature data sets showed the same degree of persistence with an exponent □□ = 0.65 in the range of time scales from 2 to 15 yr. More recently this sort of universality has been questioned since a value □ = 0.5 seems to be present over continental lands while higher values □□ = 0.65 have been found over the coastline. In order to calculate the degree of persistence, we need to distinguish between trends and correlations. Usually, to eliminate trends in the temperature data sets, the temperature anomalies are calculated. In climate studies, these are defined as the difference between the temperature measured at a given day and the temperature mean value for the same calendar day over many years of data. In such a definition of anomaly, there is the implicit assumption that the seasonal annual cycle is constant, and it is generated by a set of stationary processes. Clearly, since the response of

the climate system to external forcing, such us the solar one, is nonlinear, tthe validity of the previous assumption is often questionable. Hence, the classical definition of anomaly could not be adequate to the complex physics of the system; and, consequently, the persistence estimation. Because of the nonlinear and nonstationary character of temperature time series the seasonal contribution has been identified through a novel technique, the Empirical Mode Decomposition. This tool recovers a set of orthogonal empirical modes called IMFs. The anomalies have been thus obtained through partial reconstructions by excluding IMFs associated to obvious persistence effects such as the urban warming and the seasonal cycle. Results from monthly historical temperature records measured for about 250 yr in Prague and Milan indicate persistence on scales from 3 to 10 yr with similar values for the detrended fluctuation analysis indices thus indicating that a suitable definition of anomalies is fundamental when persistence effect in climate is investigated. The dynamics of the climate system has been investigated, through the EMD, by analyzing the seasonal oscillation of monthly averaged temperatures recorded at 1167 stations covering the whole USA. We found the presence of an orbit-climate relationship on time scales of about 20 yr related to the nutational forcing. The relationship manifests itself through occasional destabilization of the phase of the seasonal component due to the local changing of balance between direct insolation and the net energy received by the Earth. The local intermittent dynamics is modulated by a periodic component of 18.6 yr due to the nutation of the Earth, which represents the main modulation of the Earth's precession. The global effect in the last century results in a cumulative phase-shift of about 1.74 days towards earlier seasons, in agreement with the phase shift expected from the Earth's precession. The climate dynamics of the seasonal cycle has been described through a nonlinear circle-map, indicating that the destabilization process can be associated to intermittent transitions from quasi-periodicity to chaos.

1.3 MAGNETOSPHERIC PHENOMENA AND NONLINEAR GEOPHYSICS

Proton acceleration in the Earth's magnetotail

Ion beams with energies of the order of several tens of keV are frequently observed in the Earth's magnetotail. We consider two possible acceleration mechanisms, the cross tail electric field Ey (due to the large-scale coupling between solar wind and magnetosphere, along dawn-dusk direction) and the stochastic acceleration due to the electromagnetic fluctuations present in the magnetotail. A 2D test particle simulation has been performed in order to reproduce the interaction between charged particles and electromagnetic fluctuations and the constant dawn-dusk electric field, Ey, in the magnetotail current sheet. Electromagnetic perturbations are generated byrandom oscillating "clouds" moving in the x-y plane (in GSM coordinate system). Protons are accelerated via a stochastic Fermi-like process and, by varying the features of the electromagnetic fluctuations, along with the value of the normal magneticcomponent and other physical parameters, we can explain a range of energetic ion observations. In order to have a more realistic description of ion acceleration, a three-dimensional (3D) model which takes into account the magnetic structure of the current sheet has to be developed. The main findings are: (a) the presence of a large scale magnetic field tends to decrease the efficiency of the Fermi-like interaction between test particles and moving clouds. (b) The ion energization grows with the (x, y) size of the magnetic clouds, while it is slightly influenced by the thickness of the clouds along z, implying that the majority of the interaction takes place in the (x, y) plane. (c) Assuming parameters of the model corresponding to those of the Earth's magnetotail, protons are accelerated to energies comparable to those observed in the plasma sheet boundary layer, and it is found that many features, like the formation of a beam in velocity space, can be reproduced.

Magnetic turbulence in the geospace environment.

Magnetic turbulence is found in most space plasmas, including the Earth's magnetosphere, and the interaction region between the magnetosphere and the solar wind. Recent spacecraft observations of magnetic turbulence in the ion foreshock, in the magnetosheath, in the polar cusp regions, in the magnetotail, and in the high latitude ionosphere are reviewed. It is found that:

1. A large share of magnetic turbulence in the geospace environment is generated locally, as due for instance to the reflected ion beams in the ion foreshock, to temperature anisotropy in the magnetosheath and the polar cusp regions, to velocity shear in the magnetosheath and magnetotail, and to magnetic reconnection at the magnetopause and in the magnetotail.
2. Spectral indices close to the Kolmogorov value can be recovered for low frequency turbulence when long enough intervals at relatively constant flow speed are analysed in the magnetotail, or when fluctuations in the magnetosheath are considered far downstream from the bow shock.
3. For high frequency turbulence, a spectral index ~ 2.3 or larger is observed in most geospace regions, in agreement with

what is observed in the solar wind.
4. More studies are needed to gain an understanding of turbulence dissipation in the geospace environment, also keeping in mind that the strong temperature anisotropies which are observed show that wave particle interactions can be a source of wave emission rather than of turbulence dissipation.
5. Several spacecraft observations show the existence of vortices in the magnetosheath, on the magnetopause, in the magnetotail, and in the ionosphere, so that they may have a primary role in the turbulent injection and evolution. The influence of such a turbulence on the plasma transport, dynamics, and energization has been described, also using the results of numerical simulations.

1.4 LABORATORY PLASMAS

Turbulence in pure electron plasmas

Highly magnetized pure electron plasmas confined in Malmberg-Penning traps allow for the experimental study of two-dimensional fluid turbulence, when the experimental conditions are such that the cold non-relativistic guiding center approximation is valid. The dynamics and statistics of the freely decaying 2D turbulence in a pure electron plasma has been studied by analyzing the results of experiments performed in the Malmberg-Penning trap ELTRAP of the Plasma Physics group of Milano University. Time sequences of 2D fluid vorticity (electron density) measurements, obtained from different types of initial conditions, namely annular vorticity and spiral vorticity distributions, have been analyzed. The role and evolution of coherent structures have been studied through the Proper Orthogonal Decomposition (POD) technique. In the case of annular initial conditions, the structure of the eigenfunctions of the POD modes with the major enstrophy content and the evolution of the corresponding temporal coefficients can be attributed to the emergence of the fastest growing diocotron modes originating from the initial annulus of vorticity. In the case of spiral initial conditions, the enstrophy is more equally distributed among the POD modes and the behavior of the POD eigenfunctions and modal coefficients indicate that spiral vorticity initial conditions give rise to a fairly developed turbulent cascade process. The intermittency properties of this turbulence have been studied by analyzing the scaling properties of vorticity increments. It has been shown that intermittency increases as turbulence develops, due to the formation of strong vorticity fluctuations which give rise to non-Gaussian tails in the PDFs of vorticity increments.

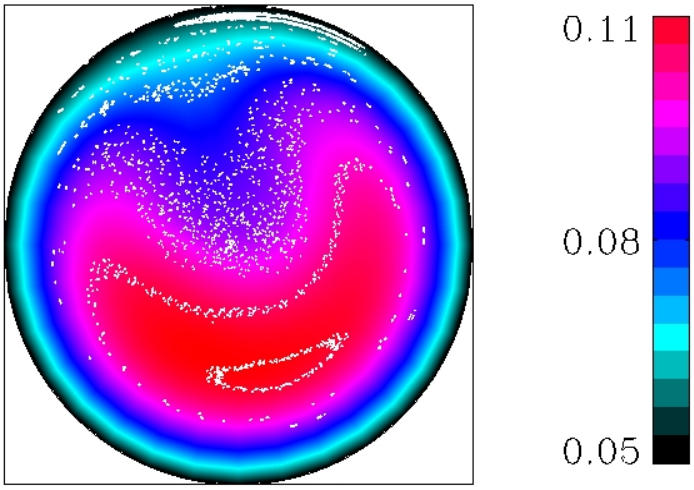

Fig. 1.4: *Poincaré section of magnetic field lines (white dots) and color plot of the temperature in a section at z constant of a RFP simulation with anisotropic thermal conductivity. A quasi-single helicity state is represented. A chaotic region and closed magnetic surfaces are present at the same time. Magnetic fieldlines are approximately isothermal.*

Compressible magnetohydrodynamic simulations of the Reversed Field Pinch

A reversed field pinch is a toroidal configuration used to confine plasmas in fusion machines. The poloidal and toroidal components of the magnetic field in an RFP are mostly generated by electric currents flowing in the plasma and they are of the same order of magnitude. The configuration is characterized by a reversal of the toroidal magnetic field close to the wall. Besides the interst of this kind of machines as potential fusion reactors, they are also useful for the study of fundamental issues like plasma relaxation, plasma turbulence and its effects on plasma confinement. We studied the reversed field pinch through the numerical solution of the compressible magnetohydrodynamic equations.

Two kinds of compressible magnetohydrodynamics simulations of the reversed-field pinch have been performed, with isotropic and anisotropic thermal conductivity. We developed a numerical method to reproduce the effect of a large parallel thermal conductivity using a multiple-time analysis, which makes magnetic field lines almost isothermal. We showed that the anisotropic thermal conductivity causes the formation of a hot island when closed magnetic surfaces exist, while temperature becomes almost uniform when the magnetic field is chaotic. The simulations show the effects of the anisotropic thermal conductivity on the system evolution. Including the anisotropy in the thermal conductivity is necessary to obtain more reliable numerical results. The simulation with anisotropic thermal conductivity shows that, after a transient single-helicity state that is formed in the initial phase (Fig. 1.4), a stationary state is reached where the RFP configuration exists in a multiple helicity state, even though the Hartmann number is below the threshold found in previous simulations for the formation of multiple helicity states.

1.5 COMPLEX SYSTEMS

Stochastic polarization switching in ferroelectric thin films

The repolarization phenomenon in a ferroelectric film has been investigated. The ferroelectric sample used was lead zirconate titanate (PZT) obtained by sol-gel synthesis and deposited by spin coating on ITO/glass substrate. A series of repolarizations were induced in the ferroelectric film by applying a triangular wave and the current peaks related to the switchings of the ferroelectric domains were acquired for statistical analyses. It has been shown that the dynamics and statistics of polarization switchings are well simulated by a simple mean-field model in which a double-well, asymmetric potential is included to describe the asymmetry at the PZT-ITO interface.

A PUBLICATIONS ON SCIENTIFIC JOURNALS

A.1 Publications on international journals

A.1.1 Publications on international journals printed in 2010

1. Greco, A., Perri S., and G. Zimbardo,
   Stochastic Fermi acceleration in the magnetotail current sheet: A numerical study
   Journal of Geophysical Research, **115**, A02203 (2010).

2. Dolgonosov M., Zimbardo G., Greco A.,
   Influence of the electric field perpendicular to the current sheet on ion beamlets in the magnetotail
   Journal of Geophysical Research, **115**, A02209 (2010)

3. Dalena S., Greco A., Zimbardo G., Veltri P.,
   Role of oxygen ions in the formation of a bifurcated current sheet in the magnetotail
   Journal of Geophysical Research, **115**, A03213 (2010).

4. Onofri M., Malara F., Veltri P.,
   Temperature evolution in a magnetohydrodynamics simulation of a reversed-field pinch
   Nuclear Fusion, **50**, 055003 (2010)

5. Servidio S., Matthaeus, W. H., Shay M. A., Dmitruk P., Cassak P. A., Wan M.,
   Statistics of magnetic reconnection in two-dimensional magnetohydrodynamic turbulence
   Physics of plasmas, **17**, 032315 (2010).

6. Greco A., Servidio S., Matthaeus W. H., Dmitruk P.,
   Intermittent structures and magnetic discontinuities on small scales in MHD simulations and solar wind
   Planetary and Space Science, **58**, 1895-1899 (2010).

7. Bitane R., Zimbardo G., Pommois P. N., Veltri P.,
   Magnetic field line diffusion coefficient and Kolmogorov entropy in the percolation regime
   Communications in Nonlinear Science and Numerical Simulations, **15**, 79-85 (2010).

8. Marino S., Lepreti F., Carbone V., Scaramuzza N.,
   Stochastic ferroelectric switching of lead zirconate titanate thin films
   The European Physical Journal B, **74**, 475-477 (2010).

9. Vecchio A., Laurenza M., Carbone V., Storini M.,
   The quasi-biennial modulation of solar neutrino flux, solar and galactic cosmic rays by the solar cyclic activity
   The Astrophysical Journal Letters, **701**, L1-L5 (2010).

10. Veltri P., Vecchio A., Carbone V.,
    Proper Orthogonal Decomposition analysis of spatio-temporal behaviour of renal scintigraphy
    Physica Medica, **26**, 57-70 (2010).

11. Valentini F., Iazzolino A., Veltri P.,
    Numerical study of ion-cyclotron resonant interaction via hybrid-Vlasov simulations
    Physics of Plasmas, **17**, 052104 (2010).

12. Valentini F., Califano F., Veltri P.,
    Two-dimensional kinetic turbulence in the solar wind
    Physical Review Letters, **104**, 205002 (2010).

13. Sorriso-Valvo L., Carbone V., Marino R., Noullez A., Bruno R., Veltri P.,
Reply to Forman et al. Comment
Physical Review Letters, **104**, 189002 (2010).

14. Sorriso-Valvo L., Yordanova E., Carbone V.,
On the scaling properties of anisotropy of interplanetary magnetic turbulent fluctuations
EuroPhysics Letters, **90**, 59001 (2010).

15. Marradi L., Valentini F., Califano F.,
Kinetic evolution of the perpendicular turbulent cascade in the solar wind
EuroPhysics Letters, **92**, 49002 (2010).

16. Nisticò G., Bothmer V., Patsourakos S., Zimbardo G.,
Observational features of equatorial coronal hole jets
Annales Geophysicae, **28**, 687-696 (2010).

17. Zimbardo, G.,
Heavy ion reflection and heating by collisionless shocks in polar solar corona
Planetary and Space Science, DOI: 10.1016/j.pss.2010.03.010 (2010).

18. Bitane R., Zimbardo G., Veltri P.,
Electron transport in coronal loops: the influence of the exponential separation of magnetic field lines
The Astrophysical Journal, **719**, 1912-1917 (2010).

19. Zimbardo G., Greco A., Sorriso-Valvo L., Perri S., Voeroes Z., Aburjania G., Chargazia K., Alexandrova O.,
Magnetic Turbulence in the Geospace Environment
Space Science Reviews, **156**, 89-134 (2010).

20. Perri S., Balogh A.,
Characterization of Transitions in the Solar Wind Parameters
The Astrophysical Journal, **710**, 1286-1294 (2010).

21. Perri S., Balogh A.,
Stationarity in solar wind flows
The Astrophysical Journal, **714**, 937-943 (2010).

22. Carbone V., Perri S., Yordanova E., Veltri P., Bruno R., Khotyaintsev Y., Andrè M.,
Sign-singularity of the reduced magnetic helicity in the solar wind plasma
Physical Review Letters, **104**, 181101 (2010).

23. Perri S., Balogh A.,
Differences in solar wind cross-helicity and residual energy during the last two solar minima
Geophysical Research Letters, **37**, L17102 (2010).

24. Perri S., Carbone V., Veltri P.,
Where does fluid-like turbulence break down in the solar wind?
Astrophysical Journal Letters, **725**, L52-L55 (2010).

25. Nigro G. , Carbone V.,
Magnetic reversals in a modified shell model for magnetohydrodynamics turbulence
Physical Review E, **82**, 016313 (2010).

26. Malara, F.; Nigro, G.; Onofri, M.; Veltri, P.,
Fluctuating Energy Storage and Nonlinear Cascade in an Inhomogeneous Coronal Loop
The Astrophysical Journal, **720**, 306-327 (2010).

27. Onofri M., Malara F., Veltri P.,
Effects of anisotropic Thermal conductivity in magnetohydrodynamics simulations of a reversed-field pinch
Physical Review Letters, **105**, 215006 (2010).

28. Vecchio A., Capparelli V., Carbone V.,
The complex dynamics of the seasonal component of USA's surface temperature
Atmospheric Chemistry and Physics, **10**, 9657-9665 (2010).

29. Vecchio A., Carbone V.,
Amplitude-frequency fluctuations of the seasonal cycle, temperature anomalies, and long-range persistence of climate records
Physical Review E, **82**, 066101 (2010).

A.1.2 Publications on international journals accepted in 2010

1. Wan M., Servidio S., Oughton S., Matthaeus WS. H.,
The third-order law for magnetohydrodynamic turbulence with shear: Numerical investigation
to appear on Physics of Plasmas.

2. Perri S., Carbone V., Yordanova E., Bruno R., Balogh A.,
Scaling law of the reduced magnetic helicity in fast streams
to appear on Planetetary Space Science

3. Korth H., Anderson B.J., Zurbuchen T.H., Slavin J.A., Perri S., Boardsen S.A., Baker D.N., Solomon S.C., McNutt Jr. R. L.,
The Interplanetary Magnetic Field Environment at Mercury's Orbit
to appear on Planetary Space Science

4. Malara F., Nigro G. Veltri P., Onofri M.,
Alfvén Waves: Coherent Phenomena in Coronal Loops and Open-Field Regions
to appear on Space Science Reviews

B PUBLICATIONS ON CONFERENCE PROCEEDINGS

B.1 Publications on international conference proceedings in 2010

1. Greco A., Matthaeus W. H., Servidio S., Dmitruk P., Wan M., Oughton S., Chuychai P.,
Statistical properties of solar wind discontinuities, intermittent turbulence, and rapid emergence of non-Gaussian distributions
Twelfth International Solar Wind Conference, M. Maksimovic, K. Issautier, N. Meyer-Vernet, M. Moncuquet, F. Pantellini Eds., American Institute of Physics, pp. 202-205 (2010).

2. Wan M., Oughton S., Servidio S., Matthaeus W. H.,
The third-order law for magnetohydrodynamic turbulence with constant shear
Twelfth International Solar Wind Conference, M. Maksimovic, K. Issautier, N. Meyer-Vernet, M. Moncuquet, F. Pantellini Eds., American Institute of Physics, pp. 172-175 (2010).

3. Matthaeus W. H., Servidio S., Dmitruk P.,
Dispersive Effects of Hall Electric Field in Turbulence
International Solar Wind Conference, M. Maksimovic, K. Issautier, N. Meyer-Vernet, M. Moncuquet, F. Pantellini Eds., American Institute of Physics, pp. 184-187 (2010).

4. Servidio S., Shay M. A., Matthaeus W. H., Dmitruk P., Cassak P. A., Wan M.,
Properties of magnetic reconnection in MHD turbulence
Twelfth International Solar Wind Conference, M. Maksimovic, K. Issautier, N. Meyer-Vernet, M. Moncuquet, F. Pantellini Eds., American Institute of Physics, pp. 198-201 (2010).

5. Parashar T. N., Servidio S., Shay M. A., Matthaeus W. H., Cassak P. A.,
Orszag Tang vortex—Kinetic study of a turbulent plasma
Twelfth International Solar Wind Conference, M. Maksimovic, K. Issautier, N. Meyer-Vernet, M. Moncuquet, F. Pantellini Eds., American Institute of Physics, pp. 304-307 (2010).

6. Malara F., Nigro G., Onofri M., Veltri P.,
Large-scale energy balance and MHD turbulence in solar coronal structures
Twelfth International Solar Wind Conference, M. Maksimovic, K. Issautier, N. Meyer-Vernet, M. Moncuquet, F. Pantellini Eds., American Institute of Physics, pp. 48-51 (2010).

7. Lepreti F., Romé M., Pozzoli R., Vecchio A., Carbone V., Maero G., Paroli B., Valentini F.,
Proper Orthogonal Decomposition of Two-Dimensional turbulence in a Pure Electron Plasma
Plasmas in the Laboratory and the Universe: Interactions, Patterns, and Turbulence, Bertin G., Lodato G., Pozzoli R., Romé M., De Luca F. Eds., American Instutute of Physics, pp. 305-310 (2010).

8. Veltri P., Valentini F., Califano F.,
The evolution of solar wind turbulence at kinetic scales
International symposium of Geomagnetism and Aeronomy (IAGA), L. Damé and A. Hady Eds., p. 43 (2010).

9. Zimbardo G.,
More than mass proportional heating of heavy ions by collisionless quasi-perpendicular shocks in the solar corona,
Twelfth International Solar Wind Conference, M. Maksimovic, K. Issautier, N. Meyer-Vernet, M. Moncuquet, F. Pantellini Eds., American Institute of Physics, pp. 52-5 (2010).

10. Zimbardo G., Perri S.,
Superdiffusive transport upstream of the solar wind termination shock
Twelfth International Solar Wind Conference, M. Maksimovic, K. Issautier, N. Meyer-Vernet, M. Moncuquet, F. Pantellini Eds., American Institute of Physics, pp. 584-587 (2010).

11. Lepreti F., Romé M., Pozzoli R., Vecchio A., Carbone V., Maero G., Paroli B.,
Dynamics of two-dimensional turbulence in a pure electron plasma
Proceedings of the 37th EPS Conference on Plasma Physics, C. McKenna Ed., European Physical Society (2010).

12. Lepreti F., Romé M., Servidio S., Valentini F., Pozzoli R., Carbone V., Maero G.,
Scaling properties of two-dimensional turbulence in a pure electron plasma
Proceedings of the 37th EPS Conference on Plasma Physics, McKenna C. Ed., European Physical Society, p. 4.406 (2010)

C INVITED PRESENTATIONS

C1. Invited presentations at international conferences in 2010

1. Sorriso-Valvo L.,
   Inertial Energy Cascade in Space Plasma MHD Turbulence
   Multifractals and turbulence in geophysics and space, Bruxelles, June 9-11, 2010.

2. Greco A., Servidio A., Matthaeus W. H., Dmitruk P.,
   Magnetic discontinuities and reconnection in MHD turbulence
   Workshop on Plasma Astrophysics, Arcetri, Italy, November 22-23, 2010.

3. Zimbardo G.,
   Anomalous and percolative transport regimes in astrophysical plasmas
   International workshop 'Self-organization in turbulent plasmas and fluids', Dresden, Germany, May 11-15, 2010.

4. Zimbardo G., Perri S., Pommois P., Veltri P.,
   Superdiffusive Transport in the Heliosphere: Numerical Simulations and Experimental Evidences
   Kinetic Processes in Plasmas: Instabilities, Turbulence and Transport, Bochum, Germany, November 8-11, 2010.

5. Klimchuk, J. A.; Nigro, G.; Dahlburg, R. B.; Antiochos, S. K.,
   The Existence and Origin of Turbulence in Solar Active Regions
   American Astronomical Society, AAS Meeting 216, 302.05, Miami, USA, May 23-27, 2010.

6. Califano F. , Valentini F.,
   3D-3V Vlasov project supported by DEISA
   International Workshop Girokinetics for ITER, Vienna, Austria, March 15-28, 2010.

7. Malara F., Nigro G., Onofri M., Veltri P.,
   Alfven waves: coherent phenomena in coronal loops and open-field regions
   Coronal Heating and Solar Wind Acceleration, Bern, Switzerland, January 25-29, 2010.

C2. Invited presentations at national conferences in 2010

1. Zimbardo G.,
   Il cielo da Galileo ad oggi
   Convegno presso il Planetario Provinciale Pitagora di Reggio Calabria, Reggio Calabria, Italy, February 4, 2010.

D PRESENTATIONS AT CONFERENCES

D1. Presentations at international conferences in 2010

1. Valentini F., Califano F., Veltri P. ,
   Solar-wind turbulence at kinetic wavelengths: hybrid-Vlasov simulations
   American Geophysical Union fall meeting, San Francisco, December 13-17, 2010

2. Yordanova E., Sorriso-Valvo L., Perri S., Carbone V.,
   Scaling Properties Of Small-Scale Anisotropy In The Solar Wind Turbulence By Multipoint Measurements
   American Geophysical Union fall meeting, San Francisco, December 13-17, 2010

3. Sorriso-Valvo L., Marino R., Bruno R., Carbone V., Noullez A.,
   The magnetohydrodynamic turbulent cascade in polar solar wind: the role of local dynamic alignment

American Geophysical Union fall meeting, San Francisco, December 13-17, 2010

4. Sorriso-Valvo L., Yordanova E., Perri S., Carbone V., André M.,
Anisotropic structure fucntions in space plasma turbulence
EGU General Assembly, Vienna, May 2-5, 2010

5. Sorriso-Valvo L., Marino R., Carbone V., Noullez A., Bruno R.,
The turbulent cascade in solar wind: scaling in fast and slow wind
EGU General Assembly, Vienna, May 2-5, 2010

6. Marino R., Carbone V., Bruno R., Noullez A., Veltri P., Sorriso-Valvo L.,
Scaling laws in solar wind MHD turbulence
EGU General Assembly, Vienna, May 2-5, 2010

7. Marino R., Sorriso-Valvo L., Redondo J.M., Yague C.
Scaling and isotropy in the inertial range of atmospheric turbulence
EGU General Assembly, Vienna, May 2-5, 2010

8. Yordanova E., Sorriso-Valvo L., Perri S., Carbone V.,
Scaling Properties Of Small-Scale Anisotropy In The Solar Wind Turbulence By Multipoint Measurements
American Geophysical Union fall meeting, San Francisco, December 13-17, 2010

9. Sorriso-Valvo L., Marino R., Bruno R., Carbone V., Noullez A.,
The magnetohydrodynamic turbulent cascade in polar solar wind: the role of local dynamic alignment
American Geophysical Union fall meeting, San Francisco, December 13-17, 2010

10. Greco A., Servidio S., Matthaeus W. H., Dmitruk P.,
Emergence of intermittent structures and reconnection in MHD turbulence
274 IAU Symposium, Advances in Plasma Astrophysics conference, Giardini Naxos, September 6-10, 2010

11. Lepreti F., Carbone V., Vecchio A., Reardon K., Capparelli V., Rossi C.,
Turbulence in the solar chromosphere and its role in small scale energy deposition
American Geophysical Union fall meeting, San Francisco, December 13-17, 2010

12. Greco A., Osman K., Servidio S., Matthaeus W. H., Dmitruk P.,
Magnetic discontinuities on small scales in MHD simulations and solar wind
52nd Annual Meeting of the APS Division of Plasma Physics, Chicago, Illinois, USA, November 8-12, 2010

13. Greco A., Servidio S. , Matthaeus W. H., Dmitruk P.,
Statistical properties of solar wind discontinuities and intermittent turbulence
EGU General Assembly, Vienna, May 2-5, 2010

14. Greco A., Perri S., Zimbardo G.,
Stochastic Fermi acceleration in the Earth's magnetotail current sheet: a numerical study
EGU General Assembly, Vienna, May 2-5, 2010

15. Zimbardo G., Nistico' G.,
Heating the polar corona by collisionless shocks: an example of cross-fertilization in space physics
38th COSPAR Scientific Assembly, Bremen, Germany, July 18-25, 2010

16. Nistico' G., Patsourakos S., Bothmer V., Zimbardo G.,
Classification and physical parameters of EUV coronal jets with STEREO/SECCHI
38th COSPAR Scientific Assembly, Bremen, Germany, July 18-25, 2010

17. Trotta E. M., Zimbardo G.,
Superdiffusive and ballistic propagation of protons in solar energetic particle events
274 IAU Symposium, Advances in Plasma Astrophysics conference, Giardini Naxos, 6-10 September, 2010

18. Zimbardo G., Nistico' G.,
Heating of heavy ions by collisionless quasi-perpendicular shocks in solar corona
Conference of Hinode-4: unsolved problems and recent insights, Palermo, Italy, October 11-15, 2010

19. Perrone D., Valentini F., Veltri P.,
Hybrid-Vlasov simulations for alpha particles heating in the solar wind
274 IAU Symposium, Advances in Plasma Astrophysics conference, Giardini Naxos, September 6-10, 2010

20. Perrone D., Nigro G., Veltri P.,
A Shell Model Turbulent Dynamo
Self-Organization in Turbulent Plasmas and Fluids, Dresden, Germany, May 10-14, 2010.

21. Nigro G., Perrone D., Carbone V. and Veltri P.,
A Shell Model For Turbulent Magnetic Dynamo
Self-Organization in Turbulent Plasmas and Fluids Workshop, Dresden, Germany, May 10-14, 2010.

22. Nigro G., Perrone D. and Veltri P.,
A shell model for turbulent dynamos
274 IAU Symposium, Advances in Plasma Astrophysics conference, Giardini Naxos, September 6-10, 2010

23. Lepreti F., Reardon K., Carbone V., Vecchio A.,
Evidence of turbulence and intermittency in line of sight velocity fields of the solar chromosphere
274 IAU Symposium, Advances in Plasma Astrophysics conference, Giardini Naxos, September 6-10, 2010

24. Lepreti F., Romé M., Pozzoli R., Vecchio A., Carbone V., Maero G., Paroli B.,
Dynamics of two-dimensional turbulence in experiments with pure electron plasmas
274 IAU Symposium, Advances in Plasma Astrophysics conference, Giardini Naxos, September 6-10, 2010

25. Lepreti F., Romé M., Pozzoli R., Vecchio A., Carbone V., Maero G., Paroli B.,
Dynamics of two-dimensional turbulence in a pure electron plasma
37th EPS Conference on Plasma Physics, Dublin (EIRE), June 21-25, 2010.

26. Lepreti F., Romé M., Servidio S., Valentini F., Pozzoli R., Carbone V., Maero G.
Scaling properties of two-dimensional turbulence in a pure electron plasma
37th EPS Conference on Plasma Physics, Dublin (EIRE), June 21-25, 2010.

27. Lepreti F.,
The inertial range of the turbulent cascade in laboratory and space plasmas
37th EPS Conference on Plasma Physics, Dublin (EIRE), June 21-25, 2010.

28. Lepreti F., Carbone V., Spolaore M., Martines E., Antoni V., Cavazzana R., Serianni G., Veltri P., Vianello N., Zuin M.,
Observation of the inertial energy cascade of electrostatic turbulence in the RFX-mod reversed field pinch plasma
"Theory of Fusion Plasmas" Joint Varenna - Lausanne International Workshop, Varenna, Italy, August 30-September 3, 2010.

29. Onofri M., Malara F. Veltri P.,
Compressible MHD simulations of the RFP with anisotropic thermal conductivity
14th IEA RFP Workshop, Padova, Italy, April 26-28, 2010.

30. Onofri M., Malara F. Veltri P.,
Heat transport in magnetohydrodynamics simulations of the reversed field pinch
Self-Organization in Turbulent Plasmas and Fluids Workshop, Dresden, Germany, May 10-14, 2010.

31. Vecchio A.,
The dynamics of the solar magnetic field: polarity reversals, butterfly diagram and quasi-biennial oscillations
274 IAU Symposium, Advances in Plasma Astrophysics conference, Giardini Naxos, September 6-10, 2010

32. Vecchio A. , Capparelli V., Carbone V.,
The complex dynamics of the seasonal component of USA surface temperature
American Geophysical Union fall meeting, San Francisco, December 13-17, 2010

33. Vecchio A., Laurenza M., Meduri D., Carbone, V., Storini M.,
The dynamics of the solar magnetic field: polarity reversals, butterfly diagram and quasi-biennial oscillations
American Geophysical Union fall meeting, San Francisco, December 13-17, 2010

34. Lepreti F., Carbone V., Vecchio A., Reardon K., Capparelli V., Rossi C.,
Turbulence in the solar chromosphere and its role in small scale energy deposition
American Geophysical Union fall meeting, San Francisco, December 13-17, 2010

2. THEORETICAL PARTICLE PHYSICS AND APPLICATIONS

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Introduction

The research activity during the AA 2009-10 included the following subjects:

- phenomenology of hadron collisions and Quantum Chromodynamics (QCD) in the high-energy limit;
- non-perturbative properties of gauge theories discretized on a space-time lattice;
- field theory of correlated devices;
- integrability in the N=4 supersymmetric Yang-Mills theory
- physics of kaon-nucleon interactions.

A major part of this activity has been carried on in collaboration with other research groups in Italy and abroad. For the part concerning the non-perturbative study of gauge theories on a space-time lattice, a large use has been done of the PC farm "Majorana" of the Istituto Nazionale di Fisica Nucleare (INFN) – Gruppo Collegato di Cosenza, hosted by the Physics Department.

2.1 QCD IN THE HIGH-ENERGY LIMIT AND HADRON PHENOMENOLOGY

2.1.1 QCD in the high-energy limit

We demonstrated that the ambiguity of the low-x evolution kernels in the next-to-leading order (NLO) permits one to match the Möbius form of the BFKL kernel and the kernel of the colour dipole model and to construct the Möbius invariant NLO BFKL kernel in N=4 supersymmetric Yang-Mills theory.

The calculation in the next-to-leading approximation of the jet vertex for the cases of incoming quark and gluon has been completed in the BFKL approach and a paper will appear soon. This vertex is a necessary ingredient for the double differential cross section for the production of two Mueller-Navelet jets in the proton-proton collision.
The study of the inclusive production of two high transverse momentum hadrons h_1, h_2 in proton-proton collisions with "Mueller-Navelet" kinematics is at an advanced stage and a paper will appear soon.

A new framework for transverse-momentum dependent parton distribution functions, based on a generalized conception of gauge invariance which includes into the Wilson lines the (spin-dependent) Pauli term is proposed. The relevance of this nonminimal term for unintegrated parton distribution functions, pertaining to spinning particles is discussed, and its influence on their renormalization-group properties is analyzed. It is shown that while the Pauli term preserves the probabilistic interpretation of twist-two distributions---unpolarized and polarized---it gives rise to additional pole contributions to those of twist-three. It turns out that the crosstalk between the Pauli term and the longitudinal and the transverse parts of the gauge fields, accompanying the fermions, induces a constant, but process-dependent, phase which is the same for leading and subleading distribution functions. We include Feynman rules for the calculation with gauge links containing the Pauli term and comment on the phenomenological implications of our approach.

The long-range (in rapidity) correlations between pairs of charged particles, produced in the collisions of hadrons at high energy---recently reported by the CMS Collaboration---are considered, and their origin is attributed to quantum entanglement. It is argued that the observed correlations can be understood in terms of non-local interactions of path-dependent phase factors that include the effect of the primordial separation of a charged particle from its partner with the opposite polarity. Phase factors also enter the definition of the transverse-momentum dependent parton densities used in the factorization formulas for semi-inclusive processes in QCD. In this latter case, the nonlocal correlations result from the interaction of Wilson loops in the so-called soft factors.

2.1.2 Hadron Phenomenology

An eikonalized elastic proton-proton and proton-antiproton scattering amplitude $F(s,t)$, calculated from QCD as a finite sum of gluon ladders, has been compared with the existing experimental data on the total cross section and the ratio $\rho(s,0)=ReF(s,0)/ImF(s,0)$ of the real part to the imaginary part of the forward amplitude. Predictions for the expected LHC

energies have been given.

Exclusive J/psi electroproduction has been studied in the framework of the analytic *S*-matrix theory. The differential and integrated elastic cross sections have been calculated using the Modified Dual Amplitude with Mandelstam Analyticity (M-DAMA) model. The model has been applied to the description of the available experimental data and proves to be valid in a wide region of the kinematical variables s, t and Q^2.

2.2 LATTICE GAUGE THEORIES

2.2.1 Finite density QCD

We have revisited the determination of the pseudo-critical line of QCD with four degenerate quarks at non-zero temperature and baryon density by the method of analytic continuation. We have determined the pseudo-critical couplings at imaginary chemical potentials by high-statistics Monte Carlo simulations and revealed deviations from the simple quadratic dependence on the chemical potential visible in earlier works on the same subject. Finally, we have studied the implications of our findings for the shape of the pseudo-critical line at real chemical potential, comparing different possible extrapolations.
Work is in progress on the study of the same phenomenon in QCD with two degenerate flavors and at finite baryon or isospin density.

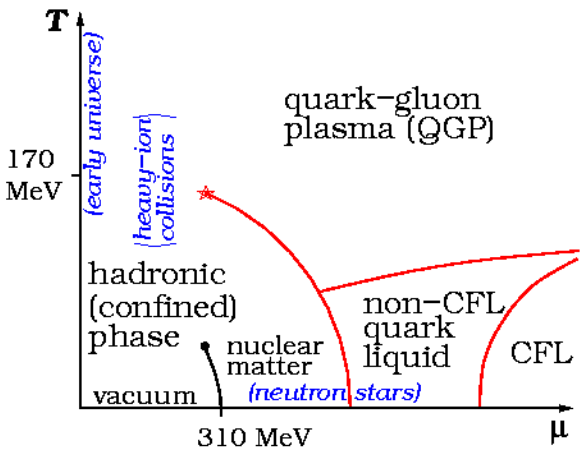

Figura 1: QCD phase diagram on the baryon chemical potential - temperature plane.

2.2.2 QCD flux tubes and deconfinement transition

The confinement mechanism based on the hypothesis of QCD vacuum as dual superconductor brings along the formation of flux tubes of the chromoelectric field between static color sources (dual Meissner effect). We have studied by Monte Carlo numerical simulations some relevant parameters of a flux tube, such as the space distribution of the field amplitude and the London penetration length, in pure gauge SU(3). The adopted method relies on the evaluation of the v.e.v. of a gauge-invariant operator made of a plaquette and a Wilson loop connected by Schwinger lines. We plan to move to the study of the flux tube structure at finite temperature, which calls for the use of a different gauge-invariant operator, with Polyakov loop correlators replacing Wilson loops.

2.2.3 Confinement and deconfinement in other gauge theories

We have studied the deconfinement transition in compact 3d U(1) gauge theory at finite temperature. Universality arguments support the conjecture that the this transition is of Berezinsky-Kosterlitz-Thouless (BKT) type, in the 2d XY universality class. A first step in the proof of this conjecture was carried on last year, when it was shown numerically that the transition is compatible with BKT in the theory with zero coupling between spatial plaquettes. This year we have considered the case of theory on isotropic lattices, finding that everything goes similarly, except for the behavior of the critical index eta, which shows large deviation from the expected universal value. Possible reasons for such behavior are discussed.

Similar considerations can be done for the 2d Z(N) gauge theory for N>4, where two phase transitions exist, a first order transition of order/disorder type and a BKT one. Owing to universality, both transitions should occur also in the 3d SU(N) gauge theory at finite temperature. The investigation of these aspects in 2d Z(5) has being completed this year and a paper has been produced and submitted for publication.

2.2.4 Two-dimensional spin models with a theta-term

The method of analytic continuation can be used also to study gauge theories and spin models in presence of a topological theta-term: simulations can be done at imaginary theta, where the Euclidean action is real and the Monte Carlo sampling is well-defined, and results are extrapolated to real theta.

This method has been used to verify the Haldane conjecture on the vanishing of the mass gap in the non-linear 2d O(3) σ-model at $\theta=\pi$. Work is in progress on the application of this method to study possible excited states in the region of real θ, recently conjectured by Controzzi and Mussardo.

2.3 FIELD THEORY OF CORRELATED DEVICES

2.3.1 Boundary field theory of Josephson devices

We have derived the effective field theory description of a tetrahedral Josephson network. Once connected to three one-dimensional Josephson junction chains, working as leads, the whole system is effectively mapped onto a 1+1 dimensional boundary field theory, in which the connected tetrahedral network is traded for an appropriate boundary interaction between the leads, regarder as one-dimensional, spinless Luttinger liquids. We show that the symmetries of the system protect its twofold groundstate degeneracy, thus letting it work as a ``symmetry protected" two-level quantum device. Moreover, we show that the interaction of the tetrahedral network with low-energy, long-wavelength plasmon modes of the leads renormalizes the system parameters, and eventually makes the network operate nearby a finite coupling fixed point of the boundary interaction Hamiltonian. As it happens in similar devices tuned nearby a
finite coupling fixed point, the interactions with the collective modes of the leads frustrate decoherence effects, thus making the system robust against fluctuations of the environmental parameters.

2.3.2 Strong coupling, spin-1/2 representation of the one-dimensional Bose-Hubbard model

We have shown that the one-dimensional Bose-Hubbard Hamiltonian, which is thought of to describe, for instance, cold atoms trapped within a one-dimensional optical lattice, taken at half-filling and in the strong Boson repulsion limit, maps onto the spin-1/2 XXZ model, with pertinently taken parameters. The careful derivation allowed us to draw a one-to-one correspondence between the parameters of the Bose-Hubbard model and the ones of the XXZ Hamiltonian. We numerically verified that the one-to-one correspondence extends to real space correlation functions of the corresponding operators in the two models. This opens the way to simulate, in a controlled way, the physics of spin-1/2 one-dimensional models, which are prototypical models of correlated one-dimensional systems, with bosons in optical lattices, whose parameters can, in principle, controlled at wish. The possibility of simulating impurities embedded in magnetic chains, as well, might possibly open the way to design, in a controlled envirnment, experiments concerning both fundamental physics problems (such as the detection of the Kondo cloud), and applications to quantum computation (such as the propagation of entanglement between impurities in a spin chain).

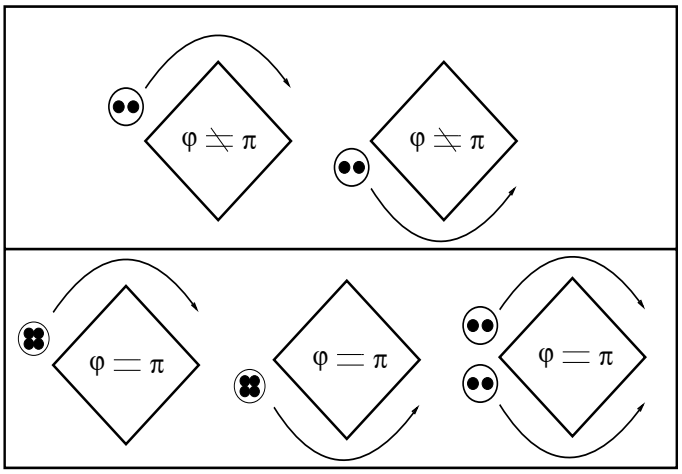

Figura 2: (Top) Tunneling of a single Cooper pair across an impurity in a Josephson network; (bottom) coherent tunneling of pairs of Cooper pairs across the same device.

2.3.3 Entanglement properties of the Haldane-Shastry spin chain

The ground state entanglement properties of a spin-1/2 spin chain with $1/r^2$-interaction (Haldane-Shastry model) have been investigated, in the presence of an applied magnetic field. Having explicitly constructed the ground spin for the chain with a finite number of sites N, various estimates of the entanglement have been computed at zero temperature, resorting afterwards to the thermodynamic limit ($N \to \infty$). The results about the behavior of the quantum correlations in the system have been related with the condensation of spin-1/2 "fractionalized" excitations (spinons), occurring when the applied field reaches its saturation value.

2.4 NON-EQUILIBRUM CORRELATED SYSTEMS

2.4.1 AC Josephson effect in a normal electronic chain connected to two superconductors

An adiabatic formalism has been derived, to study the DC, as well as the AC current, induced across an interacting quantum wire, regarded as a one-dimensional Luttinger liquid with pertinent parameters, connected to two superconductors at finite voltage bias V. While the adiabatic formalism allows for computing the current for any value of the tunneling amplitude between the contacts and the leads, resorting to a Luttinger liquid description of interacting one-dimensional electronic systems, allows for computing the current by also taking into account the interaction at the central region. Resorting to the boundary field theory formalism, then, allows for describing the effects of electron interaction onto the subgap current, due to multiple Andreev reflection processes.

2.5 INTEGRABILITY IN THE N=4 SUPERSYMMETRIC YANG-MILLS THEORY (SYM)

The first one was the study of high spin behaviour of anomalous dimensions in the planar sl(2) sector of N=4 SYM. This was done using the integrability properties of this problem, in specific the mapping of the dilatation operator to the Hamiltonian of a quantum integrable model, completely defined by a set of Bethe equations. This mapping is exact for long operators, but in general is affected by the so-called wrapping problem. The high spin anomalous dimension at fixed twist was studied, in its first subleading dependence on the spin (the so-called virtual scaling function). Afterwards, the scaling limit in which both the logarithm of the spin and the twist go to infinity, while their ratio is kept constant, was studied, still in its first subleading dependence. Finally, both analysis were completed and the computation of all subleading terms going as inverse powers of the logarithm of the spin was finalised.

The second subject of investigation concerns the recently discovered formulation of the problem of computing anomalous dimensions in N=4 SYM in terms of a set of Thermodynamic Bethe Ansatz equations. This allows to overcome the 'wrapping' problem plaguing the previously described Bethe Ansatz equations and thus gives exact results.
At present, work is still in progress and no papers have been written.

2.6 PHYSICS OF KAON-NUCLEON INTERACTIONS

We continued the revision of the programs of analysis of low-energy Kaon-Nucleon reactions. A new analysis will include results from KLOE, and hopefully from this experiment new data will be provided for low energy KN reactions, improving considerably the knowledge of this interaction. A poster about this perspectives has been submitted to a Conference in Tsukuba. Some progress has been made, though the situation is not definite about including in the
group an UNICAL Ph D student and some foreign student (in particular from Iran). We are still considering the possibility of an ambitious publication on KN physics with a contribution of all the members of INFN Project PG 21.

A PUBLICATIONS ON SCIENTIFIC JOURNALS

A.1 Publications on international journals

A.1.1 Publications on international journals printed in 2010

1. V.S. Fadin, R. Fiore, A.V. Grabovszky, A. Papa,
   Low-x evolution equations in Moebius representation,
   Phys. Part. Nucl. 41 (2010) 935-938.

2. V.S. Fadin, R. Fiore, A.V. Grabovszky,
   Matching of the low-x evolution kernels,
   Nucl. Phys. B831 (2010) 248-261; arXiv:0911.5617 [hep-ph].

3. R. Fiore, L.L. Jenkovszky, E. Kuraev, A. Lengyel, Z. Tarics,
   Predictions for high-energy pp and p_bar-p scattering from a finite sum of gluon ladders,
   Phys. Rev. D81 (2010) 056001; arXiv:0912.4955 [hep-ph].

4. I.O. Cherednikov, A.I. Karanikas, N.G. Stefanis,
   Wilson lines in transverse-momentum dependent parton distribution functions with spin degrees of freedom,
   Nucl. Phys. B840 (2010) 379-404; arXiv:1004.3697 [hep-ph]

5. P. Cea, L. Cosmai, M. D'Elia and A. Papa,
   The phase diagram of QCD with four degenerate quarks,
   Phys. Rev. D81 (2010) 094502, arXiv:1004.0184 [hep-lat].

6. O. Borisenko, R. Fiore, M. Gravina and A. Papa,
   Critical behavior of the compact 3d U(1) gauge theory on isotropic lattices,
   J. Stat. Mech. (2010) P04015; arXiv:1001.4979 [hep-lat].

7. D. Giuliano, P. Sodano,
   Competing Boundary Interactions in a Josephson Junction Network with an Impurity,
   Nucl. Phys. B837 (2010) 153-185.

8. D. Giuliano, A. Sindona, G. Falcone, F. Plastina and L. Amico,
   Entanglement in a spin system with inverse square statistical interaction,
   New J. Phys. 12, 025022 (2010).

9. D. Fioravanti, P. Grinza, M. Rossi,
   The generalised scaling function: a note,
   Nucl. Phys. B827 (2010) 359-380.

10. D. Fioravanti, P. Grinza, M. Rossi,
    On the logarithmic powers in sl(2) SYM4,
    Phys. Lett. B684 (2010) 52-60.

11. D. Fioravanti, M. Rossi,
    The high spin expansion of twist sector dimensions: the planar N=4 super Yang-Mills theory,
    Advances in High Energy Physics, vol. 2010, Article ID 614130, 30 pages, 2010.

A.1.2 Publications on international journals accepted in 2010

1. M.S. Cardaci, P. Cea, L. Cosmai, R. Falcone and A. Papa,
   Chromoelectric flux tubes in QCD,
   to appear on Phys. Rev. D, arXiv:1011.5803 [hep-lat]..

B PUBLICATIONS ON CONFERENCE PROCEEDINGS

B.1 Publications on international conference proceedings in 2010

1. A. Prokudin, R. Fiore, L.L. Jenkovszky, V.K. Magas, S. Melis,
   Exclusive J/psi photo- and electroproduction in a dual model,
   PoS DIS2010 (2010) 171; arXiv:1011.5924 [hep-ph].

2. N.G. Stefanis, I.O. Cherednikov, A.I. Karanikas,
   Role and properties of Wilson lines in transverse-momentum-dependent parton distribution functions,
   PoS (LC2010) 053; arXiv:1010.1934 [hep-ph].

3. P. Cea, L. Cosmai, M. D'Elia and A. Papa,
   The critical line of QCD with four degenerate quarks,
   PoS(Lattice 2010)173/1-7, arXiv:1012.4908 [hep-lat].

4. O. Borisenko, R. Fiore, M. Gravina and A. Papa,
   Critical behavior of the compact 3D U(1) gauge theory at finite temperature,
   PoS(Lattice 2010)188/1-7, arXiv:1012.4942 [hep-lat].

5 O. Borisenko, G. Cortese, R. Fiore, M. Gravina and A. Papa,
   Critical properties of the two-dimensional Z(5) vector model,
   PoS(Lattice 2010)274/1-7, arXiv:1101.0512 [hep-lat].

C PRESENTATIONS AT SCHOOL AND CONFERENCES

C.1 Presentations at international schools and conferences in 2010

1. I. Cherednikov,
   What we need to evolve TMD correctly? Recent progress,
   invited talk given at the "Gluons and the quark sea at high energies: distributions, polarization, tomography",
   Seattle (WA), USA, 13 Sept - 19 Nov 2010

2. I. Cherednikov,
   Developments on unintegrated PDFs,
   invited talk given at the 40th International Symposium on Multiparticle Dynamics,
   Antwerp (Belgium), 21 - 25 Sep 2010

3. I. Cherednikov,
   Transverse momentum parton distributions: recent progress in theory,
   talk given at "Diffraction 2010", Otranto (Lecce), Italy, 10 - 15 Sep 2010

4. I. Cherednikov,
   TMD parton densities: light-cone gauge calculations,
   invited talk given at the International Workshop "Hadron Structure and QCD: from low to high energies",
   Gatchina, St. Petersburg, Russia, 5 - 9 Jul 2010

5. I. Cherednikov,
   TMD factorization in light-cone gauges,
   invited talk given at the International Workshop on Transverse Momentum Distributions (TMD 2010),
   Trento, Italy, 21 - 25 Jun 2010

6. I. Cherednikov,
   Transverse-momentum dependent parton densities: definition, renormalization and evolution,
   talk given at the 4th Workshop on Exclusive Reactions at High Momentum Transfer,

Thomas Jefferson National Accelerator Facility Newport News (VA), USA, 18 - 21 May 2010

7. O. Borisenko, R. Fiore, M. Gravina and A. Papa,
Critical behavior of the compact 3D U(1) gauge theory at finite temperature,
poster presented by R. Fiore at LATTICE 2010, XVIII International Symposium on Lattice Gauge Theories, Villasimius, June 14 - 19, 2010.

8. O. Borisenko, G. Cortese, R. Fiore, M. Gravina and A. Papa,
Critical properties of the two-dimensional Z(5) vector model,
poster presented by G. Cortese at LATTICE 2010, XVIII International Symposium on Lattice Gauge Theories, Villasimius, June 14 - 19, 2010.

9. D. Giuliano,
Local pairing of Cooper Pairs in Josephson junction networks,
Plenary talk given at the ESF Research Conferences "Quantum Engineering of States and Devices: Theory and Experiments",
Obergurlg (Austria), 5-10 June 2010.
10. M. Rossi,
Integrability in N=4 SYM: the non linear integral equation approach,
poster presented at the international workshop RAQIS 2010, Annecy-le-Vieux (France), 15-18 June 2010.

11. M. Rossi,
Beyond cusp anomalous dimension from integrability in SYM4,
talk given at "Diffraction 2010", Otranto (Lecce), Italy, 10 - 15 Sep 2010.

ORGANIZATION OF INTERNATIONAL CONFERENCES IN 2010

1. Diffraction 2010, International Workshop on Diffraction in High-Energy Physics,
Otranto, September 10-15, 2010, M. Capua, R. Fiore, A. Papa and E. Tassi (Univ. Calabria) *et al.*,
http://www.cs.infn.it/diff 2010

3. EXPERIMENTAL PARTICLE PHYSICS

Professors and Researchers M. Capua
G. Crosetti
L. La Rotonda
A. Mastroberardino
M. Schioppa
G. Susinno
E. Tassi

Postdoc fellows C. Adorisio
S. Fazio
D. Salvatore

PhD students V. Lavorini
G. Morello
T. Venturelli

Technicians: F. Pellegrino, V. Romano, P. Turco

Experimental particle physics studies the fundamental constituents of matter and the forces that cause their mutual interactions. Studies in experimental energy physics are made by means of particle accelerators and particle detectors. The first ones rise the energy of beam particles (in the most powerful accelerators the energy can reach values as large as a few TeV) and allow them to collide against each other or a target. The detectors are designed to reconstruct the particles produced as a consequence of the primary particle interactions. The need of innovative from the technological point of view has wide implications in many areas of applied physics.

The researches on high energies physics to which the physicists of this University take part are:

30. Study of the proton structure in deep inelastic scattering processes with the ZEUS experiment at the lepton-proton accelerator HERA of the DESY Laboratory (Hamburg, Germany).
31. Study of proton-proton interactions with the ATLAS experiment at the LHC accelerator of the CERN laboratory (Geneva, Switzerland).
32. Studies of a forward physics detector for ATLAS (AFP) and medical applications.
33. Hadronic calorimetry: analysis and development of hadronic calorimeter modules based on the Dual Readout Method (DREAM).
34. Study of the electron-positron interactions at the centre of mass energy 1020MeV with KLOE apparatus at DAFNE collider (Frascati, Italy).
35. Project for the realization of a ground-based apparatus to detect the muon content of the showers employing the last generation high precision drift chamber (UNICAL, Italy).

3.1 THE ZEUS EXPERIMENT AT THE HERA E-P COLLIDER (DESY, HAMBURG-GERMANY)

Physicists: M. Capua
S. Fazio
A. Mastroberardino
M. Schioppa
G. Susinno
E. Tassi

Technicians: F. Pellegrino

International collaboration

ZEUS is a collaboration running a large particle detector at the electron-proton collider, HERA, at the DESY laboratory in Hamburg. The participating scientists are pushing forward our knowledge of the fundamental particles and forces of nature, gaining unsurpassed insight into the exciting laws of the microcosm.
The ZEUS detector is a sophisticated tool for studying the particle reactions provided by the high-energetic beams of the HERA collider. At the HERA collider two separate magnet systems guide the electron (*e*) and proton (*p*) beams around the 6,3 km long ring and two independent superconducting RF systems accelerate the *e* and *p* bunches up to 30GeV and 920GeV energy respectively.
The High Energy Experimental Physics (HEP) group of the UNICAL has been involved in the ZEUS Collaboration, since 1988, in the design, construction, testing, calibration, alignment, running and maintenance of three components of ZEUS experiment: Forward Muon Spectrometer (FMUON), Leading Proton Spectrometer (LPS) and MicroVertex (MVD). Furthermore the UNICAL HEP researchers participate, since 1991 when the detector started operating, to the data taking as well as the physics analyses.

At the maximum beam energies the centre of mass energy is ~320GeV, much larger than previously achieved in such collisions, and allowing to probe the proton structure down to distance scales as low as 10^{-18}m which is a factor 1000 smaller than the proton radius. With this resolving power exciting physics topics can be studied, such as proton structure, neutral and charged current processes, tests of Quantum Chromodynamics, studies of diffraction and searches for physics beyond the Standard Model. At large momentum transfers (the kinematical limit at HERA is 10^5 GeV^2/c^2) there is a direct interaction of the electron with one of the quarks in the proton. For this reason HERA is often addressed as the world's only lepton-quark collider.

ZEUS collected 0.5fb-1 of data and new results are in progress and the UNICAL members of the Collaboration are actively involved. During the 2010 year we have continued to contribute to:

- the combination of the ZEUS and H1 inclusive results and determination of the proton parton distribution functions;
- the studies of Deeply Virtual Compton Scattering in diffractive processes with the complete HERA data set.

One of the most important goal of the HERA research program is to capitalize the experience gained in the study of inclusive and diffractive processes and apply it to future measurements at the LHC experiments.

3.2 ATLAS Experiment at the LHC proton-proton collider (Geneva – Switzerland)

Physicists: G. Crosetti
M. Capua
S. Fazio
L. La Rotonda
V. Lavorini
A. Mastroberardino
E. Meoni
G. Morello
D. Salvatore
M. Schioppa
G. Susinno
E. Tassi
T. Venturelli

Technicians: F. Pellegrino, V. Romano, P. Turco

International collaboration

Nature has given us more than one elementary particle (6 leptons, 6 quarks and the carriers of the four fundamental interactions), whose masses range in a wide interval of values from the mass-less gauge bosons to the top quark mass, M_t=170 GeV/c^2. The mechanism that determines the particle masses is still unknown and many experiments with particle accelerator have been undertaken to give an insight into it and explain the mass origin.

In 1964 Peter Higgs first proposed a clever solution to this puzzle: an undetectable field, similar to the electromagnetic one,permeates the whole space. As particles move in space they travel through this field, and interaction

with this field allows them to acquire their masses. This is similar to the action of viscous forces felt by particles moving through any thick liquid: the stronger the interaction of the particles with the field, the bigger the mass they seem to have. We know from quantum theory that fields have particles associated with them, so a Higgs boson should be associated to the Higgs field.

Up to now no one has ever observed the Higgs boson in an experiment to confirm the theory. Finding this particle would give an insight into why particles have certain mass, and help to develop subsequent physics. The technical problem is that we do not know the mass of the Higgs boson itself, which makes it more difficult to identify. Physicists have to look for it by systematically searching a range of mass within which it is predicted to exist. The yet unexplored range is accessible using the Large Hadron Collider (LHC).

This collider provides 10 times higher center of mass energy and 100 times higher p-p collision rates than previous colliders and is fully operative since November 2009. This opens up a new frontier of physics and the LHC experiments, ATLAS, CMS, ALICE and LHCb, are ready to explore this great potential.

ATLAS is a general-purpose experiment. Designed to see a wide range of particles and phenomena produced in LHC collisions, it involves approximately 2,000 physicists from some 35 countries. These scientists use the data collected from the complex detectors to search for new phenomena, including the Higgs boson, super-symmetry and extra dimensions. They also measure the properties of previously-discovered quarks and bosons with unprecedented precision, and are on the lookout for completely new, unpredicted phenomena.

The basic design concept to achieve these goals includes three detector systems:

Inner Tracker, with semiconductor pixel and strip detectors for very high accuracy measurements of the charged particle trajectories, followed by straw tube detectors giving independent electron identification. The tracker is confined to a cylinder 6.8 m long and with a radius of 1.1 m in a 2 T magnetic field, provided by a superconductive solenoid

Calorimeter, with an inner cylinder in highly granular liquid argon technology with Pb absorber, followed at large radius by an iron-tile scintillator calorimeter providing good resolution in a very cost-effective manner

High precision standalone **Muon Spectrometer**. Its conceptual layout is based on the magnetic deflection of muon track in a system of three large superconducting air-core toroid magnets instrumented with separate-function trigger and high-precision tracking chambers.

The researchers of the experimental high energy physics (HEP) group of UNICAL have been strongly involved in various aspects of the design, construction, installation and test of the muon spectrometer since 1994. During this period the contribution from many undergraduate, graduate and PhD students and postdoc researchers has been substantial to this end.

Our group is also involved in the design and simulation of the ATLAS Forward Physics (AFP) apparatus. The AFP is a proposed project which comprises a new generation of 3D silicon detectors, to be inserted along the beam pipe, at a distance of 220 m and 420 m from the interaction point. The installation of the detectors will allow the ATLAS experiment to study diffractive processes including the very important diffractive production of the Higgs boson.

During 2010 the Unical HEP group gave a major contribution to many ATLAS activities:

- Participation in the maintenance and improvement task force of the muon precision chambers at CERN. This is a small group of expert physicists taking care of the whole detector performance, overlooking the functionality of gas, readout, alignment, data control, high and low-voltage systems

- Development and maintenance of the Gnam package, the low-level data acquisition software for the ATLAS sub-detector online monitoring. The Gnam package is a low-level data acquisition software, capable to promptly spot if sub-detectors are not working properly. It decodes the raw data coming from sub-detectors and shows the relevant quantities through histograms: as an example, it reveals dead or noisy channels, which may affect the data taking itself and subsequent reconstruction and pattern recognition processes.

The Cosenza HEP group is involved in the design and development of the Gnam tool since the 2004 combined test beam of a slice of the ATLAS Muon Spectrometer. Highly appreciated, it was widely used during the installation and commissioning phase of the spectrometer and has been inserted into the official Trigger and Data Acquisition software of the ATLAS experiment. Now that LHC activity has started, most of the ATLAS sub-detector collaborations use Gnam online histograms to establish the quality of acquired data.

- Contribution to the Standard Model physics group: study of the production of the W and Z bosons and top quark.

The study of the production of the W and Z gauge bosons constitutes an important part of the ATLAS physics program at the LHC. The measurement of the their large production cross sections, that are known at the next-to-next-to-leading order (NNLO) in QCD, will allow to perform stringent tests of the predictions of the Standard Model and to study the properties of the gauge bosons in a hitherto unexplored kinematic region.

Our group is contributing to the measurement of the total and single differential cross sections for the production of the W and Z bosons, decaying in the leptonic (electron and muon) channel. The analyses are based on the full data sample collected by the ATLAS experiment in the year 2010. Our group is also working on a precise measurement of the W and Z charged asymmetries that have the potential, when included in Altarelli-Parisi QCD fits, to improve our understanding of the proton's parton distribution functions.

The top quark, the heaviest of all known elementary particles, was discovered in 1995 at the Fermilab Tevatron collider.

Studying top quarks is important for several reasons. With its large mass, the top quark is the only fermion at the electroweak scale; it is therefore of great interest for the studies of electroweak symmetry breaking. Accurately measuring the top quark mass also helps to put constraints on the SM Higgs boson mass. Additionally, top quarks will constitute a significant background process to many beyond SM searches.

Our group is also involved in the study of top pairs production with the top quarks decaying in the semileptonic mode, where events in the electron/muon plus jets channel are isolated.

- Contribution to the Long-Lived particle and Hidden Valley group and Exotics physics group.

Several extensions of the SM predict the existence of neutral, weakly coupled unstable particles with macroscopic decay lengths. Among these the Hidden Valley (HV) scenario predicts neutral long-lived particles, the so-called π_V, that decay to heavy quark pair and τ pairs. These particles can be produced in Higgs boson decays, supersimmetric processes and Z decays.

At the time of design, the ATLAS apparatus was not optimized to reveal neutral particles with long decay paths and di-jet final states displaced throughout the overall detector. As such these events, which might signal physics beyond the SM, would be undetected.

In collaboration with the INFN Rome1 group and the Seattle University, Washington, our group is involved in the study of the ATLAS detector performance for the Higgs decay into two π_V. The group is responsible of the search of the Higgs boson in the leptonic decay channel of the HV particle, in particular is active in the study of the acceptance of the existing as well as new ad-hoc designed triggers for this process. The leptonic decay channel represents the favourite decay mode for light Higgs boson and has a very clean topological signature. The group is also deeply involved in developing a realistic analysis strategy to reconstruct events from such unexplored physics.

Our group is also involved in the design and simulation of the ATLAS Forward Physics (AFP) apparatus. The AFP is a proposed project which comprises a new generation of 3D silicon detectors, to be inserted along the beam pipe, at a distance of 220 m and 420 m from the interaction point. The installation of the detectors will allow the ATLAS experiment to study diffractive processes including the very important diffractive production of the Higgs boson. Our group has organized, in April, an International Meeting dedicated to the ATLAS Forward Physics and Detectors Program.

3.3 HADRONIC CALORIMETRY

Physicists: L. La Rotonda
G. Susinno
T. Venturelli

Technicians: F. Pellegrino, V. Romano

International collaboration

High-precision measurements of hadrons and hadron jets have become increasingly important in experimental particle physics. The energy resolution of a hadron calorimeter is in general much worse than what can be achieved for e.m. shower detection. The wide variety of possible interaction processes and the effects associated with excitation of the absorber nuclei are considered responsible for this.

In compensating hadron calorimeters a dominant source of fluctuations that comes from π^0 production in the shower is eliminated by equalizing the calorimeter response to e.m. and purely hadronic shower component.

In recent years, R. Wigmans (Texas Tech) in collaboration with other groups have developed an alternative technique: The Dual Readout Method (DREAM). DREAM calorimeters are based on a simultaneous measurement of different types of signals which provide complementary information about details of the shower development.

The DREAM prototype, that has been successfully tested at CERN, is a copper absorber structure, equipped with two types of active media. Scintillating fibres measure the total energy deposited by the shower particles, while Quartz fibres measure the Cerenkov light that is only produced by the charged, relativistic shower particles.

Since the latter are almost exclusively found in the e.m. shower component (dominated by π^0 s produced in hadronic showers), a comparison of the two signals makes it possible to measure the energy fraction carried by this component, fem, event by event.

Once the effects of the dominant source of fluctuations, *i.e.,* fluctuations in the e.m. energy fraction fem, are eliminated, the performance characteristics are determined (and limited) by other types of fluctuations. In the described detector, a prominent role is played by the small number of Cerenkov photoelectrons constituting the signals (8 p.e./GeV) due to the small sampling fraction used in the prototype.

Moreover, for the measurement of electromagnetic showers and photons, it could be convenient to place in front to a DREAM-like calorimeter a high resolution electromagnetic homogenous calorimeter. In such a calorimeter it would be important to preserve the possibility of dual readout in order to correct the energy measurement of the fraction of hadrons developing electromagnetic showers already in this detector.

So, in order to improve the DREAM setup different ways are practicable:

a) Increase the sampling fraction in DREAM-like calorimeters, to increase the light collected

b) production of crystal electromagnetic calorimeters with dual readout to be placed in front of DREAM-like calorimeters, to improve the energy resolution of electromagnetic showers, keeping the possibility of measuring the electromagnetic fraction of hadrons showers that start in the electromagnetic calorimeter that can then be compensated on an event-by-event basis.

To this last projects, with U.S. researchers an Italian collaboration: Bologna - Cagliari - Cosenza - Roma1 -Pavia is working from 2006.

In a homogeneous calorimeter the two light components can be disentangled by:

(1) Directionality. The Cerenkov light is emitted at a fixed angle with respect to the momentum vector of the particle that generates it, while the scintillation light is isotropically emitted.

(2) Time structure. The Cerenkov light is prompt, whereas scintillation processes have one or several characteristic decay times.

(3) The spectrum. The Cerenkov light is emitted with a characteristic λ^{-2} spectrum, while the scintillation processes have their own characteristic spectra.

(4) Polarization. Contrary to scintillation light, Cerenkov light is polarized

Very promising results have been obtained in case of single doped BGO crystals and a small electromagnetic calorimeter made of lead tungstate (PbWO4) crystals tested in conjunction with the DREAM calorimeter mentioned above, and exposed to high energy particle beams at CERN's Super Proton Synchrotron.

Time structure and spectrum of signals like to be the most interesting characterization of two signals.

The study of new crystals more efficient to discriminate scintillation and Cerenkov light and the development of a faster electronic are going on.

The last additional feature that might in principle be used to distinguish scintillation from Cerenkov light is the fact that the latter is polarized. In 2010 we investigated the possibilities in this respect. High-energy pions were used to generate signals in a BGO crystal, and the effects of polarization filters on the two types of light generated in this crystal have been measured.

Respect to point a) in 2010 the first four prototype modules of a new DREAM-like calorimeter have been constructed and successfully tested. MIUR as considered this project as a PRIN (Progetto di Ricerca di Interesse Nazionale) project and has funded it in the period 2010-2012

The Cosenza Group participate to the Test Beam, data analysis and to the new modules construction and is involved in the Geant simulation .

3.4 3D PIXEL COLLABORATION

Physicists: M. Capua
S. Fazio
A. Mastroberardino
G. Susinno

Technicians: none

International collaboration

The 3D pixel Collaboration was approved in July 2007 and includes 4 processing facilities: CNM Barcelona (Spain), FBK Trento (Italy) and the 3DC Consortium with SINTEF (Norway) and Stanford (USA). The main goals of these studies are the development, industrial fabrication, characterization and testing, with and without front-end readout chips, of full-3D with active-edge and mod (double side)-3D silicon pixel sensors of extreme radiation hardness and high speed for the Super-LHC ATLAS upgrade and the ATLAS B-layer replacement (IBL).

A specific goal is to demonstrate the design implementations of 3D as a safe sensor solution for the IBL in the high radiation environment expected during the full period between the LHC phase-1 and phase-2 upgrades.

Using data sets collected in dedicated test beams, taken in 2009, to which our group actively contributed, our group has this year published new results on the performance of the 3D sensor prototypes

3.5 KLOE-2 EXPERIMENT AT DAFNE E-E+ COLLIDER (National Laboratory of Frascati)

Physicists: M. Schioppa
G. Morello

Technicians: none

International collaboration

The DAFNE collider accelerates stores electrons and positrons of 510MeV energy each to produce PHI-mesons via the reaction e^+e^- -> gamma* -> PHI. This meson is made of strange – anti-strange quanrks, has 1020 MeV/c2 mass, has the photon quantum numbers: $J^{PC}=1^{--}$. It decays at rest and the final state contains mainly charged and neutral kaon pairs (branching ratio BR=49.5% and BR=34.3% respectively), RHO-PI and PI+PI-PI0 (BR=15.5%), ETA-GAMMA (BR=1.3%), ETA'-GAMMA (BR=0.00012). The neutral kaon pairs are produced in a well-defined quantum and kinematical state with negative charge parity. The kaons are monochromatic (127MeV/c for charged kaons and 110MeV/c for the neutral one) and are emitted back to back to be detected in an almost background free environment. With the integrated luminosity of 2.5fb-1 (2001-2006) the collider has produced 10^10 PHI-mesons and than about 10^10 kaon pairs.

The experiment KLOE is a general purpose detector designed to study all kinds of kaon, PHI, RHO, ETA and ETA' decays emphasizing tests of discrete symmetries (CP-, CPT-, T-invariance) and measurements of hadronic cross sections and tests of chiral perturbation theory.

The detector is a huge (4m diameter, 4m long), transparent drift chamber in 0.5Tesla magnetic field produced by a superconductive solenoid, with 55000 stereo wires, in helium based gas mixture, surrounded by a lead-scintillating fibre calorimeter, 15X0 thick, 98% solid angle coverage with a resolution of 54ps/SQRT(E)+140ps (E in GeV) in time and 5.7%/SQRT(E) in energy .

During 2008 the INFN has approved the KLOE-2 proposal at the improved DAFNE luminosity performance. The

data taking campaign (20-50fb-1) will start on spring 2011.

The contribution to KLOE-2 project of the UNICAL's researchers has been focused on CCALT LYSO calorimeter performance studies by GEANT4 simulations, QCALT tile calorimeter tests with UV pulsed LED on photodiodes, tiles and fibres, cylindrical GEM inner tracker detector gas gain simulations and prototypes test beams and the study of light boson weekly coupled with standard matter using initial state radiation events.

3.6 AIR SHOWER OBSERVATORY WITH SCINTILLATOR DETECTORS ARRAY

Physicists: M. Schioppa
Technicians: none

During the last 20 years the Astroparticle research has considerably contributed to the better understanding of the laws that govern the Universe but it has also leaved many open questions (i.e. the origin, the acceleration mechanism and the elementary composition of the Cosmic Rays) that can be coped only with ground based experimental apparatus that are the only capable to detect those CR coming from galactic and extragalactic exotic astrophysical sources and directly from the Big Bang. Indeed these particles have energy greater than 100TeV (UHE) and interact with the nuclei of the atmosphere generating extensive air showers (EASs). During the last years the ground-based apparatus have reached goals unattainable with the other techniques to explore the Universe. For example it has put in evidence a very large number of gamma-sources from our galaxy and from other galaxy, it has demonstrated the existence of very complex gamma sources, and it has discovered extragalactic gamma source at distance never explored previously.

The researchers of UNICAL physics department, with the precious collaboration of physics students, have designed and realized an EAS observatory made of 3 large scintillator counters placed at the vertex of an equilateral triangle, 20m side. The apparatus detects EAS produced by CR of energy greater than PeV and can measure the direction of the primary CR with a resolution of 5°. During 2010 the apparatus has collected about half million EAS and the data analysis is in progress. The apparatus is particularly suitable also for didactics purpose.

A PUBLICATIONS ON SCIENTIFIC JOURNALS

A.1 Publications on international scientific journals

A.1.1 Publications on international scientific journals published on 2010

1. Capua M., Fazio S., Mastroberardino A., Schioppa M., Susinno G., Tassi E., Zeus C.,
   Measurement of high-Q^2 charged current deep inelastic scattering cross sections with a longitudinally polarised positron beam at HERA,
   European Physical Journal C, 2010, Vol. 70, n. 4, pp. 945-963

2. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Morello G., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C.,
   Drift Time Measurement in the ATLAS Liquid Argon Electromagnetic Calorimeter using Cosmic Muons,
   European Physical Journal C, 2010, Vol. 70, n. 3, pp. 755-785.

3. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Morello G., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C.,
   Charged-particle multiplicities in pp interactions at sqrt(s) = 900 GeV measured with the ATLAS detector at the LHC,
   Physics Letters B, 2010, Vol. 688, pp. 21-42.

4. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Morello G., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C.,
   Readiness of the ATLAS Tile Calorimeter for LHC collisions,
   European Physical Journal C, 2010, Vol. 70, n. 4, pp. 1193-1236.

5. Schioppa M., et al.,
   Luminosity and background measurements at the e+e− DAΦNE collider upgraded with the crab waist scheme, Nuclear instruments & methods in physics research. Section A, Accelerators, spectrometers, detectors and associated equipment, 2010, Vol. 621, pp. 121-129.

6. Schioppa M., et al.,
   Description and performances of luminosity and background detectors at the upgraded e+e- DAFNE collider, Nuclear instruments & methods in physics research. Section A, Accelerators, spectrometers, detectors and associated equipment, 2010, Vol. 621, pp. 157-170.

7. Schioppa M., et al.,
   Detectors for absolute luminosity measurement at DAFNE,
   Nuclear instruments & methods in physics research. Section A, Accelerators, spectrometers, detectors and associated equipment, 2010, Vol. 617, pp. 453-456

8. Capua M., Fazio S., Mastroberardino A., Schioppa M., Susinno G., Tassi E., Zeus C.,
   Measurement of J/psi photoproduction at large momentum transfer at HERA,
   Journal of High Energy Physics, 2010, Vol. 1005, n. 085, pp. 1-38.

9. Schioppa M., Morello G., et al.,
   Activity of CERN and LNF groups on large area GEM detectors,
   Nuclear instruments & methods in physics research. Section A, Accelerators, spectrometers, detectors and associated equipment, 2010, Vol. 617, pp. 151-154.

10. Adorisio C., Capua M., Crosetti G., Fazio S., La Rotonda L., Mastroberardino A., Morello G., Salvatore D., Schioppa M., Susinno G., Atlas C.,
    Measurement of the W -> l ν and Z/gamma -> ll production cross sections in proton-proton collisions at sqrt(s) = 7*

TeV with the ATLAS detector,
Journal of High Energy Physics, 2010, Vol. 2010, n. 12, pp. 1-65.

11. Capua M., Fazio S., Mastroberardino A., Schioppa M., Susinno G., Tassi E., Zeus C.,
Events with an isolated lepton and missing transverse momentum and measurement of W production at HERA, Journal of High Energy Physics, 2010, Vol. 1003, n. 035, pp. 1-19.

12. Capua M., Fazio S., Mastroberardino A., Schioppa M., Susinno G., Tassi E., Zeus C.,
Inclusive dijet cross sections in neutral current deep inelastic scattering at HERA,
European Physical Journal C, 2010, Vol. 70, n. 4, pp. 965-982.

13. Capua M., Fazio S., Mastroberardino A., Schioppa M., Susinno G., Tassi E., Zeus C.,
Combined measurement and QCD analysis of the inclusive e± p scattering cross sections at HERA,
Journal of High Energy Physics, 2010, Vol. 1001, n. 109, pp. 1-55.

14. Capua M., Fazio S., Mastroberardino A., Schioppa M., Susinno G., Tassi E., Zeus C.,
A QCD analysis of ZEUS diffractive data,
Nuclear Physics B, 2010, Vol. 831, pp. 1-25.

15. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Morello G., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C.,
Readiness of the ATLAS Liquid Argon Calorimeter for LHC Collisions,
EUROPEAN PHYSICAL JOURNAL C, 2010, Vol. 70, n. 3, pp. 723-753.

16. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Morello G., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C.,
The ATLAS Inner Detector commissioning and calibration,
European Physical Journal C, 2010, Vol. 70, n. 3, pp. 787-821.

17. Capua M., Fazio S., Mastroberardino A., Schioppa M., Susinno G., Tassi E., Zeus C.,
Measurement of D^+ and Λ_c^+ production in deep inelastic scattering at HERA,
Journal of High Energy Physics, 2010, Vol. 2010, n. 11, pp. 1-27.

18. Capua M., Fazio S., Mastroberardino A., Schioppa M., Susinno G., Tassi E., Zeus C.,
Measurement of charm and beauty production in deep inelastic ep scattering from decays into muons at HERA,
European Physical Journal C, 2010, Vol. 65, pp. 65-79.

19. Capua M., Fazio S., Mastroberardino A., Schioppa M., Susinno G., Tassi E., Zeus C., "
Measurement of dijet photoproduction for events with a leading neutron at HERA,
Nuclear Physics B, 2010, Vol. 827, pp. 1-33.

20. Capua M., Fazio S., Mastroberardino A., Schioppa M., Susinno G., Tassi E., Zeus C.,
Measurement of beauty production in DIS and F-2(b(b)over-bar) extraction at ZEUS,
European Physical Journal C, 2010, Vol. 69, pp. 347-360.

21. Capua M., Fazio S., Mastroberardino A., Schioppa M., Susinno G., Tassi E., Zeus C.,
Measurement of isolated photon production in deep inelastic ep scattering ZEUS Collaboration,
Physics Letters B, 2010, Vol. 687, pp. 16-25.

22. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Morello G., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C.,
Performance of the ATLAS Detector using First Collision Data,
Journal of High Energy Physics, 2010, Vol. 2010, n. 9, pp. 1-66.

23. Capua M., Crosetti G., La Rotonda L., Mastroberardino A., Morello G., Salvatore D., Schioppa M., Susinno G., Tassi E., Atlas C.,
Search For New Particles in Two-Jet Final States in 7 TeV Proton-Proton Collisions with the ATLAS Detector at the LHC,
Physical Review Letters, 2010, Vol. 105, pp. 1-19.

24. Capua M., Fazio S., Mastroberardino A., Schioppa M., Susinno G., Tassi E., Zeus C.,
Inclusive-jet cross sections in NC DIS at HERA and a comparison of the k(T), anti-k(T) and SIScone jet algorithms,
Physics Letters B, 2010, Vol. 691, pp. 127-137.

25. L. La Rotonda, G. Susinno, T. Venturelli and DREAM Collaboration,
Optimization of crystals for applications in dual-read out calorimetry,
Nuclear instruments & methods in physics research. Section A, Accelerators, spectrometers, detectors and associated equipment, 2010, Vol. 621, pp. 212-221.

A.1.2 Publications on international journals accepted in 2010

1. Capua M., Fazio S., Mastroberardino A., et al.,
3D-FBK pixel sensors: Recent beam tests results with irradiated devices,
Accepted by Nuclear Instruments and Methods In Physics Research A, doi:10.1016/j.nima.2010.12.209.

2. L. La Rotonda, G. Susinno, T. Venturelli and DREAM Collaboration,
Polarization as a tool for dual-read out calorimetry,
Accepted by Nuclear Instruments and Methods In Physics Research A.

3. L. La Rotonda, G. Susinno, T. Venturelli and DREAM Collaboration,
A *Comparison of BGO and BSO Crystals Used in the Dual-Readout Mode,*
Accepted by Nuclear Instruments and Methods In Physics Research A.

A.1.3 Public international notes in 2010

1. G. Morello, M.Schioppa, et al.,
Technical Design Report of the Inner Tracker for the KLOE-2 experiment,
LNF-10-3-P, feb. 2010, 77pp, arXiv:1002.2572.

2. G. Morello, M.Schioppa, et al.,
Proposal for taking data with the KLOE-2 detector at the DAFNE collider upgraded in energy,
LNF-10-17-P, jul. 2010, 22pp, arXiv:1007.5219.

B PUBLICATIONS ON CONFERENCE PROCEEDINGS

B.1Publications on international conference proceedings in 2010

1. M. Capua,
Perturbative and non-perturbative diffraction at HERA,
30th International Symposium On Physics In Collision, 1-4 Sep 2010 Karlsruhe, Germany arXiv: 1101.1561, to be published.

2. M. Schioppa, et al.,
Test of a LYSO matrix with an electron beam between 10MeV and 500MeV for KLOE-2,
Prepared for the XI Pisa Meeting on advanced detectors: Frontier Detectors for Frontier Physics, La Biodola, Italy, 24-30 May 2009. Published in Nucl.Instrum.Meth.A 617, pag. 109-112, 2010

3. M. Schioppa, et al.,
   Activity of CERN and LNF groups on large area GEM detectors,
   Prepared for the XI Pisa Meeting on advanced detectors: Frontier Detectors for Frontier Physics, La Biodola, Italy, 24-30 May 2009.
   Published in Nucl.Instrum.Meth.A 617, pag. 151-154, 2010.

4. M. Schioppa, et al.,
   Detectors for absolute luminosity measurement at DAFNE,
   Prepared for the XI Pisa Meeting on advanced detectors: Frontier Detectors for Frontier Physics, La Biodola, Italy, 24-30 May 2009.
   Published in Nucl.Instrum.Meth.A 617, pag. 453-456, 2010.

PRESENTATIONS AT SCHOOLS AND CONFERENCES
C.1 Invited presentations at international schools and conferences in 2010

1. M. Capua,
   Perturbative and non-perturbative diffraction at HERA,
   30th International Symposium On Physics In Collision 1-4 Sep 2010 Karlsruhe, Germany arXiv: 1101.1561.

2. E. Tassi,
   Convener of the section "Hadronic Structure, Parton Distributions, soft QCD, Spectroscopy" of the 35th International Conference on High Energy Physics, 22-28 Jul 2010. Paris, France.

3. S. Fazio,
   From DVCS to Vector Meson Electroproduction,
   Workshop on Diffractive and Electromagnetic Processes at the LHC, Trento (Italia), 4-8 gennaio 2010.

4. S. Fazio,
   Vector Meson Production and DVCS at HERA on behalf of ZEUS ed H1,
   Low-x Meeting 2010, Kavala (Grecia), 23-27 giugno 2010.

4. SURFACE ELECTRON SPECTROSCOPY (SPES)

Professors and Researchers	Elio Colavita (*Group Leader*) Gennaro Chiarello Raffaele Giuseppe Agostino Vincenzo Formoso Tommaso Caruso
Postdoc fellows	Enrico Maccallini Alfonso Policicchio
PhD students	Antonio Marino Georgios Kalantzopoulos Myrsini Antoniou
Technicians	Salvatore Abate (*Lycril/CNR*) Giovanni Desiderio (*Lycril/CNR*) Vito Fabio Eugenio Li Preti
Collaborators	P. Milani *(University of Milano, Italy)* P. Rudolf *(Material Science Center, University of Groningen, The Netherlands)* C.E. Bottani *(Politecnico of Milan, Italy)* J. bNagy *(Dept of chemical and material engineering, Univ. of Calabria)* G. Golemme *(Dept of chemical and material engineering, Univ. of Calabria)* A. Goldoni *(Elettra, Trieste, Italy)* S. La Rosa *(Elettra, Trieste, Italy)* S. Scalese *(CNR, Catalina, Italy)* D. Gournis *(University of Ioannina, Greece)* F. Alamgir *(Brookhaven National Laboratory, New York, USA)* G. Froudakis *(University of Crete, Greece)* P. Trikalitis *(University of Crete, Greece)* F. Alamgir *(Georgia Institute of Technology, Atlanta, Georgia, USA)* G. Valenti *(University of Bari, Italy)* A. Politano *(Universidad Autonoma de Madrid, Cantoblanco, Spain)*

Research subjects:

4.1 CHEMISORPTION ON METAL SURFACES
- 4.1.1 Enhancement of hydrolysis in alkali ultrathin layers on metal substrates in the presence of electron confinement
- 4.1.2 Alkali coadsorption with oxygen on gold thin film
- 4.1.3 Alkali-promoted stabilization of subsurface oxygen on Cu(111)
- 4.1.4 CO-promoted formation of the alkali-oxygen bond on Ni(111)

4.2 ELECTRONIC COLLECTIVE EXCITATIONS OF METAL SYSTEMS
- 4.2.1 Low-energy bulk plasmon of nickel
- 4.2.2 Plasmonic modes confined in nanoscale thin silver films deposited onto metallic substrates
- 4.2.3 Sputtering-induced modification of the electronic properties of of Ag/Cu(111)

4.3 SPECTROSCOPIC AND MICROSCOPIC STUDIES OF CARBON AND METAL-OXIDE NANOSTRUCURES

Introduction

The Group carried out his research activity on vibrational and electronic properties of surfaces and on ultra thin films and, moreover, on TiO_2 nanostructures by photoemission and absorption investigations.

Vibrational studies of alkali atoms and their coadsorption with carbon monoxide, oxygen and water on Ni(111) and Cu(111) surfaces allowed to shed more light on some long standing problems as the relationship between chemical reactivity and electron quantum confinement and the presence of subsurface oxygen species in alkali-modified copper surfaces. The research activity involved also the preparation and the investigation of the electronic properties of ultra-ultrathin films of Ag and Au supported on the Ni(111) and Cu(111) surfaces. We also studied the influence of defects introduced by ion bombardment on the electronic response of such films. Low-energy electronic collective excitations were studied for the bare Ni surface. We found the existence of a low-energy bulk plasmon.

Metal-oxide nanostructures spectroscopic studies deal with photoemission and absorption investigations on nanostructured TiO_2 grown by a pulsed laser deposition method. In addition we characterized by environmental scanning electron microscopy the wetting properties of these TiO_2 nanostructures hierarchically organized in a columnar structure. The samples were grown with different synthesis parameters in order to understand their relationship with the hydrophobic-hydrophillic properties and their structural evolution by thermal annealing. This work was realized in collaboration with the group of Prof. Carlo Bottani of the Politecnico di Milano.

4.1 CHEMISORPTION ON METAL SURFACES

4.1.1 Enhancement of hydrolysis in alkali ultrathin layers on metal substrates in the presence of electron confinement

Vibrational spectroscopy has been used to study the interaction at room temperature of H_2O with ultrathin alkali films grown on Cu(111), Ni(111) and Ag/Ni(111). We find strongly enhanced dissociation efficiency in the monolayer regime of Na/Cu(111), indicative of an active role of the existing Na-derived quantum wells in hydrolysis. No water adsorption has been observed for alkalis (Na, K) adsorbed on Ni(111), very likely due to the absence of electron confinement in these systems. On the other hand, partial water dissociation has been revealed in K-doped silver thin layers on Ni(111), in the presence of Ag 5sp-derived quantum wells.

4.1.2 Alkali coadsorption with oxygen on gold thin film

We have investigated the catalytic properties of Na-doped Au monolayer grown on Cu(111). The presence of Na atoms allows the dissociation of oxygen molecules and the stabilization of atomic oxygen. The strong reduction of the dissociation barrier for O_2 promoted by Na could readily favor many surface chemical reactions, due to the key role of atomic oxygen in many oxidation processes catalyzed by gold.

4.1.3 Alkali-promoted stabilization of subsurface oxygen on Cu(111)

The coadsorption of alkalis (Na, K) with O on Cu(111) and Ni(111) surfaces was studied by vibrational measurements. We found that doping the Cu(111) surface with small amounts of alkalis reverses the energetic conditions for oxygen adsorption so as to render energetically favorable the population of subsurface sites. Such mechanism is not effective for the alkali-modified Ni(111) surface.

4.1.4 CO-promoted formation of the alkali-oxygen bond on Ni(111)

We have studied the coadsorption of alkali metals (Na, K) and oxygen on clean and CO-modified Ni(111) surfaces. We unambiguously show that on an alkali-precovered surface, the alkali-O bond was not formed upon O2 exposure. On the contrary, the alkali-O bond was readily observed by exposing to O2 the Ni(111) surface precovered with an alkali+CO phase. This enhanced oxidation rate of alkali metals in the presence of CO molecules was ascribed to the short-range CO-induced modification of the electronic charge of alkali-metal adatoms.

4.2 ELECTRONIC COLLECTIVE EXCITATIONS OF METAL SYSTEMS

4.2.1 Low-energy bulk plasmon of nickel

High-resolution electron energy loss spectroscopy has been used to study low-energy bulk excitation modes of planar-bound electrons (bulk plasmons) in nickel. We observed for the first time a bulk plasmon at about 1.2 eV, in agreement with dielectric theory. The behavior of its amplitude with the off-specular angle ensures the dipolar nature of such mode. On the other hand, the intensity of the plasmon peak is vanishing upon ion bombardment due to the sputtering-induced modification of dielectric function.

4.2.2 Plasmonic modes confined in nanoscale thin silver films deposited onto metallic substrates

Collective electronic excitations in nanoscale thin Ag layers adsorbed on Cu(111) and Ni(111) at room temperature have been investigated by angle-resolved electron energy loss spectroscopy.

Surface plasmon was found to be confined within grains on Ag thin films on Cu(111) nanostructured in islands. Annealing removed surface plasmon confinement and induced a negative linear term of the dispersion relation. On the other hand, on flat thin films on Ni(111) the dispersion of Ag surface plasmon was found to be fully quadratic. Landau damping processes of the plasmonic excitation were found to be dependent on the growth mode. Ag multipole surface plasmon at 7.7 eV was observed only under stringent kinematic conditions enhancing surface sensitivity.

4.2.3 Sputtering-induced modification of the electronic properties of of Ag/Cu(111)

We have investigated the electronic properties of Ag thin films deposited on Cu(111) and modified by Ar^+ sputtering. Ion sputtering strongly modifies the loss function in the region of single-particle transition as deduced from the appearance of sputtering-induced spectral features in the valence band. In contrast to unmodified Ag systems, in the sputtered films the centroid of the induced charge of the surface plasmon lies in the close vicinity of the jellium edge. In these modified Ag films, Landau damping processes are activated beyond a critical energy of 3.83 eV and a threshold wave vector of 0.2 $Å^{-1}$. Moreover, we find that plural plasmonic losses arise upon increasing the Ar^+ dose.

4.3 SPECTROSCOPIC AND MICROSCOPIC STUDIES OF CARBON AND METAL-OXIDE NANOSTRUCURES.

4.3.1 Photoemission and X-ray absorption investigations on nanostructured TiO_2 grown by pulsed laser deposition

Titanium dioxide is widely employed in photocatalysis, electronics and biotechnology. Many TiO_2 properties strongly depend on its nanostructure and electronic properties; hence, for the production of technological devices, it is crucial to develop nanoscale control of the morphology and structure of the material as well as of its surface properties. Pulsed Laser Deposition (PLD), that permits to control both size (from atom to clusters) and chemical state of the deposited films building blocks, can achieve this goal.

Titanium oxide nanostructured thin films, synthesized by pulsed laser deposition (PLD) at the Politecnico di Milano in collaboration with the C.E. Bottani group (NanoLab), were characterized with a multi-technique approach to investigate the relation between surface electronic, structural and morphological properties. Home laboratory and synchrotron radiation experiments were performed.

Depending on the growth parameters, these films present characteristic morphologies ranging from compact to columnar and to an extremely open structure. As-deposited films have a disordered structure both in the bulk and on the surface, as shown by Raman spectroscopy and by the fine structure of X-ray absorption spectra near the Ti and O edge (NEXAFS). The surface reactivity towards the atmosphere was analyzed by photoemission spectroscopy, formation of surface hydroxyl terminal groups was observed and turns out to be dependent not only on the effective surface but also on the surface structure. By ultraviolet photoemission spectroscopy, we observed that, depending on the sample structure and morphology, defect states at 1 eV binding energy in the valence band can be induced by exposing the samples to an intense synchrotron photon beam. After annealing at 673 K, the structural order increases towards a mainly anatase phase in which the presence of rutile increases in films with a more open morphology. Such structural modifications influence the surface stability since the defect formation in the valence band is strongly reduced in all the annealed films, and it is completely hindered in the most compact films.

These studies were partially carried out, following acceptation of official proposals, by different experiments at the

ELETTRA Synchrotron (Materials Science beamline).

In addition in collaboration with the same group we submit two Italian FIRB, PROGRAMMA "FUTURO IN RICERCA", projects with titles “Oxide Meso and Nanostructured Surfaces for Innovative light HArvesting (OMNIHA)” and “SHINING - Surfaces and hybrid interfaces for innovative nanoengineered solar cells” where our group was involved as local coordinator unit. On these projects the electronic, morphological and structural characterization of TiO_x and TCO indium free thin films, and TiOx/dye interfaces, will be performed and completed with electric measurements to test the photovoltaic efficiency of these materials.

4.3.2 Electronic and structural characterization of carbon nanotubes

The electronic, chemical and structural properties of Carbon NanoTubes (CNTs) growth by Chemical CVD (CCVD) were analyzed. The CNTs were grown by Prof. Dimitrios Gournis of University of Ioannina, Greece. The CCVD process is governed by the choice of carbon source, catalyst and growth temperature although in many studies other parameters, such as growth time, have been also proved to be crucial to the resulting carbon materials. SWCNTs, DWCNTs and mixtures of those two have been grown over Fe-Co bimetallic catalysts using various combinations of support material and hydrocarbon gases. We studied samples obtained by the synthesis of SWCNTs in high yields by catalytic decomposition of acetylene over MgO supported Fe-Co bimetallic catalysts without performing any pre-reduction treatment. Transmission electron images were obtained with High Resolution Transmission Electron Microscope (HRTEM) LEO 922. The electronic and chemical structure of the synthesized carbon products were analyzed by Energy Filter Transmission Electron Microscope (EFTEM). The data have been reprodeuced by FEFF program in order to understand the local electronic and structural properties. In addition, as a comparison, valence band measurements have been carried out at ELETTRA synchrotron facility in Trieste.

Recently our group started another collaboration on the synthesis and the characterization of CNTs with Prof. J. B. Nagy, Department of Chemistry and Materials Engineering, University of Calabria, about the synthesis of CNT by chemical vapour deposition (CVD) technique, supported on zeolites substrates impregnated with Fe and Co catalytic nanoparticles. The characterizations have been obtained by SEM and micro-Raman spectroscopy. The samples show different morphologies due to the synthesis conditions (catalytic nanoparticle size and composition, supporting substrate, gas carrier pressure…). The novelty lies on the synthesis of CNTs into the sepiolite substrate, which is new result in the literature. The goal is also the production of single walled CNT with open ends and well determined diameter for hydrogen storage application. The use of open CNTs should enhance the hydrogen storage capacity because in this way outer and inner surface of CNT will be utilized for H_2 adsorption.

4.4 MORPHOLOGICAL AND STRUCTURAL CHARACTERIZATION AND VOLUMETRIC GAS ADSORPTION EVALUATION OF MESO AND MICROPOROUS MATERIALS WITH HIGH SURFACE SPECIFIC AREA

4.4.1 New silicalite carbon nanostructures materials for hydrogen storage

The SPES group has been involved since 2007 studies the gas adsorption on porous materials in collaborations with both academic (University of Ioannina and Crete (*Greece*)) and industrial (INNOVA Technology Solutions (*Italy*)) partnerships. The materials under investigation are MCM-41 like, which have a hexagonal ordering of the pores. SEM and XRD measurements were carried out on those materials by the several equipments present in our Department. The experimental system (PcT) developed in our group to measure the hydrogen capacity up to 80 bar. We study the storage capacity dependence on the pore size and the chemical species present on the surface. Furthermore, we depict the dependence of the hydrogen storage capacity on the surface specific area (SSA) of the sample. Usually higher SSA means higher storage capacity. However we observed important stored amount of hydrogen molecules in sample with smaller SSA because of the substitution of peculiar atoms into the sample surface enhancing in this way the physical interaction with H_2. On the same samples preliminary results on CH_4 adsorption have been obtained.

4.4.2 Hydrogen storage capacity at high pressure of organo-silane modified silicalite

The PcT apparatus has been utilized to obtain the adsorption isotherms of modified zeolite by organo-silane molecules. This modification, which is well known in the literature, is external to the zeolite surface. The modification is introduced in order to change the dynamical adsorption properties of the samples by changing the diameter pore size. In this way the diffusion time of hydrogen molecules is different depending on the modification. The next step is the testing of the sample by CH_4 in order to observe if the diffusion time is different. If differences will be observed, that modified zeolites

can be utilized as selective membranes. The CNTs growth in CCVD is governed by the choice of carbon source, catalyst and growth temperature although in many studies other parameters, such as growth time, have been also proved to be crucial to the resulting carbon materials. SWCNTs, DWCNTs and mixtures of those two have been grown over Fe-Co bimetallic catalysts using various combinations of support material and hydrocarbon gases. We studied samples obtained by the synthesis of SWCNTs in high yields by catalytic decomposition of acetylene over MgO supported Fe-Co bimetallic catalysts without performing any pre-reduction treatment. Transmission electron images were obtained with High Resolution Transmission Electron Microscope (HRTEM) LEO 922. The electronic and chemical structure of the synthesized carbon products were analyzed by Energy Filter Transmission Electron Microscope (EFTEM).

A PUBLICATIONS ON SCIENTIFIC JOURNALS

A.1 Publications on international journals

A.1.1 Publications on international journals printed in 2010

1. Politano A. , Chiarello G. ,
O_2 dissociation in Na-modified gold ultrathin layer on Cu(111),
Gold Bulletin, 2010, Vol. 43, pp. 267-274.

2. Politano A. , Formoso V. , Chiarello G. ,
Plasmonic modes confined in nanoscale thin silver films deposited onto metallic substrates,
Journal of Nanoscience and Nanotechnology, 2010, Vol. 10, pp. 1313-1321.

3. Politano A. , Marino A. R. , Chiarello G. ,
CO-promoted formation of the alkali-oxygen bond on Ni(111),
Journal of Chemical Physics, 2010, Vol. 132, n. 4, pp. 044706-1-044706-5.

4. Politano A. , Chiarello G. ,
Sputtering-induced modification of the electronic properties of of Ag/Cu(111),
Journal of Physics D: Applied Physics, 2010, Vol. 43, pp. 085302-1-085302-9.

5. Politano A. , Chiarello G. ,
Enhancement of hydrolysis in alkali ultrathin layers on metal substrates in the presence of electron confinement,
Chemical Physics Letters, 2010, Vol. 494, pp. 84-87.

6. Politano A. , Marino A. R. , Chiarello G. ,
Alkali-promoted stabilization of subsurface oxygen on Cu(111),
Chemical Physics, 2010, Vol. 367, n. 1-2, pp. 148-151.

7. Politano A. , Chiarello G. ,
Low-energy bulk plasmon of nickel,
Solid State Sciences, 2010, Vol. 12, pp. 2096-2099.

8. Maccallini E. , Tsoufis T. , Policicchio A. , La Rosa S. , Caruso T. , Chiarello G. , Colavita E. , Formoso V. , Gournis D. , Agostino R. G. ,
A spectro-microscopic investigation of Fe–Co bimetallic catalysts supported on MgO for the production of thin carbon nanotubes,
Carbon, 2010, Vol 48 pp. 3434-3445.

A.1.2. Publications on international journals accepted in 2010

1. Politano A. , Chiarello G. ,
Change of the Adsorption Site for CO Molecules on Nickel Surfaces upon Coadsorption: A Comparative Study,
The Journal of Physical Chemistry C, 2011, pp. xxx-xxx.

2. Politano A. , Chiarello G. ,
Carbon monoxide interaction with oxygenated nickel single-crystal surfaces studied by vibrational spectroscopy,
Vibrational spectroscopy, 2011, Vol. 55, pp. 295-299.

3. Fusi M. , Maccallini E. , Caruso T. , Casari C. , Li Bassi A. , Bottani C. , Rudolf P. , Prince K. C. , Agostino R. G. ,
Surface electronic and structural properties of nanostructured titanium oxide grown by pulsed laser deposition,
Surface Science, 605 (2011) 333–340

4. M. Fusi, F. Di Fonzo, C. S. Casari, E. Maccallini, T. Caruso, R. G. Agostino, C. E. Bottani and A. Li Bassi*, *Island Organization of TiO2 Hierarchical Nanostructures Induced by Surface Wetting and Drying*, Langmuir 2011, 27(5), 1935–1941.

International and National Projects

a) Proposal full title: SHINING - Surfaces and hybrid interfaces for innovative nanoengineered solar cells
Italian FIRB - PROGRAMMA "FUTURO IN RICERCA" project
Name of the coordinating person: Dr. C.S. Casari
List of participants:
1 (Coordinator) Politecnico di Milano
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Application in 2010

b) Proposal full title: Oxide Meso and Nanostructured Surfaces for Innovative light HArvesting (OMNIHA)
Italian FIRB - PROGRAMMA "FUTURO IN RICERCA" project
Name of the coordinating person: Dr. A. Li Bassi
List of participants:
1 (Coordinator) Politecnico di Milano
2 Physics Dept, Università della Calabria
Application in 2010

International patent

a) D. Gournis, P. Trikalitis, G. Froudakis, R.G. Agostino,
Functional nanoporous materials for gas storage applications,
International Patent n. PCT WO20119889A2, deposited on 21/07/2010,
pubblished on 27/01/2011

5. CONDENSED MATTER PHYSICS

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The research activity of the group is oriented in seven closely related directions, which are briefly described in the following sections:

5.1 Surface Nanoscience
5.2 Secondary Electron emission and charge transfer processes in the interaction of slow ions and electrons with solids
5.3 Photon-matter interaction: electronic properties of graphene and related materials
5.4 Quantum coherence and correlations in condensed matter systems
5.5 Ion interaction with nanostructures and solids
5.6 Multimedial education

5.1 SURFACE NANOSCIENCE

Understanding the interaction of epitaxial monolayer graphite (MG) grown on transition metal (TM) with the substrate is an important step from both fundamental and technological point of view. Recently, we address our research on the fabrication and study of graphene overlayers epitaxially grown on metallic surfaces, in order to develop a fundamental understanding of the graphene-substrate interaction. We investigate electronic structure of the MG/metal system by surface spectroscopic techniques based on different probes: Auger electron spectroscopy (AES), high-resolution (HR) electron energy loss spectroscopy (EELS) and photoelectron spectroscopies (XPS, UPS).

Angle resolved (AR) EELS is mainly used to obtain information about the valence band structure and the momentum-space-dependence of collective excitations in graphene foils grown on metallic substrates. Electron emission from well ordered thin films, excited by photons or monochromatized electrons, follows the conservation laws of energy and momentum parallel to the surface. This means that the parallel component of the wave vector of either the valence electrons or the excited plasmons can be obtained together with the energy. In particular, we are focusing on two-dimensional (2D) plasmons, whose charge fluctuations are strongly localized at a monolayer. Graphene is a significant testing ground of the microscopic dielectric theory of 2D systems, being its electronic states confined in one atomic-layer thickness. For this reason, it has been recently indicated as a promising material also for nanoplasmonics, an emerging field that deals with the employment of collective excitations for developing new devices. Plasmonic components can be used to improve the resolution of microscopes, the sensitivity of chemical detectors, the efficiency of Light-Emitting Diodes (LEDs).

One of the outstanding features of a 2D free electron gas is the square-root dependence of plasmon energy on the parallel wave vector, in contrast with the parabolic dispersion law typical of 3D systems. The 2D collective electron excitation modes, determined by charge fluctuations strongly localized at a monolayer, have been discussed theoretically for a long time. However, few experimental data have been reported and no clear experimental evidence of the anomalous dispersion was found, likely because of the weak localization of electronic states of the atomic overlayers under study. The electronic states of MG/metal systems are instead characterized by a very strong localization at the overlayer plane, due to the large anisotropic chemical C-C bond of graphite, thus leading to 2D electronic states confined in one atomic-layer thickness.

We found that the influence of the substrate induces a change in the charge distribution, and consequently in the collective electronic excitations properties of the overlayer in comparison to a free standing graphene sheet or to a 3D graphite stack.

The occurrence of new electronic states, distinct both from the graphite and the substrate band structure, have been clearly detected. We measured an intraband 2D plasmon in the (0-3) eV energy region, with square root energy dispersion on the parallel wave vector, and assigned another branch at energies above 6.0 eV to the longitudinal 2D plasmon related to interband transitions. The hybridization of π orbital of MG with *d* bands of the substrate induces a partial population of conduction band states near the Fermi level, leading to the observed 2D plasmon at lower energy. Therefore, the strength of the interaction between MG and the underling substrate can be determined by monitoring the Fermi surface in the graphene overlayers.
We expect, in fact, that the intensity of this intraband electronic excitation and the value of its energy strongly depends on the number of charge carriers occupying hybrid electronic states. On the other hand, the localization of these states in one atomic layer give a 2D character to the plasmon, allowing us to add more experimental evidence for the dispersion relations. It is worth noting that this collective excitation cannot occur in the zero-gap free-standing graphene, unless either temperature is non-zero or graphene is driven away from the charge neutrality point by doping or gating. The MG-substrate coupling is responsible of the onset of this collective excitation; nevertheless, the presence of the substrate does not alter the plasmon 2D nature, and tunable hybridization between electronic states of graphene and the metal surface can be exploited to modify the plasmon behaviour, as it depends on the charge carriers distribution.

5.2 SECONDARY ELECTRON EMISSION IN THE INTERACTION OF SLOW IONS AND ELECTRONS WITH SOLIDS

The research activity focused on many body excitation induced by slow ions and electrons interacting with metal surfaces and nano-structured materials. The main lines of research and the obtained results can be summarized as follows:

5.2.1 Charge transfer processes

Resonant neutralization of hyperthermal alkali metal ions impinging on clean metal surfaces was studied, focussing on the correlations between the final charge fraction of scattered atoms and the type of collision. A wave-packet propagation algorithm was developed to calculate the neutralization probability of the outgoing atoms. Excellent agreement was found with measurements of 10-50 eV Na^+ ions incident on Cu(100) surfaces. The next step was trying to determine how low energy ion scattering off metal nanoclusters may reveal unique information about the electronic structure of the target materials. Indeed, The neutral fraction of 1 keV Na^+ scattered from nanosize Au islands deposited on TiO_2 was found to significantly increase with decreasing the cluster size, reaching values as high as 50% in contrast with the low value 3% observed for metallic Au. Based on time-dependent Hartee-Fock simulations, we considered a semi-empirical potential for the valence Na-electron and applied the wave-packet method to obtain the neutralization probability of the scattered atomic level. Preliminary calculations are consistent with available measurements. We began to study and characterize nanostructured targets grown on inert substrates. In particular, we investigated the electronic properties of graphene adsorbed on a Ni(111) surface via secondary electron emission spectroscopy. Auger core-valence-valence transitions from single wall Carbon nanotubes were studied focussing on the high kinetic energy region of the spectra, where we have tried to characterize the many body shake-up of pi electrons. The calculations were found in good agreement with available experiments.

5.2.2 Electron Emission Spectra from Clean and Cesiated Al Surfaces

We investigated the role of plasmon decay in secondary electron emission through measurements of energy spectra of electrons emitted by 130 eV and 2 keV electron impact on clean and cesiated Al surfaces. Electron emission from the clean metal surface appears to be dominated by plasmon decay features. The electron collision cascade excited by plasmon decay appears not to be as important as considered in theoretical calculations. Modification of the surface by adsorption of Cs shows that the main channel for plasmon excitation is indirect, by fast secondary electrons travelling inside the solid.
The data allow also to discuss an issue that is important in many phenomena and applications, where electron emission is a relevant process. The analysis of electron energy distributions measured as a function of surface modification allowed us to separate the spectrum of rediffused electrons from the continuum background of

cascade electrons. The results show that values of yields of rediffused electrons currently used in several applications may be significantly overestimated. More generally, our work shows that the interplay between different emission mechanisms in many cases cannot be neglected, as electrons of different origin can have the same characteristic energy. This implies that application of data analysis techniques to experimental spectra is required whenever there is the need to disentangle different contribution to the electron emission yield.

5.2.3 Molecular dynamics study of kinetic electron emission induced by slow sodium ions incident on gold surfaces

Electron excitation and emission phenomena, due to Na+ ion impact on Au (1 0 0) surfaces, are studied at incident projectile energies below the threshold for kinetic electron emission (0.1÷2.0 keV). The trajectories and velocities of the projectile and the target atoms are simulated with molecular dynamics. This information are used to calculate the energy loss by electronic stopping as a series of discrete events, localized in space and time, that are treated as sources of excitation energy. We observed that the energy lost by the moving atoms decreases exponentially with increasing the initial inverse velocity of the projectile. The same trend is followed by the experimental electron yield, although the two quantities seem to be non-linearly correlated. Nevertheless, the logarithmic slopes of the two curves are of the same order of magnitude.
We used the information on the trajectories and the velocities of the moving atoms to calculate the electron yield as function of the incident projectile energy, via a diffusion equation where each surface atom is treated as a source of excitation energy. The theoretical yield has the same trend as the measured yield, even though it depends critically on the choice of the energy diffusion coefficient, which is indeed the crucial parameter of the model.

5.2.4 Secondary Electron Emission from Graphene on Metal Surfaces

We use the spectroscopy of secondary electrons emitted in the interaction of slow singly charged helium ions and electrons with the sample surface as a probe for excited states of graphene on Ni(111). Spectra of electrons emitted under the impact of electrons and He^+ reveal structures that are consistent with excitation of valence electrons into high lying conduction band states, from which electrons are detected into vacuum. In the case of electron impact, excitation occurs by electron scattering processes during the collision cascade developed by primary electrons. The reported observations open the prospect for detailed band-structure measurements and calculations at much higher energy than those covered by existing literature. The sensitivity of the fine structure to disorder or radiation damage implies that secondary electron spectroscopy is a suitable technique for the *simultaneous* characterization *in situ* of both the electronic properties and the crystalline quality of the graphene sample. In the case of slow singly charged Helium ions, valence electron excitations into conduction states is produced by electron promotion, establishing slow ions as an efficient probe for electronic properties of the graphene overlayer.

5.3 PHOTON-MATTER INTERACTION: ELECTRONIC PROPERTIES OF GRAPHENE AND RELATED MATERIALS

This research line concerns with the study of the electronic properties of graphene (G) and related materials by means of synchrotron radiation. Specifically, graphene sheets prepared by the exfoliation method and epitaxially grown on transition metals have been studied through the photoemission and photoabsorption process induced by a synchrotron light source.

In collaboration with the *Istituto di Struttura della Materia*-CNR of Trieste, we have investigated the electronic structure of G epitaxially grown on selected transition metals at the beam line *VUV Photoemission* of the Synchrotron *Elettra*, by means of Angle-Resolved Photoemission Spectroscopy (ARPES). This technique has probably contributed more than any other experimental tool to verify the notion of the electronic bands and of some other fundamental concepts, like crystal momentum, Umklapp processes or the Brillouin zone. Thanks to the development of experimental equipments, nowadays ARPES can explore subtle many-body effects, which challenge our understanding of band theory. A photoemission spectrum is in fact directly related to the one particle spectral function $A(k, \omega)$, a fundamental theoretical quantity which contains exhaustive information on the excitation spectrum of a many body system, and therefore of the nature and strength of the interactions. In particular, if the experimental energy and momentum resolution are sufficiently high, ARPES can probe the fundamental quasiparticle states (or signal their absence), which determine the thermodynamic properties of a material. This method is ideal to investigate the conical dispersion of the π band of graphene at the K point of the

Brillouin zone. The properties of the quasiparticles may be altered through periodic potentials or destroyed by interaction with the substrate. In order to investigate the intriguing effect of a modulated potential on the electronic structure of graphene, we have performed ARPES investigations of graphene epitaxially grown on Ir(111) (S. Rusponi *et al.,* Phys. Rev. Lett. 105, 246803 (2010)). We have successfully perturbed the G/Ir(111) system by self-assembled Ir cluster superlattices. We showed that the cluster superpotential induces highly-anisostropic Dirac cones and affects the electronic band dispersions and the bandgaps of graphene. Further, we have recently investigated the effects of Na doping on G/Ir(111) and the same system precoated with metal clusters. Our results show that Na ad-atoms quench the graphene moiré and Ir superlattice potentials, suppress replica bands along with the minigaps, and restore the trigonal warping of the bands. Moreover, we gave evidence of a large gap (740 meV) between graphene states when Na and Ir are co-adsorbed on graphene, due to a strong inequivalence between C atoms.

We are also interested in studying magnetic effects on G and carbon-based materials. New carbon-based materials would greatly extend the limits of technologies relying on magnetism. Even more promising is the applications of such materials in the design of nanoscale magnetic and spin electronics devices. Electrical spin injection in normal metals is routinely achieved by contacting ferromagnets like Fe, Ni, and Co with metals, and driving a current through the system. Interestingly, one of the potential application of graphene is use of it as junction layer in spin-filtering devices. We have recently studied the effect of magnetic thin films of Ni and Co put in chemical contact to Ir(111) and the G layer by intercalation. Our results show how the linear dispersion of the π band of G/Ir(111) is perturbed by the interaction with thin magnetic films. We were able to tune the electronic behavior of π electrons from the free-standing like character of G/Ir(111) to the hybridized one of G/Ni(111), through an intermediate step where magnetic films only 1ML thick are bound to the G layer.

Concerning graphene flakes prepared by the exfoliation method (thus free-standing) we have many projects in course on the characterization of the electronic properties by means of spatially resolved electron spectroscopies. Recently, we have performed a near-edge X-ray absorption fine-structure (NEXAFS) and transmission electron microscopy (TEM) investigation of freely suspended graphene flakes and graphene oxide (GO) sheets (D. Pacilé *et al.,* Carbon 49, 966 (2011)). Our investigation provided the structure and chemical composition of GO, showing as well a new and efficient route to study the electronic structure of suspended membranes. Of more recent interest is the electronic behaviour of twisted double-layer graphene flakes. It is well known that changing the rotational angle between adjacent graphene planes has a drastic effect on the low-energy electronic properties of multilayer graphene. Rotational stacking faults of an arbitrary angle induce a momentum mismatch between Dirac cones of adjacent layers, suppressing coherent interlayer motion at low energy. In this description multilayer graphene behaves in an approximate manner like decoupled single layers, thus accessing two-dimensional physics in a family of three-dimensional materials. We are planning spatially resolved photoemission experiments of twisted double-layer graphene flakes, in order to investigate the correlation between definite twist angles and corresponding low-energy quasiparticle spectral function.

5.4 QUANTUM COHERENCE AND CORRELATIONS IN CONDENSED MATTER SYSTEMS

In this research line, we theoretically investigate the role of quantum coherence and correlations (entanglement and discord) in the wuantum optical and condensed matter physics of mesoscopic systems, on the two cases of few- and many-bodies. The two main themes of the research performed in 2010 have been: (1) Quantum correlations in spin systems; (2) Decoherence and Entanglement in spin-boson systems.

5.4.1 Quantum correlations in spin systems

We have studied the properties of various spin systems. In particular, the entanglement properties of the ground state of a spin-1/2 chain with 1/r^2-interaction (Haldane-Shastry model) have been investigated, in the presence of an applied magnetic field. Having explicitly constructed the ground state for the chain with a finite number of sites N, various estimators of the entanglement have been computed at zero temperature. The results about the behavior of the quantum correlations in the system have been related with the condensation of spin-1/2 "fractionalized" excitations (spinons), occurring when the applied field reaches its saturation value.
Furthermore, we investigated the behavior of both one- and two-qubit systems coupled to an interacting spin chain environment, by focusing, in particular, on the role of the quantum phase transition in the environment and on the control achieved by modifying the external magnetic field, either witnessed by the decohering qubit or by

the dynamically disentangling pair.

5.4.2 Decoherence and Entanglement in spin-boson systems

We have studied the behavior of quantum coherence and entanglement for qubits coupled to non-markovian environments and discussed ways to avoid the decoherence. Specifically, we studied the dynamics of two atoms (a qubit pair) spontaneously emitting into a lossy cavity, and showed that the entanglement decay can be controlled by detuning the atoms from the cavity field. We also studied the possibility of modifying the dynamics of both classical and generic quantum correlations, as measured by the discord, by means of the quantum Zeno effect.
We have found, in particular, that some frequency region exists for which the anti-Zeno effect is obtained, and even that oscillations between the Zeno and anti-Zeno regimes may occur.
We have then focused on the cooperative behavior of a large number of qubit coupled to a boson mode (Dicke model) and established a formal connection with a class of collective spin models (uniaxial models) that enabled us to obtain analytic expressions for various measures of quantum correlations.

5.5 ION-MATTER INTERACTION

5.5.1 Ion interaction with nanostructures

We studied electron spectroscopy study on Na+ ion implantation and Na atom deposition on carbon structures. Our results show that, for implanted Na at the same ion dose, the Na surface concentration decreases with the structure order, while deposited Na particles readily diffuse in the bulk. Interaction of alkali metal atoms with carbon structures actually holds an important role in scientific research because of its implications in advanced technological applications. Graphite is a highly anisotropic material in terms of its structural and electronic properties, due to the relatively strong in-plane forces between carbon atoms, and to the weak interplanar forces between adjacent graphene layers. Atoms of various chemical species, intercalated or implanted within graphite layers, form atomic or molecular bonds. The interest in these intercalated compounds is due to changes in electronic and mechanical properties induced by the intercalates, which can lead to technological applications of the new materials. Further, the resistivity of carbon nanotubes decreases upon exposure to alkali metals denoting a progressive sample metallization; the most significant change in resistivity occurring for sodium exposure. Low energy Na^+ ion implantation and Na atom intercalation exhibit a quite different dopant spatial distribution, as implanted alkali atoms remain on the surface while intercalated alkali particles readily diffuse into the bulk. These results suggested to us to study the changes in carbon structure properties after sodium exposure and implantation at room temperature. As for carbon nanotubes, we employ the CEAES technique (Collisionally Excited Autoionization Electron Spectroscopy. This electron spectroscopy induced by atomic collisional processes, allows us to monitor the amount of implanted ions by observing the change in intensity of such atomic features as a function of the dose of sodium projectile ions. Through this spectroscopy we are able to study changes of the sample local electrostatic potential (work function) by observing the spectral lines shift under Na irradiation, since the kinetic energy of electrons emitted by atomic particles near the surface, is strictly related to the electrostatic potential difference between the sample and the analyser. The full width at half maximum (FWHM) of observed lines can provide information about the homogeneity of the sample region beneath the decaying atoms. In fact the de-excitation should take place at a distance of $\sim$10 Å from the surface. The electrostatic potential seen by the emitted electron is thus an average over the (macroscopically very limited) underlying sample region, and the presence of impurities (for example, Na implanted atom) on the surface should inevitably cause a broadening of the spectral lines. From the intensity of the electron peaks it is found that implantation is more effective on disordered carbon structure (amorphous graphite) rather than on ordered carbon features (HOPG or SWNT). The effectiveness refers to the alkali concentration on the surface. On the other hand, if we compare to the techniques used, we observe a difference between implantation and evaporation. Independent of the carbon structure used (ordered or disordered) our results show again that the implantation technique leads to a higher surface concentration of alkali atoms, or, in the case of evaporation, the alkali diffusion into the bulk is more probable.

5.5.2 Radiation interaction with solids

Electrochromism is the property for which the color of a material changes reversibly in response to an

externally applied potential. In the last years many efforts have been concentrated in developing electrochromic [EC] devices as EC windows, car mirrors, and display panels. In our work on radiation absorbance from EC devices, we have studied the visible range spectral features of viologen inserted into a polymer plasticized matrix of electrochromic films illustrated in previous works. We used ethyl viologen instead of other viologens, having longer chemical groups linked to nitrogen, because of its greater solubility into the plastic matrix. On the other hand, the methyl viologen has been excluded due to its well-known high toxicity. A suitable polymer matrix is the polyvinyl formale (PVF) plasticized with propylene carbonate (PC), a solvent with high dielectric constant and high boiling temperature. Useful film formulations fall in 30−40% PVF, 55−65% PC composition ranges. Taking into consideration the dielectric constant of PC, ranging from about 65 at room temperature, and that of the PVF, which is around 3, the average dielectric constant of the host matrix for viologen salts falls in the range 39−42, which is almost half of the water dielectric constant. So in this case, following the conclusions of Monk, no dimer formation of the monocation species, originated by the dication reduction, should occur. This idea is strongly supported by the fact that the blue color, observed in the operations of the electrochromic devices based on the previously discussed electrochromic film, never turns into violet. Another factor that should prevent dimer formation in our system is the reduced molecular diffusion, a very viscous plastic environment, should make very improbable the contact between different monomer monocations, at least during short operation times. Despite this simplification, the spectra of the reduced species may remain quite complex due to the presence of other mechanisms. First of all the formation of the neutral species V^0 must be taken into account. Then the possibility of complex formation between viologen species and oxygen, always endemically dissolved into the solvent, must also be considered. Concerning the second point, enough literature data support the importance of this mechanism: particularly relevant are the studies carried out by Ogawa et al. and Milosavljevic.

5.6 MULTIMEDIAL EDUCATION

The use of toys in physics teaching is a common practice (Güémenez et al. 2009, Aref et al. 2007, Featonby 2005), since a lot of physics may come out of them if properly employed. In particular, there is a well known toy suitable to get many insights on magnetic field properties: the GEOMAG™ magnetic building kit. Such a kit consists of a number of strong cylindrical bar magnets (6 mm diameter and length 25 mm, completely covered in hard plastic except at their two ends) and of a number of ferromagnetic steel balls (diameter 12.7 mm). Geomags have been used in the past for educational purposes either to qualitatively elucidate some issues about magnetic force/torque (Allasia et al. 2006) and field (Defrancesco et al. 2007), or as a tool to practically illustrate the well known “method of images” in electrostatic by establishing analogies between electric and magnetic phenomena (Poon 2003). In a recent paper (Defrancesco et al. 2007) an apparent paradox involving Geomags interactions has been proposed: two like-poles may attract if properly faced through a ferromagnetic sphere. This phenomenon has been quantitatively investigated in a more recent paper (Bonanno et al. 2009a). In our work we propose a multimedia tool allowing to interactively visualize the behavior of the surface magnetization of a ferromagnetic sphere in presence of one or more little magnets, and the interaction force among them. The computational part of the simulation is based on a magnetostatics transposition of the electrostatic’s method of images, following previous literature results (Lindell 1993, Poon 2003, Redžić 2006).

A. PUBLICATIONS ON SCIENTIFIC JOURNALS

A.1 Publications on international journals

A.1.1 Publications on international journals printed in 2010

1. G. Liberti, F. Piperno, F. Plastina,
   Finite-size behavior of quantum collective spin systems
   Phys. Rev. A **81**, 013818 (2010)
   Also selected by Virtual Journal of Nanoscale Science and Technology, Vol. 21, Issue 6, 2010
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2. D. Giuliano, A. Sindona, G. Falcone, F. Plastina and L. Amico,
   Entanglement in a spin system with inverse square statistical interaction
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3. T. J. G. Apollaro, A. Cuccoli, C. Di Franco, M. Paternostro, F. Plastina and P. Verrucchi,
   Manipulating and protecting entanglement by means of spin environments
   New J. Phys. **12**, 083046 (2010).
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4. F. Francica, S. Maniscalco, F. Plastina
   Off-resonant quantum Zeno and anti-Zeno effects on the entanglement
   Physica Scripta **T140**, 014044 (2010).

5. F. Plastina, G. Falcone, F. Francica, G. Liberti, F. Piperno, and S. Maniscalco
   Cavity induced quantum cooperative phenomena
   Physica Scripta **T140**, 014008 (2010).

6. F. Francica, F. Plastina, S. Maniscalco
   Quantum Zeno and anti-Zeno effects on quantum and classical correlations
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7. A.Bonanno, M. Barberio, P. Barone, M. Camarca, D.R. Grosso, R. Vasta, F. Xu, A. Oliva,
   Changes in electronic properties of carbon structures by evaporation and implantation of alkali metals
   Vacuum **84** (2010) 1025–1028.

8. G. Chidichimo, D. Imbardelli, B.C. De Simone, P. Barone, M. Barberio, A. Bonanno, M. Camarca, A. Oliva,
   Spectroscopy and kinetic investigation of ethil viologen reduction in novel electrochromic plastic films
   J. Phys. Chem. C 2010, **114 (39)** , pp 16700–16705.

9. A.Bonanno, G. Bozzo, M. Camarca and P. Sapia
   Magnetic interactions: A multimedia interactive tutorial
   Il Nuovo Cimento C **33 (3)**, 131-136 (2010).

10. S. Rusponi, M. Papagno, P. Moras, S. Vlaic, M. Etzkorn, P. M. Sheverdyaeva, D. Pacilé, H. Brune, and C. Carbone
    Highly anisotropic Dirac cones in epitaxial graphene modulated by an island superlattice
    Phys. Rev. Lett. **105**, 246803 (2010).

11. D. Pacilé, M. Papagno, T. Skala, V. Matolìn, T. Sainsbury, T. Ikuno, D. Okawa, A. Zettl, and K. C. Prince
    Excitons at the B K edge of boron nitride nanotubes probed by X-ray absorption spectroscopy
    J. Phys.: Condensed Matter **22**, 295301 (2010).

12. M. Castriota, E. Cazzanelli, D. Pacilé, L. Papagno, C.O. Girit, J. C. Meyer, A. Zettl , M. Giarola and G. Mariotto, "Spatial dependence of observed Raman frequencies and disorder in graphene monolayers" Diam. and Relat. Mat. **19**, 608 (2010).

13. P. Riccardi, M. Pisarra, A. Cupolillo, M. Commisso, A. Sindona, R. Baragiola, C. A. Dukes, "Secondary electron emission spectra from clean and cesiated Al surfaces: the role of plasmon decay and data analysis for applications" J. Physics: Condensed matter **22**, 305004 (2010).

14. A. Cupolillo, M. Pisarra, A. Sindona, M. Commisso, P. Riccardi, "Electron excitation in the interaction of slow ions and electrons with metals and monolayer graphite on Ni(111) surfaces" Vacuum **84 (8)** , 1029-1032 (2010).

15. A. Sindona, P. Riccardi, S. Maletta, M. Pisarra, A. Cupolillo, "Wave-packet study of hyperthermal alkali ion neutralization at metal surfaces" Vacuum **84 (8)**, 1038-1042 (2010).

16. A Sindona , M Pisarra , S Maletta , P Riccardi and G Falcone, "Charge transfer in single and multiple scattering events at metal surfaces: a wavepacket study of the Na + /Cu(100) system" J. Physics: Condensed Matter **22**, 475004 (2010).

17. P. Riccardi, A. Cupolillo, M. Pisarra, A. Sindona, and L. S. Caputi "Observation of excited states of Graphene on Ni(111) by secondary electron spectroscopy", Applied Physics Letters **97**, 221909 (2010) Also Selected for the Virtual Journal of Nanoscale Science & Technology Vol.22, issue 24, 2010

A.1.2 Publications on international journals accepted in 2010

1. T.J.G. Apollaro, C. Di Franco, F. Plastina, M. Paternostro "Memory-keeping effects and forgetfulness in the dynamics of a qubit coupled to a spin chain" Accepted by Phys. Rev. A

2. M. Barberio, D. Barca, P. Barone, V. Pingitore, A. Bonanno "Cathodo-luminescence from extrinsic impurities in bundles of carbon nanotubes: a possible role" Accepted by Journal of Nanoscience and Nanotechnology

3. D. Pacilé, J. C. Meyer, A. Fraile Rodriguez, M. Papagno, C. Gomez-Navarro, R. S. Sundaram, M. Burghard, K. Kern, C.Carbone, and U. Kaiser "Electronic properties and atomic structure of graphene oxide membranes" Accepted by Carbon

4. M. Pisarra, A. Sindona, P. Riccardi, "Molecular dynamics study of kinetic electron emission induced by slow sodium ions incident on gold surfaces" Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, In Press, Corrected Proof, Available online 17 December 2010 Doi:10.1016/j.nimb.2010.12.046

5. A. Sindona, M. Pisarra, S. Maletta, P. Riccardi, A. Cupolillo, G. Falcone, "Wave packet evolution of the valence state of a hyperthermal sodium ion impinging on a copper surface", Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms, In Press, Corrected Proof, Available online 30 November 2010, Doi:10.1016/j.nimb.2010.11.068

6. M. Pisarra, A. Cupolillo, L.S. Caputi, A. Sindona, P. Riccardi,
"Secondary Electron Spectra of Graphene on Ni(111) Surface"
to appear in Journal of Nanoscience and Nanotechnology, 2011

7. A. Sindona, S. Maletta, M. Commisso, M. Pisarra, P. Riccardi, A. Bonanno, P. Barone, G. Falcone,
"Role of Many Body Shake-up in Core-Valence-Valence Electron Emission from Single Wall Carbon Nanotubes"
to appear in Journal of Nanoscience and Nanotechnology.

A.1.3 Papers submitted for publication in 2010

1. A. Sindona, M. Pisarra, P. Riccardi, G. Falcone
"Many-body effects in Auger electron emission from short-length Carbon nanotubes"
submitted to Journal of Nanoscience and Nanotechnology Letters

B PUBLICATIONS ON CONFERENCE PROCEEDINGS

B.1Publications on international conference proceedings in 2010

1. A.Bonanno, M. Camarca, P. Sapia, A. Serpe,
"Archimedes and Caustics: A twofold multimedia and experimental approach".
Proceedings of the International Conference THE GENIUS OF ARCHIMEDES – 23 CENTURIES OF INFLUENCE ON MATHEMATICS, SCIENCE AND ENGINEERING, History of Mechanics and Machine Science - volume 11. Paipetis S.A., Ceccarelli M. (eds). Springer, London (2010).

2. A.Bonanno , P. Sapia, Y.L.T. Ting
"Multimedia [science+foreign language] transfer: a tool for innovative 21st Century learning".
Proceedings of "ICERI 2010. International Conference of Education, Research and Innovation", Madrid, Spain, 15-17/11/2010. ISBN: 978-84-614-2439-9.

3. A.Bonanno, M. Camarca, P. Sapia,
"Music's Mathematical groups: A multimedia tutorial on the circle of fifths and other musical symmetries".
Proceedings of "EDULEARN 10. International Conference on Education and New Learning Technologies", Barcelona, Spain, 5th-7th July, 2010. ISBN: 978-84-613-9386-2.

4. A.Bonanno, G. Bozzo, M. Camarca, P. Sapia
"Playing with clean energies: A multimedia guide"
Proceedings of "INTED 2010. International Technology,Education and Development Conference", Valencia, Spain, 8-10/03/2010. ISBN: 978-84-613-5538-9.

5. A.Bonanno, M. Camarca, P. Sapia
"A Java tutorial on the electrostatic method of images"
Proceedings of "INTED 2010. International Technology,Education and Development Conference", Valencia, Spain, 8-10/03/2010. ISBN: 978-84-613-5538-9.

6. V.Pingitore, M. Barberio, P. Barone, A. Bonanno
"The role of intrinsic and extrinsic impurities on cathodoluminescence from carbon nanotubes"
NanoSEA 2010 28 Giugno - 2 Luglio 2010 Cassis (Francia).

7. E. Cazzanelli, M. Castriota, D. Pacilé, L. Papagno, C.O. Girit, J. C. Meyer, A. Zettl , M. Giarola and G. Mariotto,
"Raman spectral effects of edge disorder and strain distribution in monolayer graphene "
CARBOMAT 2010, Catania 6-8 Ottobre, 2010

C INVITED PRESENTATIONS

C.1 Invited presentations at international conferences in 2010

1. F. Plastina,
   "Memory-keeping effects and forgetfulness in the dynamics of a qubit coupled to a spin chain"
   Quantum Mechanics: Foundations and Open Systems II, Turku (Finland) 27-10-2010.

2. A. Sindona, "Many Body Shake-up in Core-Valence-Valence Electron Emission from Single Wall Carbon Nanotubes"
   Workshop Nanoscience and Nanotechnology 2010, Laboratori Nazionali di Frascati, September 20 – 23, 2010 .

D PRESENTATIONS AT CONFERENCES

D.1 Oral Presentations at international conferences in 2010

1. A. Sindona,
   "Many Body Shake-up in Core-Valence-Valence Electron Emission from Single Wall Carbon Nanotubes",
   3rd International Conference on Nanostructures SElf-Assembly NanoSEA 2010 Congress Center, Cassis, French Riviera, 28 June - 2 July 2010

2. P. Riccardi,
   "Electron emission in the interaction of slow ions and electrons with nanostructured surfaces",
   24th International Conference on Atomic Collisions in Solids, ICACS 2010, Kracow, Polland, july 18-23 2010.

3. M. Pisarra,
   "Wave-packet study of hyperthermal alkali ion neutralization at metal surfaces",
   24th International Conference on Atomic Collisions in Solids, ICACS 2010, Kracow, Polland, july 18-23 2010.

D.2 Poster Presentations at international conferences in 2010

1. F. Plastina
   "Perfect and efficient information transfer via quantum tunneling in a spin chain"
   Quantum Engineering of States and Devices: Theory and Experiments, Obergurgl (Austria), 7-6-2010

2. S. Lorenzo
   "Information trasmission via local modulation in spin chain"
   DPG-School and Workshop, Nanophotonics meets Quantum Optics, Bad Honnef (Germany), 21-9-2010

3. F. Francica,
   "Entanglement dynamics of two qubits near the edge of a photonic band gap"
   CEWQO 2010, St. Andrews (Scotland), June 9, 2010.

4. A. Bonanno, M. Barberio, P. Barone, M. Camarca, D. R.Grosso, R. Vasta, F. Xu, and A. Oliva
   "Transport Properties of alkali-doped carbon nanotube mats".
   5th International Conference on Surfaces, Coatings and Nano-Structured Materials (Nanosmat-5), 19-21 Ottobre 2010 Reims - Francia

5. M. Pisarra,
   "Secondary Electron Spectra of Graphene on Ni(111) Surface",
   3rd International Conference on Nanostructures SElf-Assembly NanoSEA 2010 Congress Center, Cassis, French Riviera, 28 June - 2 July 2010

6. M.Pisarra,
   "Molecular Dynamics study of electron emission induced by slow ions at metal surfaces",
   24th International Conference on Atomic Collisions in Solids, ICACS 2010, Kracow, Polland, july 18-23 2010.

7. M. Pisarra,
   "Secondary Electron Spectra of Graphene on Ni(111) Surface"
   Workshop Nanoscience and Nanotechnology 2010, Laboratori Nazionali di Frascati, September 20 – 23, 2010

D.2 Presentations at national conferences in 2010

1. V. Pingitore M. Barberio, P. Barone, A. Bonanno, A. Oliva
   "Transport properties of alkali -doped single –wall carbon nanotubes mats"
   Nanoscience & Nanotechnology 20 – 23 Settembre 2010 *INFN - Laboratori Nazionali di Frascati*

6. MOLECULAR BIOPHYSICS

Professors and Researchers: Luigi Sportelli
Rosa Bartucci
Rita Guzzi
Bruno Rizzuti *(Lab. Licryl, CNR-INFM, Cosenza)*

Graduate Student: Stefania Evoli

Technical staff: Massimo Sposato

Collaborators: D. Marsh (*MPI for Biophysical Chemistry, Goettingen, Germany*)
M. Esmann (*Aarhus University, Dept. of Biochemistry, Denmark)*
M.P. De Santo, *(Lab. Licryl, CNR-INFM, Cosenza)*
B. Zappone *(Lab. Licryl, CNR-INFM, Cosenza)*
F. Scarpelli (*at Lab. of Molecular Biophysics from Dept. of Physics, Leiden, Nederland)*
M. Pantusa, A. Stirpe (*Post-Doc)*
G. Sindona (*Dept. of Chemistry*, *University of Calabria)*
A. Russo (*Dept. of Chemistry*, *University of Calabria)*
E. Perri (*C.R.A. Centro di Ricerca per l'Olivicoltura e l'Industria Olearia, Rende*)

Introduction

In the year 2010 the research activity of the Molecular Biophysics Group has essentially been focused on the study of the molecular properties of biosystems. In particular, the following two research lines have been of interest of the group:

a) Structure and dynamics of proteins at cryogenic temperatures
b) Aggregation and molecular dynamic simulation of proteins

In the first research line, by using different EPR methods (conventional and pulsed FT-EPR spectroscopy), the librational dynamics and the structural heterogeneity of spin-labelled proteins at cryogenic temperatures (77 – 250 K) have been studied.
In the second one, the kinetics of absorption of fatty acids by human serum albumin has been investigated by molecular dynamics simulation. Finally, the investigation of the aggregation of β-lactoglobulin on solid surfaces (silicon and mica) has been carried out by using SEM and AFM techniques.

In the following, the main research results obtained during the investigation are briefly presented in the form of abstracts.

6.1. STRUCTURE AND DYNAMICS OF PROTEINS AT CRYOGENIC TEMPERATURES

6.1.1 Heterogeneity of protein substates visualised by spin-label EPR

The energy landscape of proteins is characterised by a hierarchy of substates, which give rise to conformational heterogeneity at low temperatures. In multiply spin-labelled membranous Na,K-ATPase, this heterogeneous population of conformations is manifest by strong inhomogeneous broadening of the EPR lineshapes and non-exponential spin-echo decays, which undergo a transition to homogenous broadening and exponential relaxation at higher temperatures. Here we apply these EPR methods to small water-soluble proteins, i.e., β-lactoglobulin, human serum albumin and hemoglobin for which the existence of conformational substates is well established. Both □-helical and □-sheet aqueous proteins that are spin-labelled on a single cysteine residue display spin-echo decays with a single phase-memory time T_{2M} and conventional EPR lineshapes with predominantly Lorentzian broadening, over a broad range of temperatures from 77 K to ca. 250 K or higher. Above ca. 200 K, the residual Gaussian broadening is reduced almost to zero. In contrast, both the proteins and the spin label alone when in a glycerol-water mixture below the glass transition, display heterogeneity in spin-echo phase memory time and a

stronger Gaussian broadening of the conventional lineshapes, similar to multiply spin-labelled membranous Na,K-ATPase below 200 K. Above 200 K (or the glass transition temperature), a single phase memory time and predominantly Lorentzian broadening are found in both spin-label systems. The results are discussed in terms of the ability of single spin-label sites to detect conformational heterogeneity and the desirability of exploring multiple sites for proteins with the size and complexity of the Na,K-ATPase.

6.1.2. Solvent effect on librational dynamics of spin-labelled hemoglobin by ED- and CW-EPR

Two-pulse, echo detected electron paramagnetic resonance (ED-EPR) spectra and continuous wave EPR (CW-EPR) spectra were used to investigate the solvent effect on the librational motion of human hemoglobin spin-labelled on cysteine β93 with the nitroxide derivative of maleimide, 6-MSL. Protein samples fully hydrated in phosphate buffer solution (PBS), in a 60 % v/v glycerol/water mixture and in the lyophilized form were measured at cryogenic temperature in the frozen state. The protein librational motion was characterized by the amplitude-correlation time product, $<\alpha^2>\tau_c$, deduced from the ED-EPR spectra. The librational amplitude, $<\alpha^2>$, was determined independently from the motionally averaged hyperfine splitting in the CW-EPR spectra, and the librational correlation time, τc, was derived from the combination of the pulsed and conventional EPR data.
Rapid librational motion of small amplitude is detected in all samples. In each case, the librational dynamics is restricted up to 180 K and, beyond this, it increases steeply for the hydrated protein in PBS and in the presence of glycerol. In contrast, in the dehydrated protein the librational dynamics is hindered and less dependent on temperature up to ~ 240 K. In all samples, $<\alpha^2>$ deviates from small values only for T > 200 K, where a rapid increase of $<\alpha^2>$ is evident for the hydrated samples, whereas a limited temperature variation is shown in the lyophilized samples. The librational correlation time is in the subnanosecond regime and weakly dependent on temperature. The results evidence that solvent favours protein dynamics.

6.2 AGGREGATION AND MOLECULAR DYNAMIC SIMULATION OF PROTEINS

6.2.1 Dynamics and kinetics of the anchoring of fatty acid molecules in the highest-affinity binding site of human serum albumin

Human serum albumin binds and transports long-chain fatty acids in the blood through three high-affinity and four low-affinity binding sites. The dynamics and kinetics of absorption of different fatty acid molecules has been investigated by using the Molecular Dynamics (MD) simulation technique. The key role of the two protein residues Tyr401 and Lys525 has been elucidated. In particular, Lys525 binds the charged head-group and the uncharged first portion of the lipid chain by means of both electrostatic interactions with its $-NH_3^+$ moiety and non-electrostatic interactions with the rest of its relatively long side-chain. The flexibility of Lys525, and in particular of the dihedral angle χ^3, contributes to explain differences observed in crystallography for human serum albumin complexed with different fatty acids. Results are also compared with data obtained on albumin with a number of other spectroscopic techniques, as well as with a few simulations performed on other lipid-binding proteins.

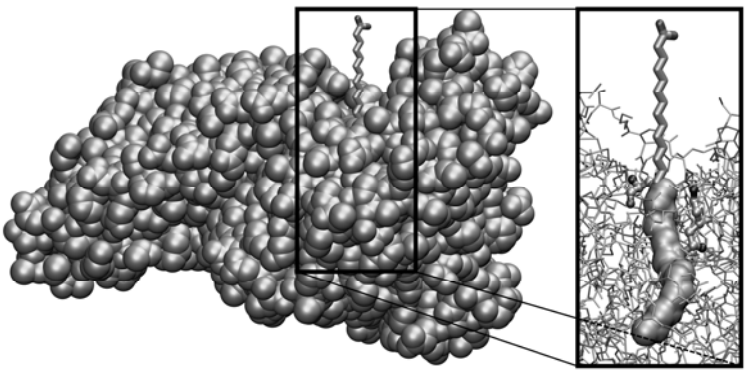

***Fig. 1**: Fatty acid molecule (licorice representation) in extended conformation, protruding from the highest-affinity binding site in human serum albumin (van der Waals representation). Inset: position of the lipid molecule with respect to the hydrophobic channel; the ligand protein residues Tyr401 and Lys525 are also shown (ball-and-stick representation) at left and right of the binding site, respectively.*

6.2.2 Aggregation and self-assembling of β-lactoglobulin on solid surfaces

Protein deposit left on silicon and mica substrates by dried droplets of aqueous solutions of bovine β-lactoglobulin has been studied under various conditions. Samples were prepared at different temperature, concentration, pH-values, and other experimental parameters. A variety of self-assembled structures were observed, such as homogeneous layers, hexagonal platelets, flower-shaped patterns, rods and fibrils. On one hand, this could be attributed to distinctive molecular features β-lactoglobulin, including its multimeric structure: aggregates may be derived by self-assembling of discotic building blocks of the protein produced by anisotropic interaction with the solid surface. On the other hand, some characteristics of the aggregation structures are in common with other proteins, such as amyloidogenic ones involved in neurodegenerative disorders, and are expected to shed light on general properties of aggregation of any polypeptide chain.

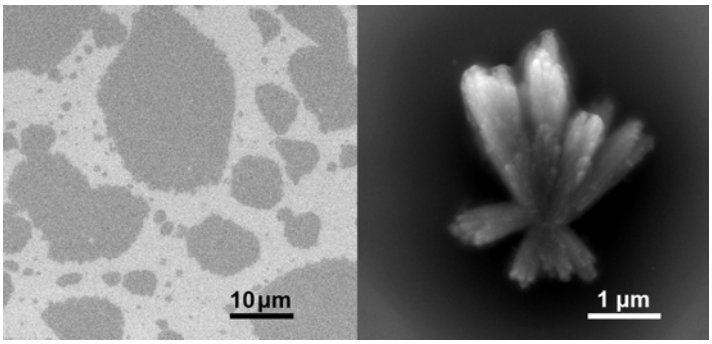

***Fig. 2**: β-lactoglobulin aggregates on silicon substrate. Homogeneous native protein layer at pH 5 (left) and multi-columnar rods formed by heat-denatured protein at pH 2 (right).*

A PUBLICATIONS ON SCIENTIFIC JOURNALS
A.1 Publications on international journals
A.1.1 Publications on international journals printed in 2010

1. B. Rizzuti, B. Zappone, M.P. De Santo, R. Guzzi
Native β-lactoglobulin self-assembles into a hexagonal columnar phase on a solid surface
Langmuir 26 1090-1095 (2010)

2. B. Rizzuti, M. Pantusa, R. Guzzi
The role of Lys525 on the head-group anchoring of fatty acids in the highest affinity binding site of human serum albumin
Spectroscopy 24, 159-163 (2010)

3. Pantusa M., Stirpe A., Sportelli L., Bartucci R.
Spontaneous transfer of stearic acids between human serum albumin and PEG:2000-grafted DPPC membranes
European Biophysical Journal 39, 921-927 (2010)

4. Russo A., Caputo S., Pantusa M., Perri E., Sindona G., Sportelli L.
Amino acids as modulators of lipoxygenase oxidation mechanism. The identification and structural characterization of spin adducts intermediates by electron spin resonance and tandem mass spectrometry
Food Chemistry 119, 533-538 (2010)

5. Pantusa M., Bartucci R.
Kinetics of stearic acid transfer between human serum albumin and sterically stabilized liposomes
European Biophysical Journal 39, 1351-1357 (2010)

A.1.2 Publications on international journals accepted in 2010

1. R. Guzzi, Babalavi, R. Bartucci, L. Sportelli, M. Esmann, D. Marsh
Spin-echo EPR of Na,K-ATPase unfolding by urea
Biochim. Biophys. Acta – Biomembranes

2. F. Scarpelli, R. Bartucci, L. Sportelli, R. Guzzi
Solvent effect on librational dynamics of spin-labelled haemoglobin by ED- and CW-EPR,
European Biophysical Journal

A.1.3 Publications on international journals submitted in 2010

1. B. Rizzuti, L. Sportelli, R. Bartucci, R. Guzzi
Kinetics of association of a single fatty acid molecule in human serum albumin.
submitted to Journal of Physical Chemistry Letters

2. A. Stirpe, M. Pantusa, B. Rizzuti, L. Sportelli, R. Bartucci. R. Guzzi
Early stage aggregation and fibrillation of human serum albumin in the presence of metal ions
submitted to International Journal of Biological Macromolecule

C INVITED PRESENTATIONS
C.1 Invited presentations at international conferences in 2010

1. B. Rizzuti, M. Pantusa, L. Sportelli, R. Guzzi, R. Bartucci
Molecular dynamics of human serum albumin complexed with fatty acids
PepCon 2010 – 3rd Protein and Peptide Conference "After a solution for the machines of life"
March 23, 2010 – Beijing (China)

D PRESENTATIONS AT CONFERENCES

D.1 Presentations at international conferences in 2010

1. B. Rizzuti, R. Bartucci, L. Sportelli, R. Guzzi
Molecular binding and recognition in human serum albumin
Meeting on: Folding and Recognition: Similarities and Differences, ISQBP 2010 – President's meeting of ISQBP (International Society of Quantum Biology and Chemistry)
June 14-16, 2010 – Cetraro (CS) (poster)

D.2 Presentations at national conferences in 2010

1. B. Rizzuti, M. Pantusa, L. Sportelli, R. Bartucci, R. Guzzi
Coordination and dynamics of fatty acids in the highest-affinity binding site of human serum albumin
SIBPA 2010 – 20th Italian conference of SIBPA (Società Italiana di Biofisica Pura e Applicata)
September 11, 2010 – Arcidosso (GR) (oral presentation)

2. F. Scarpelli, R. Bartucci, B. Rizzuti, L. Sportelli, R. Guzzi
Solvent effect on the librational motion of spin-labelled hemoglobin
SIBPA 2010 – 20th Italian conference of SIBPA (Società Italiana di Biofisica Pura e Applicata)
September 11-14, 2010 – Arcidosso (GR) (poster)

3. R. Guzzi, M. Pantusa, R. Bartucci, L. Sportelli, B. Rizzuti
Dynamical features of stearic acid binding in serum albumin
SIF 2010 – 96th National congress of SIF (Società Italiana di Fisica)
September 22, 2010 – Bologna (oral presentation)

7. PHYSICS AND APPLICATIONS OF THE SOFT MATTER

Professors and Researchers	Roberto Bartolino Riccardo C. Barberi Lev M. Blinov Enzo Cazzanelli Gabriella Cipparrone Maria Penelope De Santo Pasquale Pagliusi Nicola Scaramuzza Giuseppe Strangi Roberto Caputo Cesare Umeton Carlo Consolato Versace Antonio De Luca
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PhD students	Josue Raul Hernandez Lucia Marino
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Laboratory of Nanotechnology, UCLM *(Spain)*
Moscow State University *(Russia)*
Centre Paul Pascal - Bordeaux *(France)*
University of Colorado - Boulder *(USA)*
University of Tunis *(Tunisia)*
College de France - Paris *(France)*
University of Marseille *(France)*
University of Exeter *(UK)*
Chalmers University - Goteborg *(Sweden)*
University of Kent *(USA)*
Polytechnic of Madrid *(Spain)*
Polytechnic of Bucharest *(Romania)*
University of Gent *(Belgium)*
University of Ljublijana *(Slovenia)*
Russian Academy of Sciences *(Russia)*
University of Tblisi *(Georgia)*
Philips Research Center *(The Netherlands*)
Hewlett Packard Research Center *(UK)*
University of Nizhny - Novgorod *(Russia)*
University of California - Berkeley *(USA)*
University of Nebraska *(USA)*
University of Ohio *(USA)*
University of Mexico–UNAM *(MEX)*
European Synchrotron Radiation Facility *(France)*
Rutherford Appleton Laboratory *(UK)*
Stanford Synchrotron Radiation Laboratory *(USA)*

Introduction

The research activity of the group is going towards different fields of the soft matter using the huge experience obtained in a long standing previous activity, specifically in liquid crystals.
Generally speaking the scientific interests of the group can be resumed as in the following:

7.1 MATERIALS, IN CLOSE COLLABORATION WITH CHEMIST GROUPS, BOTH FROM UNIVERSITY OF CALABRIA AND FROM OUTSIDE: NEW LIQUID CRYSTALS, COLLOIDAL SYSTEMS, NANOPARTICLES AND LIQUID CRYSTALS, POLYMERS, PHOTOPOLYMERS, BLENDING OF LIQUID CRYSTALS AND POLYMERS….. CHARACTERISATION (DIELECTRIC, RAMAN, ELLIPSOMETRY, ELECTRON MICROSCOPY…)

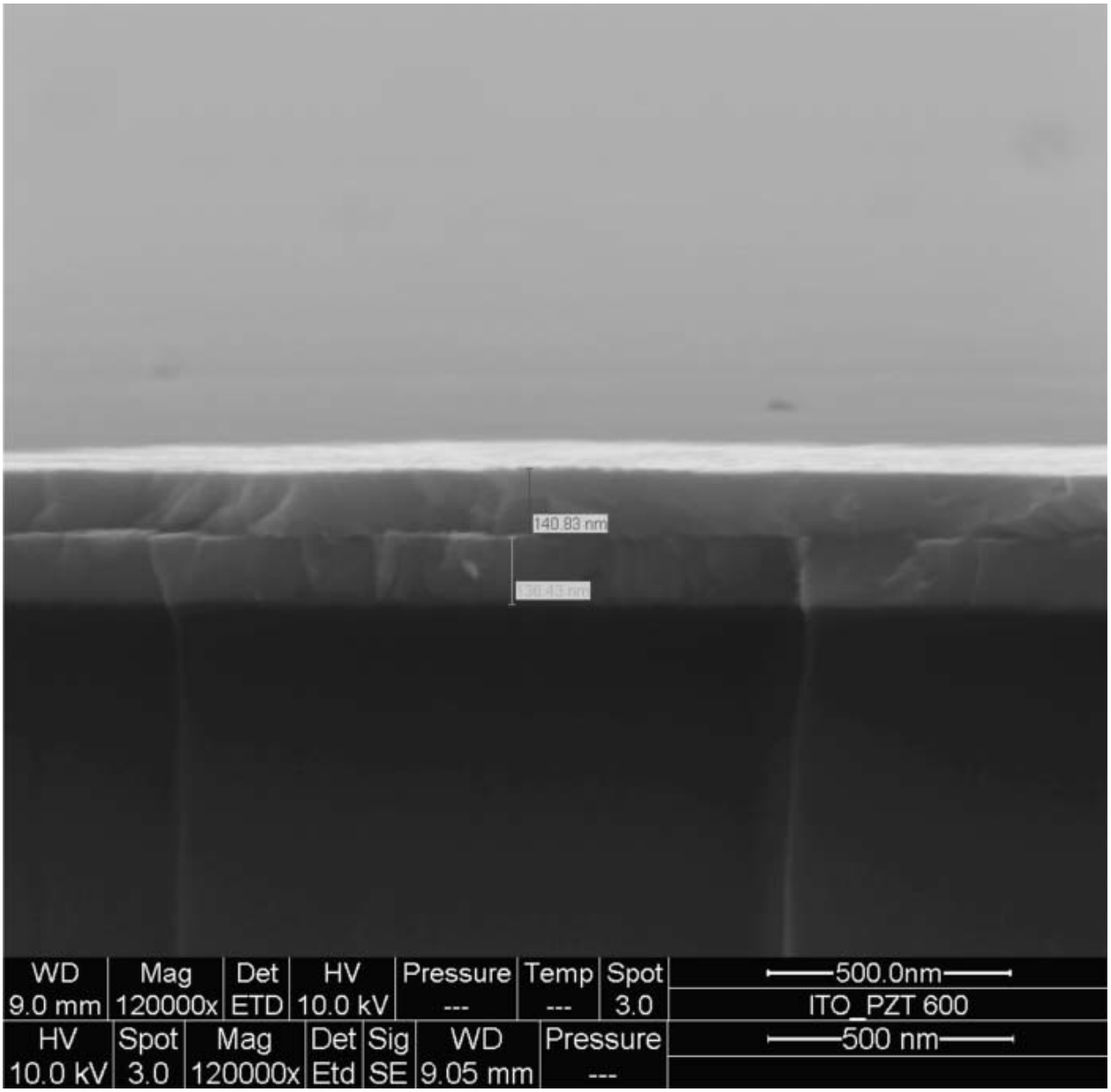
Chiral Liquid Crystals

Cholesteric liquid crystals (CLC) possess a self-organized supramolecular helicoidal periodic structure in which periodicity can be set from 100nm to infinity and which are also characterised by 100% selective reflection of circularly polarized light. CLCs can be used for several applications:
- When a photoluminescent dye is hosted in a CLC matrix which has been prepared using nematic liquid crystals and chiral dopants, the dye acts as an active material in a resonator. Laser emission can therefore be obtained from the mixture when it is illuminated with a pump laser. The possibility to modify the helical pitch and then the photonic band gap structure of CLCs together with the possibility to exploit new luminescent materials with chiral properties allows to obtain mirrorless micro lasers with a finely tunable emission. We are also investigating lasing from liquid crystalline blue phases, that appear in short pitch cholesterics and have self-assembled three-dimensional cubic structures. The application of an electric field produces a versatile effect on the blue phases, causing a distortion of the cubic lattice and a consequent shift of the Bragg peaks. We are working to demonstrate that lasing in the blue phases may be tuned and

easily controlled by an electric field and/or temperature and therefore be useful for photonic material based devices.
- Generally, if a CLC is confined between two flat plates treated to provide boundary conditions with planar anchoring, the resulting texture is uniformly twisted everywhere and the helical axis is normal to the plates. When the distance d between the two boundary plates is small compared to the pitch p of the helix, then, these boundary conditions force the director throughout the sample to be perpendicular to the plates. In the narrow range of the confinement ratio $C=d/p\approx1$ of the thickness d over the equilibrium pitch p, one observes the formation of periodic gratings. When the boundary conditions of the confining plates is homeotropic one observes the formation of "bubbles". These bubbles are defects which form and grow after an external perturbation, but that can be stable in absence of the starting perturbation, and they have been observed for the first time in 1974 by Haas and Kawachi. The forming process of these exotic structures can be achieved by using three techniques: Applying a dc or low frequency voltage to the CLC cell, so that, an electro-hydrodynamic turbulence is induced and the bubbles appear spontaneously after removal the electric field; Raising the temperature of the CLC to the isotropic phase and then suddenly cooling it to room temperature; Applying a laser beam to the CLC cell. We investigate the formation and evolution of bubble domains with the goal to demonstrate that this kind of defects may hold a great interest due to their optical properties and that they can to be used as an array of tunable micro-lenses.

Structural Transformations of PZT 53/47 Sol-Gel

PbZr0.53Ti0.47O3 (PZT) thin films were obtained by sol-gel synthesis, deposited by spin coating on ITO-coated float glass and Si wafer, and subjected to different thermal treatments. Their thermal structural evolutions have been studied by X-ray diffraction (XRD), scanning electron microscopy (SEM), and atomic force microscopy (AFM). The growth of ferroelectric perovskite phase, occurring for the highest annealing temperatures, depends on the substrate, being observed only on ITO substrate, while pyroclore phase, not ferroelectric, grows on Si substrates. The electrical properties of the perovskite phase have been investigated, on the nanoscale, by using electric force microscopy (EFM). It reveals asymmetric responses for induced polarization persistence, which can be related to phenomena of intrinsic polarization regarding the films, which changes as a function of the annealing temperature and of the duration of the annealing processes.



Lateral view of the thin PZT film deposition on ITO/glass.

Raman Spectroscopy

The current research issues of the group are electrochromic and ferroelectric thin solid films, polimeric electrolytes and ionic liquids, other kind of films, also organic, deposited on various substrates, carbon nanotubes, functionalized for material science and biomedical applications, graphen and similar systems. Finally, the group is interested to the microspectroscopic characterization of cultural heritage artifacts and minelalogical samples.

For the year 2010 are worth of mention: the study on ferroelectric oxides PZT, used as electrodes in nematic liquid crystal cells, to obtain a rectivied electro-optic response; the characterization of polymorphism of phthalocianine films , in particular tytanil phtalocianine, deposited on mica and other substrates via supersonic molecular beams.

Relevant for the basic spectroscopic development, the discovery of an anomalous amplification of Raman effect on WO3 films , correlated to the formation of sodium islands on the surface of ITO-coated glass substrates after pre-deposition thermal treatments.

In addition, investigation on carbon forms like nanotubes and graphene, and isomorphous material like BN, have been continued. In particular, Raman micro-spectroscopy allowed to map the spontaneous stresses in small grapheme sheets.
In the field of systems with bio-medical applications, micro-Raman investigations have been carried out on ligand-receptor interaction for the protein GPR30 and for ligands like G1, 17-β estradiol and similar ones.
As new research activity can be cited the micro-spectroscopic characterization of various materials entering in the assembling of POLYCRIPS (Polymer Liquid Crystal Polymer Slices), studied with the aim to obtain meta-materials when combined with gold nanoparticles. The liquid crystal E7 and the polymeric matrix NOA have been investigated, as well as the gold nano-particles coated by a thin layer of CTAB (Hexadecyltrimethylammonium bromide) and PINIPAM (Poly-N-isopropylacrylamide). Such investigation identified the liquid crystal vibration sensitive to the molecular orientation, so that a determination in situ of the liquid crystal orientation inside the POLYCRIPS was made.Moreover a reaction mechanism for the NOA polymerization has been suggested.
Beside the basic scientific research, the year 2010 has been devoted to the technology transfer activity, planned in the enterprise project NOTREDAME, include in the general university project CRESCITA (Conoscenza Ricerca e Sviluppo per l'avvio in Calabria di Imprese a Tecnologia Avanzata) proposed by the "PARCO SCIENTIFICO E TECNOLOGICO DELLA CALABRIA-CALPARK".
Within such activity , after receiving citations by the Italian newspaper "IL SOLE 24 ORE": Pag. 2, N°359 of 31 december 2009 and NOVA-IL SOLE 24 ORE": Pag. 12-13, N°215 of 18 March 2010, dr. Marco Castriota has been invited to present the project NOTREDAME (i**N**n**O**vative substrates **D**evelopment for electro-optic**A**l poly**M**eric flexible self consistent devices for applications in the field of the **E**nergy saving) at several meetings aimed to close the gap between research and business:

Realization and characterization of photonic aperiodic structures with a photo-polymerization technique.
These structures are realized using a novel approach to their fabrication based on the use of a programmable Spatial Light Modulator encoding Computer-Generated Holograms. This approach will also possibly allow (by comparison) a further understanding on the diffusion process driving the holographic realization of periodic structures such as diffraction gratings.

7.2 SURFACES AND INTERFACES: CHARACTERISATION, INTERACTION LC-SURFACES, POLYMER SURFACES, ANCHORING, EFFECTS ON EELCTROOPTICS AND PHOTONICS

Self-assembling and surface properties of chromonics
Nucleic acids and in particular guanosine derivatives can be regarded as chromonic systems, an interesting class of lyotropic mesogenic materials including various drugs ranging from antibiotics to anticancer compounds. Molecules in the chromonic liquid crystalline phases tend to stack forming columnar aggregates as a result of intermolecular interactions, first of all the □-□ interactions between aromatic rings, even in diluite solutions. Many studies have been performed in order to better understand the factors governing the stability and order of the self-organized chromonic mesogens but their structure-property relationships are still not clearly understood.
Recent studies have shown that an important application of chromonic liquid crystals is the fabrication of thin liquid crystalline films for applications in bio-photonics and as bio sensors. For applications a key issue is the inderstanding of the mechanism of the anchoring of chromonic systems to surfaces. We are currently researching on this subject using polarized optical microscopy as well as X rays diffraction/reflectometry and scanning probe microscopies (AFM, STM, ESEM, TEM). X ray reflectometry and diffraction can give information not only about the film thickness and roughness but also about its order in plane and out of plane. The morphology of a chromonic monolayer on model conductive surfaces (graphite, MoS2) can be exploited using low current scanning tunnelling microscopy. The results of these studies will be also used as a basis for the manipulation of DNA and G4 for technological applications.

Nematic order Reconstruction as new tool to overcome topological barrier
Thermotropic Liquid Crystal (LC) molecules consist essentially of rigid core units with flexible side chains and they are usually represented by physicists as simple rods with cylindrical symmetry. Most of the LCs classical phenomena are described by the director **n**, which indicates the average orientation of the calamitic molecules, and by an uniaxial scalar order parameter S that, in many cases, is considered mostly constant and independent of **n**. Nevertheless, rich and intriguing physical phenomena in highly frustrated LC systems, such as topological defects, self organized colloidal dispersions in LC , LC emulsions, LC confined in porous materials or LC confined by means of topographic patterns can not be fully explained by this simplified classical description. In all these cases, a tensor order parameter Q, which

couples **n** and S, needs to be defined, as pointed out by de Gennes.
For nematic LCs, the tensor description predicts two different ordered phases: uniaxial, which has a cylindrical symmetry with respect to the director, and biaxial, where such symmetry is broken and the system has two distinct optical axes. However, most nematogenic molecules are intrinsically biaxial even if they give rise to a uniaxial phase, which is usually a consequence of the rotational disorder around the long molecular axis. If the rotational disorder is hampered, non-uniaxial features may appear and biaxial order could arises.
In this frame, in the last few years we provided experimental investigations as well as theoretical foundation to the existence of biaxial domains within uniaxial LC systems, both in the bulk as well as at the LC interface. Recent experiments on LCs frustrated systems show that local and transient bulk biaxial order can be induced in calamitic nematics, and suggest that biaxiality should play a fundamental role in LC phenomena which take place on nanometer scale. In particular, we have proposed the biaxial order reconstruction in nematics as a new tool to describe locally transient biaxial states inside a uniaxial phase. This mechanism is capable to induce, for instance, by means of a strong electric field, a thin biaxial region, which connects two competing uniaxial nematic textures present in a symmetric □-cell. Moreover, we have also demonstrated that, the repulsive force between two surfaces confining a nematic topological defect can be influenced by biaxial states connecting competing alignments. All these phenomena are mathematically described by the eigenvalue exchange mechanism of the Landau de Gennes Q order tensor formalism.
Moreover we have developed a new numerical model based on Finite Element Method to solve ade adequately the Landau de Gennes Q tensor model. The new method consists in a new adaptive grid techniques which moves dynamically the grid points of the mesh in the space where the gradient of the order and the local and transient biaxiality become important, keeping constant their connectivity and the number of mesh points inside the integration domain.

OPTICAL METAMATERIALS
Metamaterials (MTMs) are artificial composite materials whose electromagnetic properties are induced by an appropriate structuring of the medium at scales much smaller than the operational wavelength. For visible light, this "effective medium" requirement implies typical sizes of the artificial structures around a few tens of nanometers or less. To manufacture millimeter-size MTM samples out of individual resonators, with an average density of one to ten resonators per wavelength in the visible, means assembling 109 to 1012 nano-resonators together. The individual, direct manipulation of such a huge number of nano-objects seems unrealistic for large-scale applications. Self-assembly appears as a solution to this daunting task: it is actually a highly efficient process, well known in soft condensed matter physics, whereby individual objects spontaneously organize under the effect of complex pair interactions into highly organized two dimensional (2D) or three-dimensional (3D) structures of various symmetries.
The typical sizes of self-assembled objects in soft condensed matter vary from nanometers (i.e. molecules) to hundreds of nanometers (e.g. colloids), which is precisely the range of interest for metamaterials. It is therefore natural to believe that the combination of nano-chemistry, which is able to finely engineer the required resonant nano-objects, with self-assembly techniques will open the way to new routes for the fabrication and aggregation of plasmonic nanoparticles integrated in soft materials, assuming the structure of guest-host systems.
This bottom-up approach is based on the spontaneous or directed organization of gain functionalized nano-objects, that under the effect of complex pair interactions, create 3D structures of various symmetries. The main interest arises from the extraordinary collective properties at optical frequencies of metallic nano-assemblies, in particular they are able to localize and strongly enhance the incident electromagnetic field by orders of magnitude at their plasmon resonance. The metamaterial properties arising from the sub wavelength architecture are shadowed by strong absorbance since they suffer from a strong radiation damping. These optical losses strongly limit possible applicative uses of plasmonic nano-structures. Theoretical studies have shown that bringing gain to metamaterials can reduce the radiation damping in terms of reduction of the imaginary part of the dielectric permittivity, by producing only slight modifications of the real part.
The approach that will be followed is based on the functionalization of core-shell (lossy) nanoparticles by fluorescent shell based on organic dyes or quantum dots (QDs) grafted at the surface of the nanoresonators. Such "smart" nanoparticles will have the capability of compensating their internal losses with a high efficiency by carrying built-in gain elements. Resonant energy transfer mechanisms between gain units and plasmonic nanoparticles will play a key role to compensate the optical losses of the meta-structures. In addition, a very striking feature can arise from these studies, since in case of very high gain the over-compensated losses can lead to the very fascinating and promising

physics of the SPASER (Surface Plasmon Amplified Stimulated Emission Radiation) introduced by M. Stockman in 2003.

Statistical analyses of repolarisation current of a PZT film deposited on ITO electrode with different thermal treatments

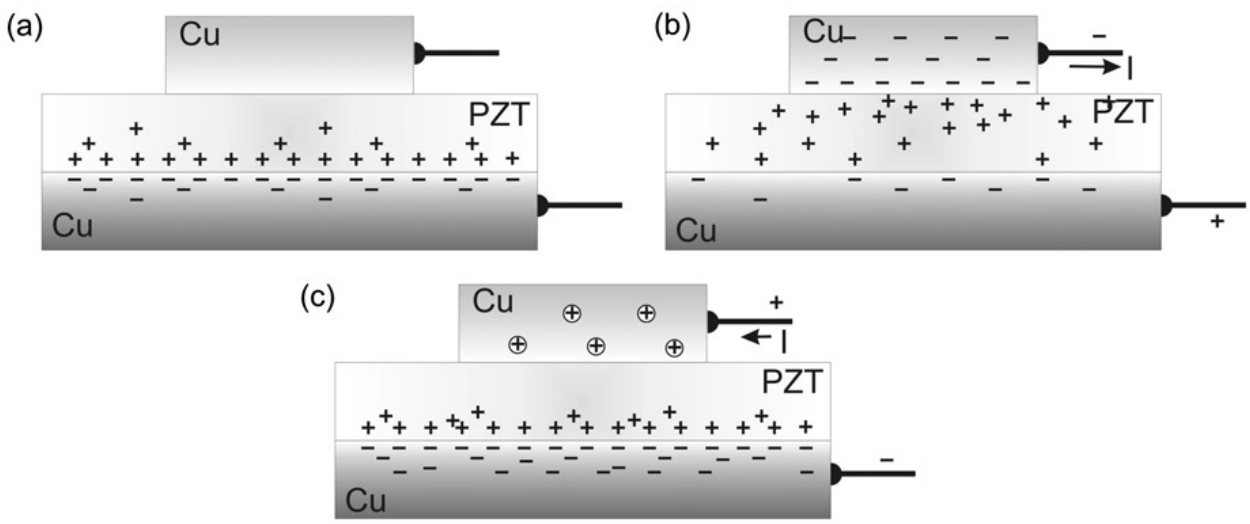
In the vast application fields of lead zirconate titanate (PZT) thin films, of particular interest are the interaction effects occurring at the ferroelectric–substrate interface. Relevant for this purpose are polarity-sensitive liquid crystals (LC) cells and micro- and nanoelectronic applications. The polarisation current was investigated of a PZT film (PbZr0.47Ti0.53O3) obtained by sol–gel synthesis and deposited by spin coating on an indium tin oxide (ITO) electrode. The different behavior exhibited by such a system when the support electrode was previously submitted to a thermal treatment was attributed to the change of the electrical properties of the ITO layer. In particular, a higher negative charge in the conductive band of the ITO electrode seems to be responsible for a higher order in the ferroelectric film.

Stochastic ferroelectric switching of lead zirconate titanate thin films

We investigate the repolarization phenomenon in a ferroelectric film. Our ferroelectric sample was lead zirconate titanate (PZT) obtained by sol-gel synthesis and deposited by spin coating on ITO/glass substrate. A series of repolarizations were induced in the ferroelectric film by applying a triangular wave and the current peaks related to the switchings of the ferroelectric domains were acquired for statistical analyses. It is shown that the dynamics and statistics of polarization switchings are well simulated by a simple mean-field model in which a double-well, asymmetric potential is included to describe the asymmetry at the PZT-ITO interface.

Anomalous conductivity in PZT thin film deposited on copper substrate electrode

Electrical properties of ferroelectric films are influenced by factors that include methods of synthesis and characteristics of the substrate electrode. Conductivity measurements were performed on PZT (lead zirconate titanate) thin films deposited by sol–gel synthesis on a copper electrode to investigate electric properties and isolate the principal charge carriers. A semiconducting PZT/Cu interface appears during thermal treatment, significantly influencing electric conduction. A power law, describing the transport mechanism across the PZT film, was found empirically.



Equilibrium distribution of copper ions in PZT and counter electrons in the copper base electrode. (b) Copper base electrode under positive voltage. (c) Copper base electrode under negative voltage

7.3 CONFINED SYSTEMS, NANOSCIENCES, PHOTONICS: LASING, GRATING, MEMORIES, HOLOGRAPHY, POLYCRIPS, SOLITONS

Study of Shock Waves in Liquid Crystals

Shock waves are a general phenomenon thoroughly investigated in disparate area of physics like fluids and water waves, plasma physics, gas dynamics, sound propagation, physics of explosions, etc. They are also expected in (non-hyperbolic) universal models for dispersive nonlinear media, such as the Korteweg-De Vries (KdV) and nonlinear Schrodinger (NLS, or analogous Gross-Pitaevskii) equations. We investigate this phenomenon in a nematic liquid crystal with twofold points ofview: numerical and experimental. Numerically we investigate the formation of typical shock profile in space and time solving the Spatial Maxwell wave equation (tipical Non linear Schrodinger equation) coupled with the Frank equation (that contain the time evolution). Experimentally we consider the conditions of numerical simulation (liquid crystal alignment, light power, spot size of light beam) in order to reproduce the shocks waves in nematic liquid crystal.

POLICRYPS Gratings with metallic nano-inclusions towards Metamaterials.

Noble metal nanoparticles (NPs) exhibiting plasmonic properties attract wide interest in research for the possibility they offer to realize metamaterials. These have been predicted in 1969 by Veselago and they are materials that gain peculiar electromagnetic properties (e.g. negative refractive index) from their structure, rather than from their chemical composition. Thanks to recent advances in nanofabrication, first examples of such materials, which exhibit particular functionalities at optical frequencies, have been realized. However, the success of these results is limited by the typical size of devices that can be fabricated, which is actually very small (few square millimetres). Alternative approaches are emerging, which propose the use of self-assembling materials in order to overcome this issue and obtain the sought for greater structures, with less difficulty [Nanogold EU project, (2009-2012); Metachem EU project (2009-2013)]. An ambitious project is to combine metallic units with host materials whose dielectric properties can be tuned by an external control; indeed, a modification of the dielectric behavior of the host could correspond to a tuning action of the plasmon resonance frequency. In this regard, by combining the tunability of POLICRYPS structures with the plasmonic response of metallic NPs could give rise to novel metamaterial devices with tunable properties.

Investigation and Applications of POLICRYPS Gratings

POLICRYPS is a structure made of perfectly aligned liquid crystal films separated by slices of almost pure polymer. Under suitable experimental and geometrical conditions, the structure is obtained by curing a homogeneous syrup of liquid crystal, monomer and curing agent molecules with a spatially modulated pattern of UV radiation. From an optical point of view, POLICRYPS is a holographic diffraction grating with a spatial periodicity that can be easily made of sub-micrometric scale, exhibiting diffraction efficiency values as high as 98%. Depending on the used substrate, the POLICRYPS grating can be utilized both in transmission or reflection, with negligible scattering losses, and can be switched ON and OFF by application of an external electric field of the order of few V/μm. Concerning this structure, in the period of observation (2008), our interest has been devoted to the following arguments:

a) POLICRYPS gratings as switchable phase modulators

POLICRYPS gratings can be used as well as electrically controlled optical phase modulators. Arbitrarily polarized light normally incident on the structure experiences a birefringence that depends on the anisotropy of the composite liquid crystalline material and on the geometrical cell parameters. The sample behaves as a retardation plate in good agreement with the Jones matrix formalism. The birefringence of the modulator can also be tuned by applying a suitable voltage, while a negligible birefringence variation is detected by increasing the incidence power. This makes POLICRYPS structures suitable as switchable phase retarders for high power laser beams.

b) All-Optical switching in (1-2)D structures

We investigate high quality azo-POLICRYPS diffraction gratings to be used for fast all-optical switching in the visible range. The polymeric microstructures, produced in a multistep chemico-physical process, confine and stabilize a well aligned nematic liquid crystal (NLC) film, which is doped with a high performance mesogenic azobenzene dye, sensitive in the visible range. The all-optical switching of the grating between highly diffractive and transparent states is realized by a photochemical phase transition between nematic and isotropic phases based on the photoisomerization of azobenzene guest molecules. The effect, which is reversible and repeatable, is triggered by a visible pump irradiation and detected through the change in the diffraction efficiency of a low power probe light. Performances of the new structures are highlighted by investigating also the correlation between switching times and pump power.

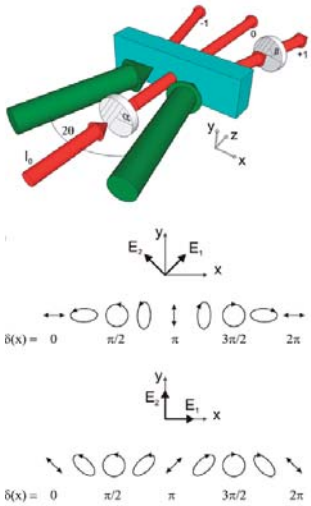
A Novel Polymer Matrix for Confinement and Alignment of Self-Organized Materials

We report about the realization and characterization of a novel polymer matrix sculptured in photosensitive material devoted to micro/nano-confinement to stabilize a wide range of organic and biological components with self-arrangement properties at the nanoscale. The high quality morphology of a 2D polymer structure is obtained by combining a nano-precision level optical holographic setup and a multi-step chemical-physical process. The sharp and uniform morphology can be conveniently used as templates to be filled with high-refractive index materials or different soft composite elements. Due to their ability as self organization materials, short pitch cholesterics LC, azo dyes LC and ferroelectrics LC have been used. Various experimental studies have been carried out in order to investigate the efficiency of such structures for the realization of electro-optical and all-optical devices. Biological materials and DNA are currently under investigation.

Photosensitive organic materials

We started the investigation of the photo-activate and photo-correlate properties of organic multifunctional molecular materials and their possible applications for photonic and optoelectronic devices. The attention to these materials, driven by their light-weight and by unique mechanical properties, as the prospect of manufacturing flexible and low-cost devices, is primarily due to the possibility to design molecules with properties tailored for specific applications, that can give rise to intermolecular interactions with high added value.

The organic materials are multifunctional polymers bearing three distinct functional groups, i.e. photosensitive azoaromatic, photoconductive and chiral groups, directly linked to the side chain. The polymers possess, all at once, the three functionality that are the basis for optical storage based on induced modulation of the refractive index, chiro-optical swhitch, non-linear optical (NLO) and photorefractive and photoconductive applications. Although the aforementioned issues was the subject of intense study in recent years, their synergistic combination and their parallel presence in the materials has not yet been studied, and could lead to the observation of new phenomena. The polymers was supplied by the Chemistry Department of the Moscow State University,(Prof. V. Shibaev) and Dipartimento di Chimica Industriale e dei Materiali, Università di Bologna (in the frame of the PRIN project "Synthesis and Functional Characterization of Photo-active Organic Semiconductors")



Photoinduced optical anisotropies

The photo-induced anisotropy obtained by irradiating the molecular materials both by single beam with different polarization states and with polarization or intensity patterns have been investigated, in order to analyze and characterize the formation of structures connected to the birth of linear and circular birefringence. Intersting results have been obtained in the case of an amorphous azo-polymers where, exploiting a method based on the vectorial holography, both linear and circular birefringence have been measured simoultaneously. Polarization grating recording in an amorphous and nonchiral azo copolymer has been investigated. The reported study shows that the amorphous polymeric film undergoes a light-guided inhomogeneous supramolecular modification as a consequence of the illumination with proper polarized light patterns, acquiring new functionalities. Both linear and circular, spatially modulated, photoinduced birefringences occur, attaining their peak values in the linearly and circularly polarized regions of the light pattern, respectively. The photoinduced anisotropic structures strongly affect the polarization state of the light propagating through them, and the characterization of their optical diffraction enables measurement of the amplitude of the linear and circular birefringences. The recorded gratings show long-time stability and full reconfigurability functional to the multiple holographic recording.

Photorefractivity

We started also the investigation of the photo-generation mechanisms and charge transport in the multifunctional polymers, paying particular attention on the association chirality-conductivity. In particular we addressed the investigations towards the influence of chiral conductors handedness on the transport phenomena and its optical control by different ellipticity and elicity light beams.

Charge localization and transport at the interface polymer-liquid crystal have been studied. Photocurrent measurements

and Two Beam Coupling experiments have been performed.

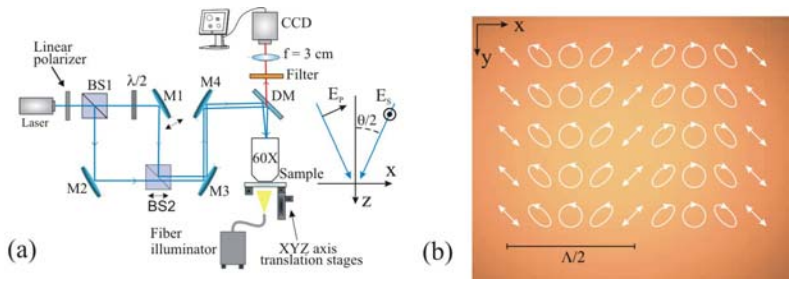
Supramolecular structuring

Supramolecular structuring has been also investigated to create structured materials with reconfigurable functionalities and photonic devices, exploiting intensity or polarization holographic techniques. The multifunctional materials have been irradiated by different interference patterns, obtained changing the number of beams, their polarization state and their intensity.

Optical trapping and manipulation

The exploitation of optical forces represents at the same time a precise, non-invasive and gentle manipulation technique of micro and nano-particles. The most powerful and widely developed tool are the optical tweezers (OT) that have shown their tremendous potentiality for the manipulation without physical contact of systems with dimension ranging from tens of nanometers to hundreds of micrometers. The OT are applied in different research fields of the life sciences since they yield a non-invasive and near-infrared radiation. Moreover the advantages of remote control of micro and nano-particles and the sensitivity of the optical trap to piconewton-scale forces make OT an extremely useful tool also in the materials science and technology.

Very suggestive techniques based on properly shaped wavefronts have been investigated to optimize the light's ability to exert forces and torques through a transfer of both linear and angular momentum. Although very sophisticated methods the intensity gradient is at the basis of their conventional trapping operation principle and none of them brings into the open optical force gradients based on the vectorial nature of the light.



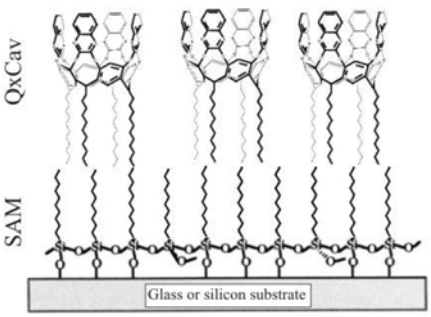
Optical sieve

We have proposed a new method where a polarization gradient, created via vectorial holography**,** offers new capabilities to optical trapping and manipulation. The simplest and pure polarization pattern has been used. In the interference region, the intensity distribution is Gaussian while, at smaller scale, a spatially periodic modulation of the polarization state occurs. This holographic tweezer allows oscillatory displacements and controls the sense of rotation of several particles inside the illuminated region. Unconventional trapping of spinning particles in circularly polarized fringes has been observed, which suggests the involvement of the lift hydrodynamic force, responsible of the Magnus effect, never revealed until now in ordinary optical trapping schemes. Liquid crystals (LC) water emulsion has been used to verify the mechanical properties of the polarized holographic optical trap; since it offers the possibility to have spherical particles of the same material with different optical properties in the same emulsion. The holographic tweezers based on the polarization gradient enable to investigate new capabilities of the technique with increased sensitivity trapping without an intensity gradient.

Polarization holography in molecular materials

Polarization gratings in LC, LC-polymers composite materials have attracted great interest because of peculiar diffraction properties which open the way to promising application in displays and photonic technologies. Several materials and configurations have been investigated.

1D and 2D LC gratings, obtained by means of different assembling of polarization holograms recorded on photo-aligning substrates, have been investigated. Near 100% efficiency has been obtained in case of 1D gratings. The 2D gratings diffract light in different directions with different polarization states, that can be optically controlled. Orthogonal circularly and linearly polarized diffraction orders are simultaneously obtained irradiating the grating with a linearly

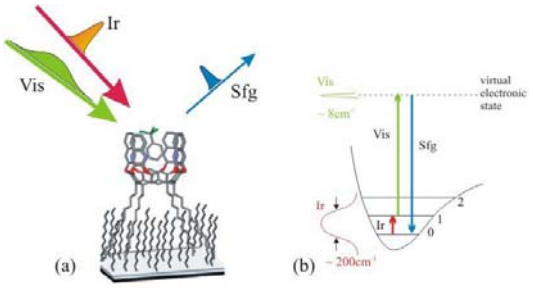


polarized beam. In both cases, an external ac voltage allows to completely control the diffracted energy distribution.

CD (circular dichroism) Spectrometer for artefacts free and real time measurements

A simple method to perform real-time measurements of circular dichroism (CD) have been developed which suppresses the artifacts introduced by anisotropic samples and non-ideal optical elements in conventional spectrometers. A single polarization holographic grating is adopted, whose first orders of diffraction have amplitudes which are proportional to the right and left circular polarization component of the input light. We demonstrate that, exploiting unpolarized white light and the intrinsic spectral selectivity of the grating, true CD spectrum is evaluated in parallel in the spectral range of interest from the intensities of the two diffraction orders, I_{+1} and I_{-1}.

A demonstrator prototype of a CD spectrograph based on this method has been developed.



Nonlinear optical investigation of molecular recognition at interfaces for environmental and bio-chemical sensing.

We explored the opportunities offered by nonlinear optics and, in particular, by the ultrafast sum-frequency generation vibrational spectroscopy (SFG-VS) in the fields of chemical and biochemical sensing. As a second-order nonlinear optical processes, SFG-VS has been proven to be a versatile analytical tool for non-invasive probing of any interface accessible by light, with intrinsic surface specificity, chemical selectivity and sub-monolayer sensitivity. With femtosecond laser pulses in the broadband scheme, it might permit the investigation of ultrafast surface dynamics and chemistry with sub-picosecond time resolution.

The SFG-VS has been used to provide a molecular-level description of surfactant-covered substrates and their hybrid bimolecular architectures with synthetic macrocyclic receptors. Molecular conformation and alignment have been deduced for both the surfactant and the synthetic receptor layer, as function of the material composition [i.e., n-octadecylsiloxane (OTS), n,n-dimethyl-n-octadecyl-3-aminopropyltrimethoxysilyl chloride (DMOAP), pyrazine-(PzCav) and quinoxaline-bridged (QxCAv) cavitands] and deposition procedures [i.e., self-assembling, Langmuir-Blodgett, Langmuir-Schaefer].

Molecular-level evidence of the receptor-analyte complexation at the solid-gas interface has been obtained. DMOAP-PzCav and DMOAP-QxCav hybrid bilayers were exposed to vapor of acetonitrile. Unexpectedly, opposite orientation for the complexed analyte molecules has been found depending on the cavity depth.

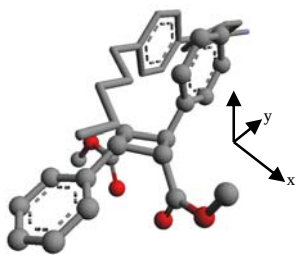
Membrane-mimetic architectures on solid substrates are extremely important for applications that include biosensor devices, preparation of biocompatible surfaces and fundamental studies of membranes. For biosensor applications, solid-supported membranes should contain both phospholipids and membrane receptors in their native conformation, be sufficiently rugged and have an high degree of stability, either in water or in air. Stabilized hybrid bilayer membranes (HBMs) have been obtained by Langmuir-Schaefer deposition of phospholipids on alkylsiloxane SAMs templates. Both OTS-DPPC and DMOAP-DPPC HBMs, supported on planar fused silica substrate, have been investigated by SFG-VS providing a description of their organization and structure.

Sum-frequency vibrational spectroscopy on polymer surfaces for liquid crystal alignment

Surface-specific sum-frequency generation vibrational spectroscopy (SFG-VS) is a unique technique that can yield vibrational spectra that are directly related to interfaces and surfaces structure. We have used it to study the photo-induced surface structural change of polyvinyl cinnamate (PVCi), which has been considered a potential polymeric material for photo-alignment of LC in real device applications.

It has been demonstrated that PVCi (and its derivatives) coated substrates after linearly polarized UV irradiation can homogeneously align an LC film in the direction perpendicular to the linear polarization. The orientation of the cinnamate side chains is believed to be responsible for the induced LC alignment. There exist, however, two proposed surface molecular structures of PVCi (and derivatives) induced by irradiation. One is photo-induced dimerization and the other trans-cis isomerization of the cinnamate side chains.

We have investigated UV-irradiated PVCi surfaces, both rubbed and unrubbed, using SFG-VS to determine their surface structural changes. The vibrational spectra of dimerized and undimerized cinnamate chains are different and their input/output



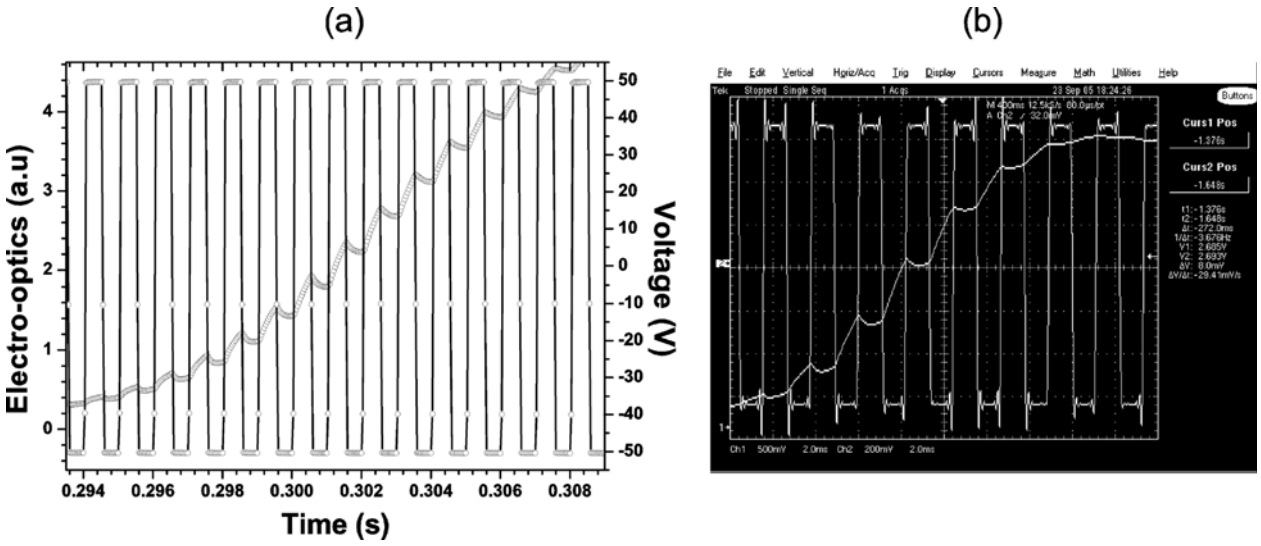
polarization dependence yields information about orientations of selected moieties.

Our SFG-VS results indicate that polarized UV irradiation dimerizes rather than isomerizes the protruding cinnamoyl side chains at the surfaces and creates significant surface structural anisotropy needed in many applications. Azimuthal anchoring energy measurements of a nematic liquid crystal film on PVCi irradiated by low UV dosages yield results in good correlation with the observed spectral anisotropy.

Laser Action in Liquid Crystals: From Random to Periodic
Extensive studies on one-dimensional (1D) PBG materials have been performed. The birefringence and natural ability to form periodic structures make cholesteric liquid crystalline (chiral nematic) materials particularly attractive as 1D PBG systems. In fact, chiral liquid crystals (CLC) possess a helical superstructure that provides a 1D spatial modulation of the refractive index, giving rise to Bragg selective reflection for circularly polarized light having the same handedness as the LC structure. If a CLC is doped with dye fluorescent molecules, in such a way that the maximum peak of fluorescence matches one of the edges of the selective stop band, the spontaneous emission is suppressed within the bandgap and enhanced at the band edges. At this spectral position the photon
group velocity approaches zero and low threshold mirror-less laser action is expected. By confining the helical super-structure of chiral liquid crystals in polymeric micro-cavity channels a tunable microcavity laser array was achieved.
In random systems, on the other hand, the propagation of the light waves is quite different, as optical scattering may induce a phase transition in the photon transport behaviour. For very weak scattering, the propagation can be described as a normal diffusion process. With an increase of the scattering intensity, recurrent light scattering events arise and the interference between the counter-propagating waves leads to enhanced backscattering, namely weak localization of light. Beyond a critical scattering level, the system makes a transition into a strongly localized state and light transmission is inhibited. This effect can be used as a photon trapping mechanism to obtain laser action in partially ordered and random systems. In the presence of a gain medium, recurrent multiple scattering and amplification substitute for the distributed optical feedback of a regular laser cavity. Due to a random walk with optical gain inside these systems, diffusive lasing action is encountered. Random lasing modes come from the eigenstates of disordered systems and open a particular chapter in the study of the interplay between localization and amplification. Here, experiments performed on systems having different order degree and confinement are presented and possible technological implications are discussed.

7.4 APPLICATIONS: SPECTROMETERS, SENSORS, DEPOLARIZING SYSTEMS, EHD, LCD, CD

Mechanisms leading to fast relaxation of liquid crystal cells aligned with conductive polymers
Using nematic liquid crystal cells aligned by conductive polymers, like polyaniline or doped polypyrrole, a very fast electro-optic response is observed. We show that when a switch that interrupts the voltage across the cell is placed between the cell and the ground, the largest voltage drop is on the switch in its open position. The voltage distribution among the nematic cell and the switch is evaluated. The role played in this very fast electro-optic response of the ionic charges built on the interfaces together with the redox processes among the free charges in the polymer-liquid crystal interface is also described. For an asymmetric cell _only one side covered with a conductive polymer_ a rectifying effect appears. In this case a circuital model is used to mimic the steplike behavior of the transmitted light during the relaxation of the system.



an expanded plot in the OFF range that shows clearly this phenomenon.

Thermal induced changes of lead zirconium titanate films and their consequences for liquid crystal devices applications

Thin films of lead zirconate titanate (PZT) were obtained by a modified sol–gel route on float glass and indium tin oxide (ITO)-covered float glass substrates. Different thermal treatments were performed on the deposited films in the temperature range 100–700_C. Spectroscopic ellipsometry was used to investigate the optical properties of the deposited films, and the changing optical absorption spectra were interpreted in terms of the growth of two different crystal phases, pyrochlore and ferroelectric perovskite, as a function of annealing temperature. Moreover, a specific resonance at 1.9nm was detected when thin PZT films are deposited on ITO substrates and was attributed to a particular charge distribution at the interface. Finally, the performance in rectifying the electro-optical response of asymmetric nematic liquid crystal cells was tested for some of the films undergoing different thermal treatments.

7.5. NANO-IMAGING OF BIOLOGICAL AND BIOCOMPATIBLE MATERIALS AND SURFACE FORCE APPARATUS (SFA)

AFM and phase imaging on membranes

AFM is used to provide a better insight in the topographical properties, on a scale not accessible to ESEM, of membranes developed at the Department of Chemical Engineering of Materials (UNICAL).

The chemical engineering group is developing membranes with ordered features made by block copolymers PS-PB (polystyrene and polybutadiene) changing the production conditions: solvents, temperature, presence of templates. The membranes are investigated in Tapping Mode AFM, with special attention to the 1st harmonic signal, to provide information on both their topographical and mechanical properties. The order in the surface morphology is correlated to the gas transport properties of the membranes. Membranes prepared using other materials are currently under investigation.

Nano-imaging of biological materials

Advanced microscopy techniques, such as Atomic Force Microscopy (AFM) and Environmental Scanning Electron Microscopy (ESEM), are finding application in biology and biomedical investigations since they are non-destructive techniques and can be performed in liquid-humid environments.

AFM and ESEM are currently used to investigate the aggregation properties of proteins such as -lactoglobulin as

influenced by the presence of a substrate. This protein is used as a "model-protein" to study the different types of aggregation that can occur i.e. globular aggregates or fibrils formation. In particular the understanding of the mechanism of fibrils formation is important since it is related to several medical diseases (Alzheimer, Parkinson).

Structural properties of hydrophobin aggregates revealed by atomic force spectroscopy in dynamic mode.
Hydrophobins are small proteins (about 100 amino-acid residues) produced by fungi as soluble forms, self assembling into an amphipatic membrane when they reach an interface (e.g. medium-air or cell wall-air).
These proteins have been split in two group, class I and class II hydrophobins, based on the differences in their hydropathy patterns, spacing of aminoacids between the cysteine residues and properties of the aggregates they form.
One distinguishing feature of class I hydrophobins is the characteristic rodlet structure observed on the hydrophobic side of an amphipathic protein film.
The interest in investigating such aggregates relies in the fact that their morphology and chemical-physical properties are reminiscent of amyloid fibrils, produced in mammals degenerative diseases; this similarity makes the hydrophobin rodlets a good model system.
We have investigated the protein vmh2 class I hydrophobin from the fungus *pleurotus ostreatus* in order to obtain informations about the structure of their assemblies, including monolayers, bilayers and aggregates under form of rodlets, with the motivation of a deeper understanding of the rodlets structure. We exploit force spectroscopy measurements in dynamic mode AFM to probe the wetting phenomenon of hydrophobin films and rodlets as a function of humidity on samples prepared by the Langmuir technique. We have demonstrated that the hydrophilicity of Langmuir-Schaefer film can be highlighted at the nanoscale by detecting the meniscus formation between the AFM tip and surface of the monolayer. On the other hand, we have demonstrated that no meniscus is formed, neither between tip and Langmuir-Blodgett monolayer, nor between tip and rodlets. These results confirm that the Langmuir-Schaefer monolayer is less hydrophobic than Langmuir-Blodgett one, as one would expect and as shown by contact angle measurements, but also demonstrate that it is less hydrophobic than rodlets. Moreover, by analyzing the phase versus distance curves performed in dry conditions for hydrophobin Langmuir-Blodgett film and rodlets, we have revealed the difference in the visco-elastic properties between Langmuir-Blodgett layers on one hand and Langmuir-Schaefer layers or rodlets on the other hand. This difference may be associated with the presence of the flexible loops that are exposed to the air in the Langmuir-Blodgett layer but interact with the substrate for Langmuir-Schaefer layer and with other molecules for rodlets. The interaction in rodlets at least partly occurs between two hydrophobins of the two layers in front of each other, as shown by the similarity between the hydrophilicity and visco-elasticity of hydrophobin bilayers and rodlets, measured by Atomic Force Spectroscopy. This similarity strongly suggests that rodlets are actually fragments of hydrophobic bilayer with molecular conformational changes with respect to simple superposed layers.

A PUBLICATIONS ON SCIENTIFIC JOURNALS
A.1 Publications on international journals
A.1.1 Publications on international journals printed in 2010

1. Ayeb H, Lombardo G, Ciuchi F, Hamdi R, Gharbi A, Durand G, Barberi R,
   Surface order reconstruction in nematics,
   Applied Physics Letters 97, 104104 (2010)

2. Amoddeo A, Barberi R, Lombardo G
   Moving mesh partial differential equations to describe nematic order dynamics
   Computers & Mathematics with Applications, 60, 2239-2252 (2010)

3. M. Buscaglia, G. Lombardo, L. Cavalli, R. Barberi, T. Bellini,
   Elastic anisotropy at a glance:the optical signature of disclination lines
   Soft Matter 6, 5434-5442 (2010)

4. Matranga MA, De Santo MP, Petriashvili G, Chanishvili, Chilaya G, Barberi R
   Frequency tunable lasing in a three layer cholesteric liquid crystal cell
   Ferroelectrics, 395, pp. 1-11(2010)

5. Chinelatto LS, del Barrio J, Pinol M, Oriol L, Matranga MA, De Santo MP, Barberi R
   Oligofluorene blue emitters for cholesteric liquid crystal lasers
   Journal of Photochemistry and Photobiology A - Chemistry JOURNAL, 210 (2-3), pp. 130-139 (2010)

6. De Santo MP, Matranga MA, Ciuchi, F, Petriashvili G, Barberi R
   Lasing Stability Enhancement in Dye Doped Cholesteric Liquid Crystals
   Molecular Crystals and Liquid Crystals, 516, pp.190-196 (2010)

7. Buonomenna MG, Golemme G, De Santo MP, Drioli E
   Direct Oxidation of Cyclohexene with Inert Polymeric Membrane Reactor
   Organic Process Research & Development ORGANIC, 14 (1), pp. 252-258 (2010)

8. Rizzuti B, Zappone B, De Santo MP, Guzzi R
   Native beta-Lactoglobulin Self-Assembles into a Hexagonal Columnar Phase on a Solid Surface
   Langmuir, 26 (2), pp. 1090-1095 (2010)

9. Armenante A, Longobardi S, Rea I, De Stefano L, Giocondo M, Silipo A, Molinaro A, Giardina
   The Pleurotus ostreatus hydrophobin Vmh2 and its interaction with glucans
   P GLYCOBIOLOGY Volume: 20 Issue: 5 Pages: 594-602 Published: MAY 2010

10. N. Coppedè, M. Castriota, E. Cazzanelli, S. Forti, G. Tarabella, T. Toccoli, K. Walzer and S. Iannotta

    Controlled Polymorphism in Titanyl Phthalocyanine thin films on mica by Supersonic Molecular Beam Deposition: a Micro-Raman analysis.
    Journal of Physical Chemistry C 114 , n 15 , pp 7038-7044 (2010)

11. M. Castriota, E. Cazzanelli, D. Pacilè , L. Papagno, C. O. Girit, J. C. Meyer, A. Zettl, M. Giarola and G. Mariotto
    Spatial dependence of observed Raman frequencies and disorder in graphene monolayers
    Diamond and Related Materials 19, n 5-6 , pp 608-613 (2010)

12. A. Mazzulla, P. Pagliusi, C. Provenzano,G. Cipparrone
    Real-Time Circular Dichroism Spectrograph Based on a Single Liquid Crystal Diffractive Element
    Molecular Crystals Liquid Crystals 516, 233-239 (2010)

13. G. Cipparrone, I Ricardez Vargas, P. Pagliusi, C. Provenzano,
Polarization gradient: exploring an original route for optical trapping and manipulation
Optics Express 18, 6008-6013 (2010)

14. C. Provenzano, P. Pagliusi, A. Mazzulla, G. Cipparrone
Method for artifact-free circular dichroism measurements based on polarization grating
Optics Letters, 35, 1822-1824 (2010)

15. G. Cipparrone, P. Pagliusi, C. Provenzano P.V. Shibaev
Polarization Holographic Recording in Amorphous Polymer with Photoinduced Linear and Circular Birefringence
J. of Physical Chemistry B, 114, 8900-8904 (2010)

16. G. Strangi, V. Barna, A. De Luca, S. Ferjani, C. Versace
Book Chapter "Random Lasing in Liquid Crystals"
TRANSWORLD RESEARCH NETWORK, Kerala , India (2010)

17. Carbone F, Yoshida H, Suzuki S, Strangi G,.
Clustering of elastic energy due to electrohydrodynamics instabilities in nematic liquid crystals
EPL Volume: 89 Issue: 4 Article Number: 46004 (2010)

18. G. Carbone, P. Salter, S. J. Elston, P. Raynes, L. De Sio, S. Ferjani, G. Strangi C. Umeton, R. Bartolino
Fast Electro-Optical Device Based on Chiral Liquid Crystals Encapsulated in Periodic Polymer Channels, MOLECULAR CRYSTALS AND LIQUID CRYSTALS Volume: 525 Pages: 55-63 (2010)

19. V. Barna, A. Petris, I. Dancus, E. S. Barna, A. De Luca, S. Ferjani and G. Strangi
Efficient Random Laser Effect In A New Dye-Nematic Liquid Crystalline Composite,
ROMANIAN REPORTS IN PHYSICS, Vol. 62, 444–454, (2010)

20. L. De Sio, A. Tedesco, N. Tabiryan and C. Umeton
Optically Controlled Holographic Beam Splitter
Applied Physics Letters 97 (2010)

21. L. De Sio, C. Umeton, S. Serak and N. Tabiryan
Full Optical Control of Holographic Gratings Realized in Composite Materials Containing Photosensitive Liquid Crystals
Molecular Crystals and Liquid Crystals 526 101 -107 (2010)

22. L. De Sio and C. Umeton,
Dual-mode control of light by two-dimensional periodic structures realized in liquid-crystalline composite materials
Opt. Lett. 35, 2759-2761 (2010)

23. G. Carbone; P. Salter; S. J. Elston; P. Raynes; L. De Sio; S. Ferjani; G. Strangi; C. Umeton and R. Bartolino
Fast Electro-Optical Device Based on Chiral Liquid Crystals Encapsulated in Periodic Polymer Channels Molecular Crystals and Liquid Crystals, 525, 41 (2010)

24. L. De Sio, J. G. Cuennet, A. E. Vasdekis and D. Psaltis
All-Optical Switching in an Optofluidic Polydimethylsiloxane - Liquid Crystal Grating Defined by Cast Molding
Applied physics letters, 2010, Vol. 96, pp. 131112-131112-3.

25. D. Donisi ; R. Asquini ; A. d'Alessandro ; B. Bellini ; R. Beccherelli ; L. De Sio ; C. Umeton
Integration and Characterization of LC/Polymer Gratings on Glass and Silicon Platform
Mol. Cryst. Liq. Cryst., 516, 152-158 (2010)

26. R.Caputo, I.Trebisacce, L. De Sio, and C.Umeton,
Jones matrix analysis of dichroic phase retarders realized in soft matter composite materials
Opt. Express 18, 5776-5784 (2010)

27. L. De Sio, A. De Luca, G. Liveri, and C. Umeton,
Observation of hysteresis effects in POLICRYPS holographic gratings
Opt. Express 18, 31-36 (2010)

28. L. De Sio, S. Serak , N. Tabiryan, S. Ferjani, A. Veltri, C. Umeton
Composite holographic gratings containing light responsive liquid crystals for visible bichromatic switching
Adv. Mater., 22, 2010

29. D. Donisi, R. Caputo, G. Cennini,
Holographic Grating Based High Sensitivity Device for Refractive Index Measurements
Opt. Exp., 18, 14, 15236 (2010)
Articolo selezionato per la pubblicazione su: Virtual Journal for Biomedical Optics, 5, 11 (2010)

30. Andrei Th. Ionescu, Anca-Luiza Alexe-Ionescu, Salvatore Marino, Marco Castriota, Giuseppe Strangi and Nicola Scaramuzza
Study of conductivity on a PZT thin film deposited on a copper substrate electrode
PHILOSOPHICAL MAGAZINE 90 (131733-1742) (2010)

31. Salvatore Marino, Andrei Th. Ionescu, Anca-Luiza Alexe-Ionescu, Gaetano Nicastro, Giuseppe Strangi and Nicola Scaramuzza
Study of repolarization current of a PZT film deposited on ITO electrode with different thermal treatments
PHILOSOPHICAL MAGAZINE 90 (12) 1575–1584(2010)

32. S. Marino, F. Lepreti, V. Carbone, N. Scaramuzza
Stochastic ferroelectric switching of lead zirconate titanate thin films
EUROPEAN PHYSICAL JOURNAL B 74 475-477(2010)

33. Marco Castriota, Stefano D'Elia, Salvatore Marino, Carlo Versace, Enzo Cazzanelli and Nicola Scaramuzza
Effects of thermal treatments on structural and optical properties of Lead Zirconium Titanate thin films obtained by sol gel
PHILOSOPHICAL MAGAZINE 90 (16) 2223-2233(2010)

34. Emanuela Bruno; Federica Ciuchi; Marco Castriota; Salvatore Marino; Gaetano Nicastro; Enzo Cazzanelli; Nicola Scaramuzza
Structural transformations of PZT 53/47 sol gel films driven by thermal treatments
FERROELECTRICS 396 49-59(2010)

35. Gaetano Nicastro, Nicola Scaramuzza, Roberto Bartolino, Anca-Luiza Alexe-Ionescu, and Andrei Th Ionescu
Mechanisms leading to fast relaxation of liquid crystal cells aligned with conductive polymers
JOURNAL OF APPLIED PHYSICS 108 (2010) 073519-1 – 073519-6

A.1.2 Publications on international journals accepted in 2010

1. Buonomenna MG, Golemme G, Choi S, Jansen J, De Santo MP, Drioli E
Surface skin layer formation and molecular separation properties of asymmetric PEEKWC membranes
Separation and purification Technology

2. E. Lacaze, A. Apicella, M. P. De Santo, D. Coursault, M. Alba, M. Goldmann and R. Barberi
Ordered interfaces for dual easy axes in liquid crystals
Soft Matter

B PUBLICATIONS ON CONFERENCE PROCEEDINGS

B.1 Publications on international conference proceedings in 2010

1. A. Aloise, G. Rotella, F. Ciuchi, F. Crea, D. Umbrello; Aloise, G. Rotella, F. Ciuchi, F. Crea, D. Umbrello
   White layer: alterazione micro strutturale"
   10° Convegno Nazionale AIMAT, Capo Vaticano (VV) 5 – 8 settembre 2010 IMPIEGO DI TECNICHE SPERIMENTALI PER L'ANALISI DELLA FORMAZIONE DI WHILE LAYER IN SEGUITO AL PROCESSO PER ASPORTAZIONE DI TRUCIOLO SU ACCIAI INDURITI (2010), Utensili ed attrezzature, Tecniche Nuove, Giugno 2010, Vol 3, pp54-56

2. D. Umbrello, F. Crea, F, Ciuchi
   Analisi Sperimentale dei Meccanismi di Formazione della White Layer durante i Processi per Asportazione di Truciolo su Acciai Induriti"
   Atti del 1° Congresso Nazionale del Coordinamento della Meccanica Italiana, 20-22 Giugno, 2010, Palermo, pp. 70-71. (lavoro completo su CD)

3. A. E. Vasdekis, J. G. Cuennet, W. Z. Song, J. W. Choi, L. De Sio, C. P. O'Neil, J. A. Hubbell, D. Psaltis
   Surface Optofluidics
   Proc. SPIE 7762, 776224 (2010)

C INVITED PRESENTATIONS

C.1 Invited presentations at international conferences in 2010

1. T. Scharf, J. Dintinger, H. Sellame, G. Mehl, G. Ungar, X. Zeng, C. Rockstuhl, S. Mühlig, T. Bürgi, A. Cunningham, L. De Sio, R. Caputo, V. Yannopapas, W. Meier, D. de Bruyn Ouboter, T. Schuster
   Self-organized bottom-up metamaterial based on spatially arranged nanoparticles: concepts and realizations
   4th International Congress on Advanced Electromagnetic Materials in Microwaves and Optics, Karlsruhe, Germany, Settembre 13-16 (2010).

D PRESENTATIONS AT CONFERENCES

D.1 Presentations at international conferences in 2010

1. M. Giarola, A. Sanson, A. Rahman, B. Rossi, M. Bettinelli, A. Speghini, E. Cavalli, E. Cazzanelli and G. Mariotto,
   Polarized Raman spectra of yttrium and lutethium orthophosphates: a comparison between experiments and simulation.
   XII International Workshop on Complex System, Andalo, Trento (Italy), 15-18 March 2010 Poster presentation.

2. M. Castriota, E. Cazzanelli, A. Fasanella, R.G. Agostino, T. Caruso and A.Policicchio,
   Raman Scattering Enhancement Associated to Sodium Oxide Formation after Thermal Treatment of Glass Substrates
   XXII International Conference on Raman Spectroscopy (ICORS 2010), 08/08 – 13/08/10 , Boston, MA, USA.

3. M. Giarola, A. Sanson, A. Rahman, M. Bettinelli, A. Speghini, E. Cazzanelli and G. Mariotto ,
   Vibrational Dynamics Of YPO_4 and $ScPO_4$ Single Crystals: An Integrated Study By Polarized Raman Scattering Experiments And Simulations
   XXII International Conference on Raman Spectroscopy (ICORS 2010), 08/08 – 13/08/10 , Boston, MA, USA.

4. Enzo Cazzanelli
   Spectroscopic techniques applied to the cultural heritage
   Oral presentation, invited, at the Department of Chemistry and Biochemistry, University of Tulsa, 17/08/10 Tulsa, Oklahoma, USA.

5. E. Cazzanelli, M. Castriota, D. Pacilè, L. Papagno, Çağlar O. Girit, Jannik C. Meyer, Alex Zettl and G. Mariotto,
   Raman spectral effects of edge disorder and strain distribution in monolayer graphene

Oral Presentation, CARBOMAT 2010, Workshop on Carbon-based low-dimensional Materials", 06/10 – 08/10/10 Catania, Italy.

6. E. Cazzanelli, M. Castriota, L. Caputi , A. Cupolillo, L. Papagno and G. Mariotto,
Linear carbon chains inside multiwalled carbon nanotubes and their temperature evolution, investigated by Raman spectroscopy
CARBOMAT 2010, Workshop on Carbon-based low-dimensional Materials", 06/10 – 08/10/10 Catania, Italy.

7. G. Cipparrone
Liquid crystal emulsions to explore optical tweezers based on polarization gradients (invited),
5th Italian Japanese Workshop on Liquid Crystals IJLC 2010, Cetraro (CS), July 6-9, 2010

8. M.G. Buonomenna, G.Golemme, A.Policicchio, F. Ciuchi, R.G. Agostino, A.Figoli
Novel mixed matrix membranes based on functionalised SBA-16 mesoporous oxide and a block copolymer of styrene and butadiene (SBS),
Oral presentation, Materials Chemistry 10 (MC10) 4 - 7 July 2011, University of Manchester, UK

9. M.G. Buonomenna, G. Golemme, E.Sardella, P.Favia, F.Ciuchi
Effects of synthesis parameters on SAPO-34 morphology and adsorption properties for CO2/CH4 separation
Oral presentation, Materials Chemistry 10 (MC10) 4 - 7 July 2011, University of Manchester, UK

10. R. Caputo, I. Trebisacce, L. De Sio and Cesare Umeton
Phase modulator behavior of a wedge-shaped POLICRYPS diffraction grating
9th Italian Liquid Crystal Society (SICL) National Meeting, Cetraro (CS), Italy, July 3-7, 2010.

11. L. De Sio, S. Ferjani, G. Strangi, C.P. Umeton, R. Bartolino
Universal Light Sculptured Soft Template For Photonic Applications: From All-Optical To Electrical Reconfigurability
9th Italian Liquid Crystal Society (SICL) National Meeting, Cetraro (CS), Italy, July 3-7 2010

OTHER PRESENTATIONS AND EVENTS

- INTESA SANPAOLO START UP INITIATIVE, 25/01-30/01/2010 MILANO,

- GREEN TECHNOLOGIES INVESTMENT FORUM, 11/02/2010 MILANO, organized by ASSOCIAZIONE IBAN (ITALIAN BUSINESS ANGELS NETWORK) and by SWEDISH BUSINESS REGION GOTEBORG AB

- TECHGARAGE CLEAN & GREEN, 26/03/2010 MILANO, organized by Associazione TechGarage, Politecnico di Milano, *Libera Università Internazionale degli Studi Sociali,* (LUISS) "Guido Gali" and dPixel

- Presently the project NOTREDAME has been selected among 20 innovative enterprises for the special incubation service center started at the University of Calabria , as planned in the project C.R.E.S.C.I.T.A."

PATENTS

C. Provenzano, P. Pagliusi, A. Mazzulla, G. Cipparrone,
"Metodo per la misura di proprietà chiro-ottiche in tempo reale basato su un reticolo di polarizzazione",
Italian Patent Office, CS2011A000003.

8 BIOMEDICAL PHYSICS

Area coordinator: L. Sportelli *(Molecular Biophysics Group)*

Professors and researchers: V. Carbone *(University of Calabria, Astrophysics Group)*
R. Guzzi *(University of Calabria, Molecular Biophysics Group)*
A. Santaniello *(Professore a contratto of Biomedical Physics)*

Post-Doc fellow: A. Vecchio *(University of Calabria, Astrophysics Group)*

Undergraduate students: I. Bonetti,, A. Curcio

Collaborators: G. Barca, R. Siciliano *(Azienda Ospedaliera di Cosenza, U. O. Fisica Sanitaria)*

Research subjects:
1. Dosimetry with new EPR-sensitive materials
2. Study of radiation effects in biomolecules
3. Transfer to medicine of theoretical models and methods

Introduction

The current research activities in Biomedical Physics concern:
1) dosimetry with novel materials for therapeutic applications at low doses,
2) modifications induced by irradiation in biomolecules,
3) analysis of complex biomedical data by means of proper orthogonal decomposition.

The investigation of the radio-induced radicals in newly developed materials expands the applicability of EPR-dosimetry to both fractionate-dose administration in conventional radiotherapy and special radiotherapeutic techniques. The low doses required by the former protocols and the high gradients present the latter approaches are, in several situations, too demanding for the current dosimetric devices, which have been designed and developed to satisfy the requirements of ordinary radiotherapy. Radio-physical applications to the biomedicine can take advantage from the high sensitivity, large spatial-sampling features and the lack of cables or housing materials of the EPR dosimeters, with a low perturbation of the sample/patient. This is guaranteed by an effective Z that can be modulated, from the average bodily value to those of its different tissue constituents, by a proper chose of the EPR-sensitive substance. More recent dosimetric materials involve sugars, dithionates and formates, among others. All of them show a higher sensitivity with respect to alanine, the EPR standard material. These materials can be modified by inclusion of paramagnetic species or isotope substitution in order to further increase low dose sensitivity below 1 Gy. We were concerned with studies of the EPR signal in Li formate irradiated with clinical and laboratory photon beams at doses in the therapeutic range. The signal was calibrated, and the effect of impurities and defects was investigated. A prototypal dosimeter was designed, to work in a phantom for beam characterisation.

The interpretation of modern medicine imaging and biomedical experiments requires the inspection and the analysis of large data sets often affected by noise, artefacts and redundancy. Algebraic treatments of the data simplify these operations and evidence details which would remain otherwise unrecognized. We make use of the proper orthogonal decomposition (POD) approach, which affords these goals by projecting the data onto a basis set derived from the data, in conjunction with an optimality criterion. No external assumptions on the data behaviour are required. POD is being applied to the analysis of cardiac magnetic resonance (CMR) images.

8.1 DOSIMETRY WITH NOVEL EPR-SENSITIVE MATERIALS

Therapeutic applications at low doses

Lithium formate monohydrate ($HCO_2Li \cdot H_2O$) was irradiated in the therapeutic dose range 0.5–150 Gy with photon beams from both a LINAC accelerator (energies of several MeV, dose rates of the order of several 10^{-2} Gy/min), and with orthovoltage beams from a laboratory equipment (X-ray irradiator, 100 keV, dose rates up to a Gy/min). The clinical irradiations were performed in collaboration with R. Siciliano and G. Barca of the AO of Cosenza. The EPR response as a function of the dose was used to build the calibration curve of pure formate, and compared for clinical and laboratory irradiations at the Molecular Biophysics Laboratory by R. Guzzi in collaboration with A. Santaniello. This was afforded as a precursor activity for the preclinical use of formate as a dosimeter for conformal beam radiotherapy (A. Curcio, Thesis in preparation). The investigation of $HCO_2Li \cdot H_2O$ modified by inclusion of paramagnetic species is under way.

8.2 STUDY OF RADIATION EFFECTS IN BIOMOLECULES

Dosimetric properties of HAp alginates

Hydroxyapatite (HAp) is a synthetic, biocompatible material, radiosensitive with respect to electron paramagnetic resonance. Biologically, it corresponds to the mineral constituent of bone and teeth, and has a relatively high effective Z value. We studied HAp alginates, in which nanograins of the radiosensitive species are embedded in a highly porous, low-Z alginate matrix. The composite material was synthesised according to the current methodologies by E. Marsich at the University of Trieste, for the purpose of biotechnological applications as osteoimplants and artificial organs. We irradiated HAp alginate scaffolds, i.e. self-sustained samples, with the orthovoltage irradiator in a wide dose interval, including therapeutic dose values. The scaffolds show an intense, stable EPR signal. The response of the pure HAp powder has been checked for comparison. HAp alginates result as feasible dosimetric materials and, in particular, are compatible with those applications in which both an intense signal and a low-density material is needed like, for instance, as lung substitutes and phantoms. Reports are in preparation.

Radioinduced modifications of carbohydrates

Foodstuff irradiation is a physical technology used to prevent the microbial deterioration and increase the shelf-life of several dietary products, according to national regulation, in several countries including Italy. The study of the radioinduced radicals in food is directly related to food dosimetry and quality assurance of irradiated aliments. A further issue in foodstuff irradiation concerns retrospective dosimetry, which may be easily implemented in case of accidents or other un-programmed exposures, given the all-pervasive presence of EPR-sensitive food, like carbohydrates, in normal households or even in working environments. Sugars show, in general, a multiple-radical spectrum, in which the single radical components present individual time-dependences, extending over time scales ranging from a few hours up to a few months. We started the study of the radioinduced modification in fructose and saccharose, in order to characterise the time dependence of the different radicals, and in particular of the stable component/components useful for dosimetry. The particular attention paid to food dosimetry triggers our interest towards the role played on the signal stability by humidity from the residual water content of the ambient atmosphere, the packaging, or the food preparation.

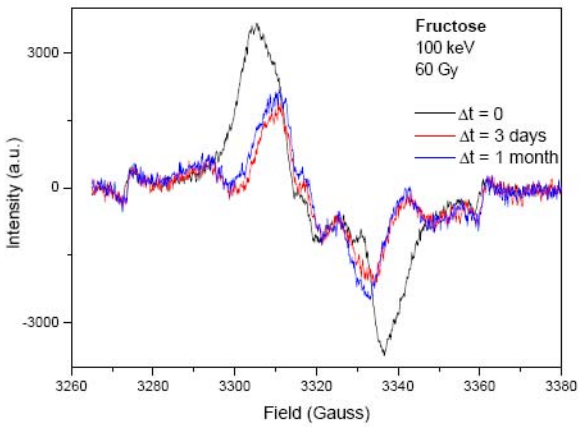


Fig. 1 Time dependence of the EPR signal in irradiated fructose. Several radioinduced components are visible, showing different temporal behaviours on the measured time scale: at least two quickly evolving features can be distinguished at about 3310 and 3337 gauss, and two slowly evolving components occur at about 3320 and 3330 gauss.

8.3 TRANSFER TO MEDICINE OF THEORETICAL MODELS AND METHODS

Proper Orthogonal Decomposition as a diagnostic technique in urology and cardiology

We analyzed data sets coming from spatial and temporal evolution of renal scintigraphy to investigate the reliability of the application of proper orthogonal decomposition (POD) in biomedical contexts.

Renal functionalities or pathologies are hardly recognized from the raw scintigraphic images and their identifications could depend on the subjective point of view of the operator. The proposed technique is able to distinguish independent events starting from a more complex phenomenon. The spatio-temporal fields, representing the radiation emitted by the radiopharmaceutical technetium-99m with mercaptoacetiltriglicin (MAG3) within the kidney, have been analyzed for six randomly selected patients. In particular our study was performed on four patients affected by renal pathologies while two scintigraphies refer to healthy patients. First of all POD represents an efficient filtering procedure to cut off noise from the raw images by only selecting the few most energetic modes. When healthy kidneys are analyzed, POD is able to separate the main processes taking place in the organ. When applied to pathological samples, POD underlines the regions of the organ interested by the troubles allowing to analyze them independently. This analysis can be complementary to the identification made by hand by the operator.

The physiologic and the pathologic behaviours of the left cardiac ventricle can be evidenced by POD analysis of the images of the beating heart obtained by cardiac magnetic resonance (CMR). In CMR the acquisition of the magnetic resonance signal is gated to the patient electrocardiogram. Hence, for a cardiac cycle with a constant rhythm, images of the myocardial spatio-temporal evolution within a heart beat are formed. The POD modes (eigenfunctions) reflect the functional and dysfunctional behaviours in the contraction-distension cycle as spatially stationary features, while the time dependent behaviour is captured by the POD eigenvalues. For instance, the first POD eigenfunction represents the average ventricular volume, and the corresponding eigenvalue describes the time-dependent volume variation, showing reduced systolic or diastolic intervals according to the occurring pathologies. A paper is in preparation.

A PUBLICATIONS ON SCIENTIFIC JOURNALS

A.1.2 Publications on international journals accepted in 2010

1. P. Veltri jr., A. Vecchio, V. Carbone,
   Proper Orthogonal Decomposition analysis of the spatio-temporal behavior of renal scintigraphies,
   Physica Medica (2010) 26, 57-70.

9. GEOPHYSICS

Professors and Researchers:	I. Guerra A. Gervasi (*Researcher from National Institute of Geophysics and Volcanology (INGV*)
PhD Student:	M. Anzidei
Postdoc fellows:	B. Orecchio
Collaborators:	A. Moretti (*Univ. of L'Aquila, L'Aquila, Italy*) G. Neri, D. Presti, and C. Totaro (*Univ. of Messina, Messina, Italy*) W.J. Kim, A. Lerner-Lam, L. Seeber, C. Stark and M. Steckler (*Lamont-Doherty Observatorv, Columbia Univ., New York, USA*) V. Carbone, A. Vecchio, P. Veltri, G. Zimbardo *(Calabria Univ., Arcavacata, Italy)* L. Sorriso-Valvo *(LICRYL, INFN/CNR, Cosenza)* S. D'Amico *(Department of Earth and Atmospheric Sciences, Saint Louis University, St. Louis, MO, USA; now at Physics Department, University of Malta)* A. Benini (*archaeologist*) G. Corrado and A. Albano (*Federico II University, Neaples, Italy*) C. Faccenna, A. Billi, L. Minelli (*RomaTre University*)
Institutional scientific agreements:	*National Institute of Geophysics and Volcanology (Rome)* *Lamont-Doherty Earth Observatory (Palisades, New York, USA)*

RESEARCH LINES

Introduction

In spite of its lean composition, the Geophysics Research Group is engaged in many lines of activity. In most cases this is due to the nature of its activities, based on the elaboration of experimental data collected by means of observations that have to be carried on over long span of time. The group indeed was established about thirty years ago in a department different from Physics with the explicit finality of answering the requirement of seismological observations in Calabria, a region characterized by a seismic risk among the highest in the Mediterranean Basin. This origin is still conditioning its programs, mainly of observational nature.

Due to the relatively great distance from the nearest centres of geophysical research and the relevance of the geodynamical problems arising from the features of the territory, the group at the Department of Physics is a reference point for both researchers, from abroad too, as well as some public administrations.

9.1 Seismotectonics

Seismotectonics is the branch of seismology that deals with the complex relations between earthquakes and geological structures and with the reconstruction of the ongoing dynamical processes. It is based on the accurate location of the seismic sources, that in turn requires a model as more realistic as possible for the elastic waves propagation in the studied area. Generally, an iterative process is performed: new seismographic data help to better constrain the velocity model that in turn leads to better locations. The maps of seismicity resulting from the above mentioned activity is then correlated to the tectonic features observed in the area. In particular the space distribution of the seismic foci can trace the position of the slip surfaces at depths not accessible to direct observation, while the propagation model includes the mechanical discontinuities met with by seismic waves along their path to the seismic stations. Seismograms contain further information that allows for determining the dynamics of the phenomena at the seismic sources. The reconstruction of the geometry of the geological bodies and their present kinematics is the result of these research activities.

Accurate seismotectonic investigations are essential in Calabria because of the peculiarity of seismic activity in the region. The area hosted in fact most of the largest earthquakes reported in Italy in historical times. However it had been practically quiescent since 1908. Moreover the adjacent Tyrrhenian Sea is the seat of deep earthquakes attributable to the interaction of the Eurasian and African plates, that represents one of the more interesting geodynamical problems in the Mediterranean

area. Therefore the monitoring of the local seismicity and its relation to the tectonic features is an important task for the scientific investigation devoted to the seismic risk assessment.

In this frame, most of the daily effort of the research group is dedicated to the management of the Calabrian Regional Seismic Network. This network has the dual role of providing an almost real time monitoring of the area and of incrementing the available waveform data bank. The first is useful in civil protection tasks, the collected information being sent to National Institute of Geophysics and Volcanology, Rome (INGV); the second is the basic instrument to conduct seismotectonic investigations.

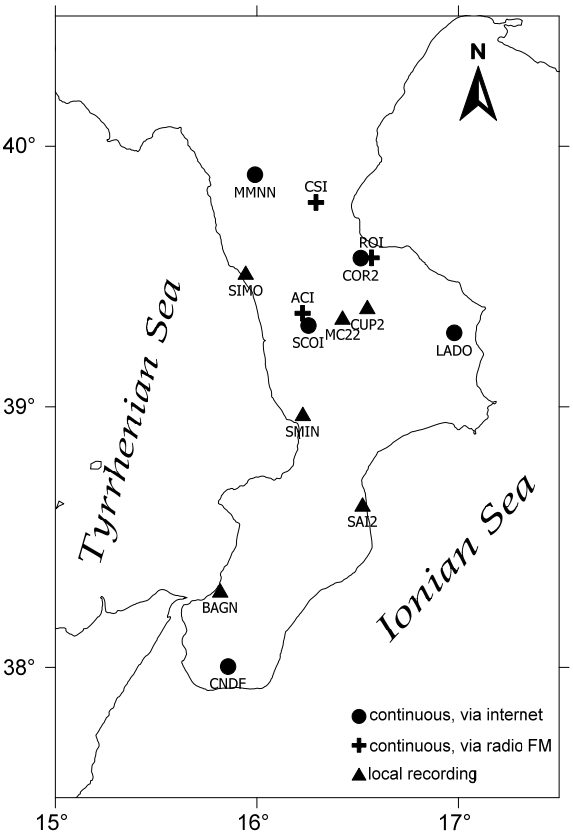


Fig.

In 2010 continued the efforts in the reorganization of the permanent Calabria Seismic Network. In the frame of the cooperation with INGV, seismic signal from seismic stations MMN and LADO are sent in real time to the national center for the seismic monitoring in Rome.
Among the results of the activity are the tests of several sites and the installation of two new stations at Condofuri (Southern Calabria) and Corigliano (Northern Calabria). The present state of the permanent seismic network is represented in fig. 1.
A special effort has been devoted to the monitoring of the local seismicity at Mormanno, a village at the north-western boundary of Calabria. Here a microseismic sequence started in September 2010, characterized by numerous earthquakes of very low energy. However their locations and focal depths are such that they are often felt by the inhabitants. A similar sequence started in December 1973 and provoked lights and diffuse damage to the buildings. In such a situation the Geophysical Group started a detailed study of the phenomenon both for scientific purposes and to answer to the request of information coming from the population. Six temporary seismometers have been installed in order to monitoring the space-time evolution of the seismic activity. Two of them are equipped with so-called "Tromino®" (www.tromino.it), instruments not properly created for seismic monitoring. They have been utilized in order to test their capability and efficiency in reveal and adequately record seismic events.
During 2010, following a research started in 2009, the Geophysical Group estimated a new 3D P-wave velocity model of crust and upper lithosphere for the Calabrian Arc region (Orecchio et al., in press). The model results from integration of all seismic velocity data available in the literature and coming from different kind of methods and analyses. The integration procedure we defined allowed us to obtain an average P-wave velocity model of the Calabrian Arc lithosphere clearly showing the first-order structural features of the area. It has the advantage to represent the simplest velocity structure consistent with all published data and therefore also an important constrain for the interpretation of the complex puzzling of

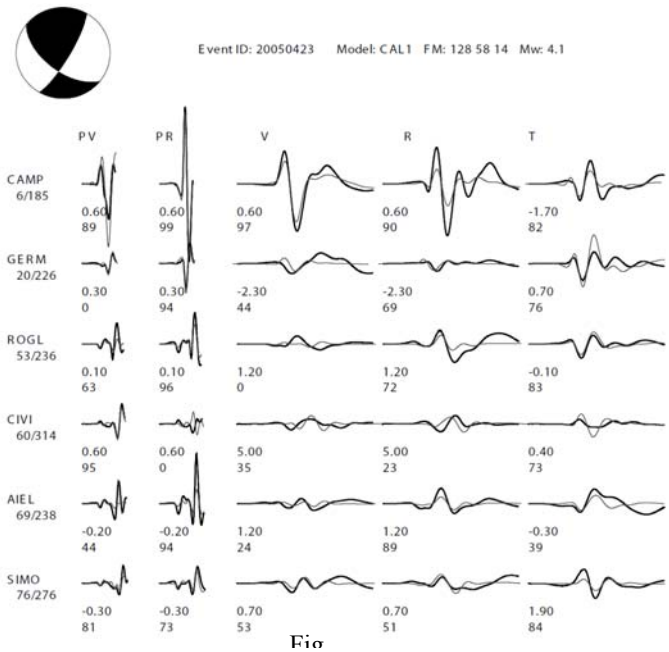


Fig.

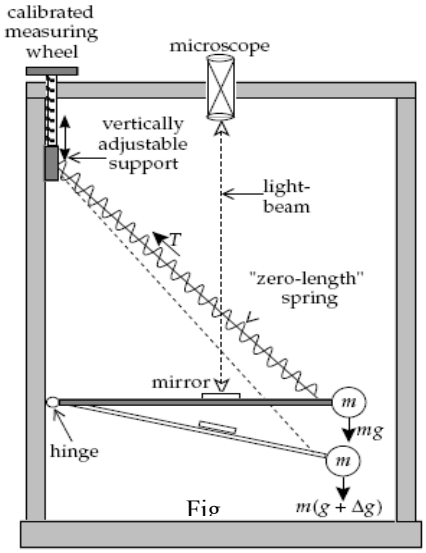
lithospheric units in the region. Moreover, with our procedure the 3D velocity model may be improved as new useful measurements will be achieve so representing a basic knowledge that can be easily extended and updated. Finally, the use of this "a-priori" model as starting velocity model in a new P-wave tomographic inversion of shallow earthquakes led to a significant improvement of hypocenter location and highlighted the relationships between the deep dynamics (related to the Ionian subduction slab) and the shallower processes occurring at crustal depths.

In the frame of a scientific cooperation with the Department of Earth and Atmospheric Sciences of the Saint Louis University we performed during 2010 a methodological study (D'Amico et al., in press) aimed to test the efficiency and stability of the "Cut And Paste" (CAP) technique for the moment tensor inversion of low-to-moderate earthquakes. As already said the Calabrian region has been interested in the last decades by moderate energy seismicity with just a few events having magnitude above 5. Therefore it clearly appears the relevance of identifying tools really capable to adequately investigate the kinematics of such low energy events. The CAP technique allows the determination of the source depth, moment magnitude and focal mechanisms using a grid search technique that identify the parameters furnishing the best agreement between the real waveforms and the synthetic ones (see an example in Fig.2).
We are now working to apply these techniques to the earthquakes of magnitude greater than 2.5 occurred in Calabria in the last decades. In particular we are following two lines of research: 1) the first devoted to study crustal earthquakes that will furnish useful information on location and kinematics of the most active seismic sources and also on the regional stress and strain fields; 2) the latter oriented to investigate intermediate and deep earthquakes that will help to better understand the state of stress of the Ionian slab and more generally the state of the whole subduction process.

9.2 Geodesy
Ground deformations is the geophysical phenomenon more frequently associated to the seismic activity in its various stages. It is detected by successive or continuous measurements of the coordinates of reference points (benchmarks). Both classical, optical and modern, GPS techniques can be applied.
In 2010 the Geophysical Group continued in caring the operation of the nine GPS sites installed in 2006 along the transect Cetraro-Crotone in the framework of the cooperation with the Lamont-Doherty Earth Observatory of the Columbia University (LDEO). During this year a new GPS site has also been added in Paola (PAOA) in order to better monitoring the movement of the Tyrrhenian coast of Calabria.

After about 3 years of recordings, the data became adequate for preliminary elaborations. For this sake we implemented in our laboratory and properly calibrated for our data the package GAMIT/GLOBK, the software developed by Bob King at the *Department of Earth Atmospheric and Planetary Sciences* of the Massachusetts Institute of Technology for GPS data analyses.
The preliminary elaborations evidenced a quite coherent movement of the GPS sites in Northern Calabria towards NNW with respect to an "Eurasia-fixed" reference frame.
We are now working in cooperation with the geologic team of the University RomaTre in Rome in order to properly frame the GPS evidences in the local geologic/seismotectonic scenario. Moreover thanks to the experience of Dr. M. Anzidei (newly acquired member of our Group) we are also deepening the investigation concerning the subsidence by means of marine archaeological data.

9.3 Micro-gravimetry
Gravimetry is the branch of Geophysics aimed to describe and utilize the Earth's gravity field both for scientific and commercial purposes. The values of the gravity acceleration (g) measured near its surface differ from those corresponding to any simple model that represents the Earth as a homogeneous rotating body, due to the real inhomogeneous density distribution of materials inside our planet. The differences between the measured values of g and the theoretical ones (the so-called *gravity anomalies*) are currently used to infer information about the geometry and nature of buried rocky bodies.
Relative motions of the Earth with respect to Moon and Sun are the origin of continuous perturbations of g in any point at the Earth surface. Modern



Fig

micro-gravimeters (fig. 3) are able to record temporal variations of the order of 10^{-8} *g*. The well-known sea-tides are their most evident consequence, but the solid part of the Earth undergoes deformations like the surface of the oceans, obviously of much smaller entity.
It is possible to study these perturbations by recording the *g*-values and the correspondingly variable inclination of the ground. It is generally believed that, due to the periodic character of the tidal phenomena, a set of observations spanned several years should be sufficient to build a mathematical model of the behaviour of a given site. These models may be useful for studying the elastic properties of the lithosphere at a regional scale and theis relationship to the structural and geodynamical context.
Microgravimetric data can be used for calculating the corrections to be applied to the observed *g*-values when they are measured during very detailed surveys, like those performed searching for underground voids, for example with archaeological purposes; for checking possible correlations among gravity variations and geodynamic phenomena; etc. Micro-gravimeters are also able to record the free oscillations of the Earth excited by the biggest earthquakes: these phenomena provides therefore for information about the elastic behaviour of the whole planetary body.

A new collaboration started in 2010 with a research-group of the University of Naples. An agreement has been signed in this frame with the Cosenza municipality and in early 2011 a micro-gravimetric and tiltmetric station will be installed in the medieval castle of the city, by using instruments made available from Naples University (La Coste & Romberg .gravimeter, mod. G; biaxial tiltmeter Applied Geomechanics mod. 712).

9.4 Dissemination and diffusion of scientific culture
Noteworthy efforts are dedicated to the diffusion of the geophysical culture, in the attempt of convincing the general public and future university students which too much frequently attribute the seismology to scientific field different from physics.
The Geophysics Laboratory is open to school visits and a set of demonstration tools is available to make seismology understandable and appealing. Every year it is visited by hundreds of pre-university scholars.
A program (ReSiSCal, Rete Sismica Scolastica Calabrese = Scholastic Calabrian Seismic Network) is underway. It is leading to the installation of a seismic network in about ten schools in the whole Calabria. From the instrumental point of view, the collected data are qualitatively equivalent to those from stations activated with purely scientific purposes.
In the framework of cooperations with Scholastic Institutes we have also cooperated with the Liceo Scientifico "G. B. Scorza" for the installation of a complete meteorological station and for developing the software interface necessary to publish the measurements in real time on a properly created web-page. After a test period the web page will be made accessible (probably at the beginning of 2011) in the home page of the municipality of Cosenza.

Concerning the dissemination of scientific progresses among the same scientific community the Geophysical Group has also cooperated with LDEO and INGV in order to organize the 35th Workshop of the International School of Geophysics focused on "Non-Steady-State Subduction: Changes in the Calabrian Arc and its Mediterranean Setting" that has been hold in Erice during October 2010.

A PUBLICATIONS ON SCIENTIFIC JOURNALS

A.1 Publications on international journals

1. Anzidei M., Esposito A., 2010:
Lake Albano: bathymetry and level changes.
In *The Colli Albani Volcano*, London Geological Society, 229-244.

2. Anzidei M., Riguzzi F., Stramondo S., 2010:
Current geodetic deformation of the Colli Albani volcano: a review.
In *The Colli Albani Volcano*, London Geological Society, 299-310

3. Anzidei M., Antonioli F., Lambeck K., Benini A., Soussi M., Lakhdar R., 2010:
New insights on the relative sea level change during Holocene along the coasts of Tunisia and western Libya from archaeological and geomorphological markers.
Quaternary International, vol. 232, 5-12.

4. Anzidei M., Antonioli F., Benini A., Lambeck K., Sivan D., Serpelloni E., Stocchi P., 2010
Sea level change and vertical land movements since the last two millennia along the coasts of southwestern Turkey and Israel.
Quaternary International, vol. 232, 13-20.

5. Anzidei M., Kurt L., Antonioli F., Ferranti L., Leoni G., Scicchitano G., Silenzi S., 2010:
Sea level change along the Italian coast during the Holocene and projections for the future.
Quaternary International, vol. 232, 250-257.

6. Billi A., Presti D., Orecchio B., Faccenna C., Neri G., 2010:
Incipient extension along the active convergent margin of Nubia in Sicily, Italy: Cefalù-Etna seismic zone, Tectonics**,** 29, TC4026, doi:10.1029/2009TC002559.

7. Billi A., Minelli L., Orecchio B., Presti D., 2010:
Constraints to the Cause of Three Historical Tsunamis (1908, 1783, and 1693) in the Messina Straits Region, Sicily, Southern Italy,
Seismological Research Letters**,** 81, 6, 907-915, doi: 10.1785/gssrl.81.6.907.

8. D'Amico S., Orecchio B., Presti D., Zhu L., Herrmann R., Neri G., 2010:
Broadband waveform inversion of moderate earthquakes in the Messina Straits, southern Italy,
Physics of the Earth and Planetary Interiors**,** 179, 97–106.

9. D'Amico S., Orecchio B., Presti D., Gervasi A., Zhu L., Guerra I., Neri G., Herrmann R., 2010:
Testing the stability of moment tensor solutions for small earthquakes in the Calabro-Peloritan arc region (southern Italy).
Bollettino di Geofisica Teorica ed Applicata, in press.

10. Ferranti L., Antonioni F., Anzidei M., Monaco C., Stocchi P., 2010:
The timescale and spatial extent of vertical tectonic motions in Italy: insights from relative sea-level changes studies.
Journal of the Virtual Explorer, vol. 36, 1-34.

11. Orecchio B., Presti D., Totaro C., Guerra I., Neri G., 2010:
Imaging the velocity structure of the Calabrian Arc region (South Italy) through the integration of different seismological data. Bollettino di Geofisica Teorica ed Applicata, in press.

D PRESENTATIONS AT CONFERENCES

D.1 Presentations at international conferences in 2010

1. D'Amico S., Orecchio B., Presti D., Gervasi A., Guerra I., Neri, G., Zhu L., Herrmann R.B., 2010:
   Broadband Source Mechanism Modeling Of Recent Earthquakes in Calabria, Southern Italy.
   Seismological Research Letters, vol. 81, 2, 372

2. Orecchio B., Presti D., Totaro C., Guerra I., Neri G.,
   P-wave tomography of the Calabrian Arc region (South Italy) using a new "a priori" three-dimensional velocity model. European Geosciences Union (EGU) General Assembly, (Vienna, May 2-7, 2010).

3. Orecchio B.,
   Velocity models and stress fields in the Calabrian Arc region,
   35th Workshop of the International School of Geophysics "*Non-Steady-State Subduction: Changes in the Calabrian Arc and its Mediterranean Setting*" (Erice, Sicily, 3-8 October, 2010).

4. D'Amico S.,
   Earthquake moment tensors,
   35th Workshop of the International School of Geophysics "*Non-Steady-State Subduction: Changes in the Calabrian Arc and its Mediterranean Setting*" (Erice, Sicily, 3-8 October, 2010).

D.2 Presentations at national conferences in 2010

1. D'Amico S., Orecchio B., Presti D., Gervasi A., Zhu L., Guerra I., Neri G., Herrmann R. B.:
   Moment tensor solutions by the "Cat and Paste" method in the Calabrian Arc region (Southern Italy)
   29th Conv. Ann. Gr. Naz. Geofis. Terra Solida, Prato, October 26-28, 2010, pp. 44-45.