

# ANNUAL REPORT 2004

*ACADEMIC YEAR 2003-2004*

*Scientific publications in 2004*

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## Introduzione

Sono ormai quasi venti anni che il Dipartimento di Fisica dell'Università della Calabria, prepara e distribuisce il suo rapporto di attività annuale. La prima edizione risale all'anno accademico 1986/87 ed era stata prodotta con una stampante ad aghi e successivamente fotocopiata e spillata nella segreteria del dipartimento. Per la prima volta quest'anno il rapporto di attività nella parte scientifica è stato redatto in inglese, per facilitarne la diffusione anche tra i centri di ricerca internazionali.

Riguardando i rapporti anno per anno è possibile farsi un'idea di quanto e come il dipartimento di fisica sia cambiato in questo periodo. A parte alcune fluttuazioni c'è un chiaro trend di crescita, del dipartimento sia in termini di personale che di pubblicazioni: il personale di ruolo è passato dalle 25 unità del 1987 alle 46 unità del 2004, ma accanto al personale di ruolo sono progressivamente comparsi, prima un consistente numero di dottorandi (dalle poche unità del 1997, fino alle 30 unità del 2004) poi un altrettanto consistente numero di assegnisti e borsisti post-doc (dalle poche unità degli anni tra il 1990 ed il 1999, fino alle 17 unità del 2004).

Oggi il dipartimento di fisica rappresenta una consistente realtà nel panorama della ricerca nazionale ed internazionale, con settori che, anche dal punto di vista della massa critica di ricercatori, hanno ormai raggiunto una notevole visibilità. All'interno del dipartimento gruppi di ricerca di assoluto rilievo internazionale sia dal punto di vista quantitativo che qualitativo, sono presenti nei campi della fisica molecolare ed in particolare dei cristalli liquidi, della fisica dei plasmi con particolare riguardo allo studio della corona solare e del mezzo interplanetario, della fisica delle alte energie, della fisica delle superfici. Ognuno di questi gruppi ha al suo attivo progetti che hanno ottenuto chiari riconoscimenti, sia nazionali che internazionali. In entrambe le tornate del bando ministeriale COFINLAB, destinato al finanziamento di centri di ricerca di eccellenza, il dipartimento di fisica è stato presente con successo: nella prima tornata è, infatti, stato finanziato il *Centro di Eccellenza per il Calcolo ad Alte Prestazioni*, cui ha contribuito in maniera determinante il gruppo di plasmi astrofisici, nella seconda tornata è invece stato finanziato il *Centro di eccellenza per la Preparazione ed il Trattamento di Materiali a struttura organizzata su scala nanometrica per applicazioni in fotonica, optoelettronica, trasformazioni e separazioni* nella realizzazione del quale ha un ruolo primario il gruppo di cristalli liquidi. Il gruppo di fisica delle Alte Energie è direttamente coinvolto nel progetto internazionale ATLAS, destinato a realizzare uno strumento da installare all'interno del *Large Hadron Collider* per rivelare il bosone di Higgs. Nell'ambito di questo progetto, nei laboratori del dipartimento di fisica sono stati realizzati i 35.000 tubi a deriva necessari alla costruzione delle camere di precisione di uno spettrometro a muoni.

Del resto il numero di pubblicazioni su riviste internazionali, dedotte dai precedenti rapporti di attività, non ha cessato di crescere dalle poche decine degli anni '80, fino alle circa 100 negli ultimi anni, mostrando che la crescita del dipartimento in termini di personale è stata accompagnata da una crescita ancora più accentuata in termini di produttività scientifica.

Gli anni che ci si prospettano debbono essere quelli del consolidamento dei risultati raggiunti e questo obiettivo richiederà lo sforzo concorde e convinto di tutto il personale del dipartimento, sforzo che, ne sono certo, sarà consapevolmente realizzato, superando in un'ottica di sviluppo e di crescita comune i problemi legati alla definizione di criteri equi ed efficaci di distribuzione delle risorse.

**Tabella: evoluzione del personale e delle pubblicazioni del dipartimento dal 1987 al 2004**

Anno	Ordinari	Associati	Ricercatori	Assegnisti Post-Doc	Dottorandi	Publicazioni
						su Riviste Internazionali
1987	5	14	6		3	20
1988	5	16	6		3	26
1989	5	15	6	3	6	21
1990	5	15	6	3	9	76
1991	5	14	10	2	10	53
1992	5	12	11	2	11	46
1993	4	17	10	2	12	52
1994	4	17	10	2	15	41
1995	5	16	12	2	11	57
1996	6	14	12		19	62
1997	6	14	12		19	63
1998	6	14	13		18	53
1999	6	14	13		19	66
2000	8	18	9	11	24	80
2001	11	19	5	12	19	92
2002						83
2003	12	20	11	11	35	103
2004	12	19	13	17	30	89

Arcavacata di Rende, 29 dicembre 2005

Il direttore del dipartimento  
(prof. Pierluigi VELTRI)

## **DEPARTMENTAL ADMINISTRATION**

### **Head of Department:**

Pierluigi VELTRI

### **Executive Board:**

Elio COLAVITA, Giancarlo SUSINNO,  
Alessandro PAPA, Cesare UMETON, Luigi  
PAPAGNO, Ignazio GUERRA, Assunta  
BONANNO, Nicola SCARAMUZZA

### **Department Council:**

12 Full Professors  
18 Associate Professors  
13 Senior Researchers  
8 Representatives of PhD students  
9 Representatives of the Technical and  
Administrative Staff

### **Administrative Secretary:**

Giocondo PERRI

## RESEARCH PERMANENT STAFF

### Full Professors

1. Roberto BARTOLINO *FIS07*
2. Lev BLINOV *FIS03*
3. Gaetano CANNELLI *FIS01*
4. Elio COLAVITA *FIS07*
5. Giovanni FALCONE *FIS01*
6. Ignazio GUERRA *GEO10*
7. Antonino OLIVA *FIS01*
8. Luigi PAPAGNO *FIS01*
9. Luigi SPORTELLI *FIS07*
10. Giancarlo SUSINNO *FIS01*
11. Cesare UMETON *FIS01*
12. Pierluigi VELTRI *FIS03*

### Associate Professors

1. Renzo ALZETTA *FIS02*
2. Riccardo BARBERI *FIS07*
3. Orazio BARRA *FIS01*
4. Assunta BONANNO *FIS01*
5. Lorenzo CAPUTI *FIS01*
6. Vincenzo CARBONE *FIS03*
7. Enzo CAZZANELLI *FIS03*
8. Gabriella CIPPARRONE *FIS03*
9. Gennaro CHIARELLO *FIS07*
10. Giovanni CROSETTI *FIS01*
11. Roberto FIORE *FIS02*
12. Laura LA ROTONDA *FIS01*
13. Francesco MALARA *FIS01*
14. Francesco PIPERNO *FIS03*
15. Nicola SCARAMUZZA *FIS07*
16. Marco SCHIOPPA *FIS01*
17. Carlo VERSACE *FIS01*
18. Galileo VIOLINI *FIS02*
19. Gaetano ZIMBARDO *FIS06*

### Senior Researchers

1. Rosa BARTUCCI *FIS07*
2. Michele CAMARCA *FIS01*
3. Marcella CAPUA *FIS01*
4. Maria DE SANTO *FIS07*
5. Vincenzo FORMOSO *FIS01*
6. Domenico GIULIANO *FIS02*
7. Rita GUZZI *FIS07*
8. Alessandro PAPA *FIS02*
9. Francesco PLASTINA
10. Leonardo PRIMAVERA *FIS05*
11. Pierfrancesco RICCARDI
12. Giuseppe STRANGI *FIS07*
13. Fang XU *FIS01*

## POST-DOCTORAL RESEARCH FELLOWS

1. Vincenzo BRUNO

2. Tommaso CARUSO
3. Francesca CASTROVILLARI
4. Federica CIUCHI
5. Antonella GRECO
6. Giuseppe LIBERTI
7. Anna MASTROBERARDINO
8. Daniela PACILÈ
9. Pasquale PAGLIUSI
10. Antonello SINDONA
11. Luca SORRISO-VALVO
12. Bruno RIZZUTI
13. Fabio LEPRETI
14. Donatella MARMOTTINI
15. Pasquale BARONE
16. Bruno ZAPPONE
17. Domenico DI GIACOMO

## PhD STUDENTS

### (XVI Cycle)

1. Roberto CAPUTO
2. Antonio DE LUCA
3. Enrico MACCALLINI
4. Evelin MEONI
5. Marco ONOFRI
6. Manuela PANTUSA
7. Andrea STIRPE
8. Francesco VALENTINI

### (XVII Cycle)

1. Cristina ADORISIO
2. Giuseppe AVOLIO
3. Rosita DE BARTOLO
4. Guido GUERINI
5. Antonio VECCHIO
6. Alessandro VELTRI
7. Paolo VETRÒ
8. Federico Pasquale ZEMA

### (XVIII Cycle)

1. Pietro GIUDICE
2. Giuseppina NIGRO
3. Francesco CAPORALE
4. Rosa ZAFFINO
5. Marco PAPAGNO
6. Adalisa TALLARICO
7. Maria Francesca DE FRANCESCHIS
8. Giuseppe AUDDINO
9. Gianluigi FILIPPELLI

### (XIX Cycle)

1. Comisso Mario
2. Apollaro Tony
3. Servidio Sergio
4. Giallombardo Claudia
5. Policicchio Antonio



**REGIONAL GRANTS**

1. Angela TUCCI

## TECHNICAL AND ADMINISTRATIVE STAFF

### Administration

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

### Secretary

5. Luigina DE ROSE
6. Luigi PARISE

### Teaching Laboratories

7. Mario LOMBARDI
8. Giovanni VIAPIANA (*Person in charge*)

### Computer Staff

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

### Research Laboratories

#### *Molecular Physics and Biophysics*

11. Bruno DE NARDO (*Person in charge*)
12. Carmine PRETE

#### *Ion-Matter Interaction and Surface Electronic Spectroscopy*

13. Eugenio LI PRETI (*Person in charge*)
14. Vito FABIO

#### *Elementary Particles*

15. Francesco SCIOMMARELLA
16. Francesco PELLEGRINO

#### *Geophysics*

17. Gerolamo LATORRE
18. Francesca SIRENA

The Physics Department hosts a INFN Section with the following staff:

- Sonia VIVONA (*Administrative Official - INFN*)  
Antonio BOZZARELLO (*Administrative Collaborator*)

### Department phonebook

(for calls from outside the Department, dial first (+39)-0984-49)

INTERNET: @FIS.UNICAL.IT

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ALZETTA Renzo	6028	PECORA Gaspare	6005
BARBERI Riccardo	6118-6150	PELLEGRINO Francesco	6102-6098
BARRA Orazio	6171	PERRI Giocondo	6004
BARTOLINO Roberto	6122	PIPERNO Franco	6058
BARTUCCI Rosina	6074-6073	PRETE Carmine	6142
BLINOV Lev	6124	PRIMAVERA Leonardo	6138
BONANNO Assunta	6170-6178	SCARAMUZZA Nicola	6113-6151
BOZZARELLO Antonio	6008	SCHIOPPA Marco	6017-6104
CAMARCA Michele	6172-6178	SCIOMMARELLA Francesco	6011
CANNELLI Gaetano	6155	SIRENA Francesca	3664
CAPUA Marcella	6022	SPORTELLI Luigi	6076-6073
CAPUTI Lorenzo	6154-6173	STABILE Fedele	6027
CARBONE Vincenzo	6131-6033	STRANGI Giuseppe	6120
CAZZANELLI Enzo	6114-6142	SUSINNO Giancarlo	6016-6104
CHIARELLO Gennaro	6157-6174	UMETON Cesare	6117-6152
CIPPARRONE Gabriella	6115-6148	VELTRI Pierluigi	6136-6033
COLAVITA Elio	6156-6174	VERSACE Carlo	6116-6147
CROSETTI Giovanni	6021	VIAPIANA Giovanni	6053
DE NARDO Bruno	6111-6106	VIOLINI Galileo	6024
DE ROSE Luigina	6001	VIVONA Sonia	6007
DE SANTO Maria Penelope	6150	XU Fang	6168-6178
FABIO Vito	6076-6166	ZIMBARDO Gaetano	6134-6033
FALCONE Giovanni	6057		
IORE Roberto	6018		
FORMOSO Vincenzo	6161		
GIULIANO Domenico	6025	<i>Network and Computer Service</i>	6035
GUARRACINO Nicola	6030	<i>Medical Physics Lab.</i>	6068
GUERRA Ignazio	3166	<i>Astrophysical Plasmas Computer Lab.</i>	6033
GUZZI Rita	6077-6073	<i>Ion-Matter Interaction Lab.</i>	6178
LA ROTONDA Laura	6014-6102	<i>Electronic Spectroscopy Lab.</i>	6174
LAMANNA Ernesto	6020-6103	<i>Biophysics Lab.</i>	6073
LATORRE Gerolamo	3664	<i>Molecular Physics Lab.</i>	6151
LI PRETI Eugenio	6179-6165	<i>Particle Physics Lab.</i>	6104
LOMBARDI Mario	6083	<i>Optics Lab.</i>	6152
MAIDA Lidia	6006	<i>Mechanical Workshop</i>	6006
MALARA Francesco	6135-6033		
OLIVA Antonino	6167-6178		
PAPA Alessandro	6015		
PAPAGNO Luigi	6158-6174		
PARISE Luigi	6002		

## SEMINARS (2004)

*January 22*

D.ssa Anna Cupolillo, Dipartimento di Fisica, Università della Calabria, *Dissociazione ed ossidazione della molecola di CO indotta da atomi di sodio depositati su una superficie di Nichel (111)*

*January 26*

Prof. Philippe Barois, *Structural studies of chiral and non chiral smectic phases by resonant scattering of x-rays*

*January 29*

Dr. Enrico Maccallini, *Nanotubi a base di carbonio: proprietà elettroniche ed applicazioni future*

*February 4*

Prof. Fabio Reale, *Coronal Loop Modeling*

*February 5*

Dott.ssa Donatella Marmottini, *Large  $N_C$  strongly coupled lattice QCD*

*February 19*

Prof. Arturo Tagliacozzo, *Aspetti generali della Superconduttività*

*February 23*

Dr. Pasquale Federico Zema, *Introduzione alla Gestione di un Sistema Operativo GNU/Linux*

*March 11*

Prof. Sergio Bertolucci, *I Laboratori Nazionali di Frascati: stato e prospettive*

*March 31*

Prof. Andre Mangeney, *Turbolenza nella magnetoguaia*

*April 1*

Prof. Alain Noullez, *Metodi numerici lagrangiani per il trasporto turbolento*

*April 18*

Proff. Emil S. Barna e Andrei Th. Ionescu, Facoltà di Fisica, Università di Bucarest, *Delocalized  $p$  electrons and physico-chemistry of liquid crystals*

*May 10*

Dr. V. Magas, *Off mass shell dual amplitude and DIS structure function*

*June 10*

Prof. Claudio FURETTA, Roma "La Sapienza", *Caratteristiche, proprietà ed applicazioni della dosimetria a termoluminescenza ()*

*June 17*

Prof. D. Marsh Max-Planck-Institut für Biophysikalische Chemie Gottingen, Germany, *Perspectives on Lipid-Protein Interactions from Crystal Structures and Magnetic Resonance*

*July 9*

Prof. Gaetano Assanto, Fac. di Ing. Roma3, *Propagazione guidata nei Cristalli Liquidi: stato dell'arte,*

*September 9*

Prof. A.B. Kaidalov, *Theoretical problems and models of high energy interactions*

*October 7*

Prof. A. Noullez , "*Fast divide and conquer methods for numerical simulations*"

*October 12*

Prof. Ettore Salusti, *Fisica del Mar Mediterraneo*

*October 13*

Prof. Alexander G. Petrov, Bulgarian Academy of Science , *Introduction to Soft Matter Physics*

*October 14*

Dr. Alessandro de Martino , *Quantum Transport in Carbon Nanotubes*.

*October 15*

Prof. Ettore Salusti, *Lo Stretto di Messina: Un interessante laboratorio*

*October 15*

Prof. Alexander G. Petrov, Bulgarian Academy of Science, *Generalized Molecular Asymmetry Concept in Soft Matter*

*October 15*

Dr. Alessandro de Martino , *Superconductivity in Carbon Nanotube Ropes*.

*October 16*

Prof. Ettore Salusti, *Vorticità potenziali*

*October 16*

Prof. B. Ginatempo, Università di Messina, *Didattica della Fisica con le nuove tecnologie: Il progetto IMF*

*October 16*

Prof. Alexander G. Petrov, Bulgarian Academy of Science , *Liquid Crystal Physics and the Physics of Living Matter*

*November 18*

Prof. Gesualdo Delfino, *Teorie di campo integrabili e fenomeni critici*

*October 28*

Prof. D. Marsh, *Interaction of lipids with beta-barrel membrane proteins: spin-label ESR and Infrared ATR spectroscopy*.

*December 7*

Prof. Eduard Kuraev, *Feynman rules for effective Regge action*

## **LAUREA THESIS' IN 2004**

*May 7*

Gianfranco DESUMMA

*Contributo alla carta magnetica della Calabria: rilievi nel graben di Catanzaro.*

Relatore: Prof. Ignazio GUERRA

Carmelina DE ROSE

*Fasi convertite da terremoti intermedi e profondi del Basso Tirreno.*

Relatore: Prof. Ignazio GUERRA

Simona TUNDIS

*Contributo alla carta magnetica della Calabria: rilievi nel settore centro-settentrionale della Catena Costiera.*

Relatore: Prof. Ignazio GUERRA

May 20

Daniela SALVATORE

*Le camere a deriva MDT per lo spettrometro a muoni dell'esperimento ATLAS: caratteristiche ed effetti sistematici nella determinazione della relazione spazio-tempo dall'analisi dei dati su fascio.*

Relatore: Prof. Giancarlo SUSINNO

Sarah Anna RUDI

*Misure di Radon disciolto in acque sorgive.*

Relatore: Prof. Antonino OLIVA

Alfonso POLICICCHIO

*Proprietà elettroniche e vibrazionali di nanotubi di carbonio drogati con sodio: caratterizzazione in funzione della temperatura.*

Relatore: Prof. Raffaele AGOSTINO

Valentino PINGITORE

*Circuiti superconduttori per calcolatori quantistici*

Relatore: Prof. Giovanni FALCONE

Mario Ariosto MATRANGA

*Miscele colesteriche per sensori UV.*

Relatore: Prof. Riccardo BARBERI

Salvatore FAZIO

*Studio delle sezioni d'urto differenziali in funzione di  $Q^2, W, t$  in processi diffrattivi di Deeply Virtual Compton Scattering.*

Relatore: Prof. Giancarlo SUSINNO

Manuela DI IORIO

*Influenza dei sistemi a larga scala sulle precipitazioni in Calabria.*

Relatore: Prof. Carlo BELLECCI

Rossana DE MARCO

*Un modello per l'interazione onda-particella in fisica del plasma.*

Relatore: Prof. Vincenzo CARBONE

Gianluca COSCHIGNANO

*Caratterizzazione di solitoni spaziali in celle di cristallo liquido.*

Relatore: Prof. Cesare UMETON

Giuseppe CODISPOTI

*Sistemi di controllo e valutazione dell'efficienza di rilevazione per particelle ad alto potere ionizzante del rivelatore centrale dell'esperimento ATLAS al CERN.*

Relatore: Prof. Giancarlo SYSINNO

Raffaele VILLELLA

*Aspetti operativi della dosimetria come strumento di verifica della tutela del personale radioesposto di una Azienda Sanitaria.*

Relatore: Prof. Ernesto LAMANNA

Ivana SURIANO

*Coadsorbimento di potassio e ossigeno sulla superficie di Ni(111) a temperatura ambiente: uno studio delle proprietà vibrazionali.*

Relatore: Prof. Gennaro Chiarello

*July 22*

Francesco SCARPELLI

*Studio dell'Emoglobina Spin-labellata Tramite EPR pulsato.*

Relatore: Prof. Luigi SPORTELLI

Luigia PEZZI

*Equilibrio forzato e riorientazione critica in cristalli liquidi, sotto l'azione di fasci laser in competizione.*

Relatore: Prof. Cesare UMETON

Giacomo BOZZO

*Imaging funzionale con risonanza magnetica : dipendenza della sensitività dal tempo di eco nelle sequenze gradient eco - EPI.*

Relatore: Prof. Franco PIPERNO

*September 30*

Maria Luisa DE BARTOLO

*La radioprotezione del paziente in terapia radiometabolica: personalizzazione della dose da somministrare nella terapia dell'ipertiroidismo.*

Relatore: Prof. Ernesto LAMANNA

*December 16*

Simona CARNEVALE

*Valutazione dei parametri biofisici dell'aria nello studio della correlazione tra arredo verde urbano e incidenza dell'allergie respiratorie nel territorio di Cosenza.*

Relatore: Prof. Giovanni FALCONE

Stefano MALETTA

*Emissione potenziale di elettroni da superfici metalliche bombardate con ioni lenti: singolarità di fermi e neutralizzazione auger.*

Relatore: Prof. Giovanni FALCONE

Giovanni POLIMENI

*Limite per densità evanescente della Teoria Quantistica dei Campi non relativistica.*

Relatore: Prof. Renzo ALZETTA

#### **1st LEVEL DEGREE THESIS' IN 2004**

*July 22*

Gianluca DE MASI

*Interazioni tra modi gravitazionali e struttura convettiva del sole.*

Relatore: Prof. Pierluigi VELTRI

September 30

Pierluigi VELTRI

*Analisi POD di dati spazio temporali di interesse biomedico*

Relatore: Prof. Vincenzo CARBONE

December 16

Raffaele MARINO

*Leggi di scala nelle precipitazioni calabresi.*

Relatore: Prof. Vincenzo CARBONE

Gabriele INFUSINO

*Studio dell'oscillatore armonico nella formulazione di Feynman della Meccanica Quantistica.*

Relatore: Prof. Alessandro PAPA

Bitane REHAB

*Modello di Tsyganenko per il campo magnetico della magnetosfera terrestre.*

Relatore: Prof. Gaetano ZIMBARDO

Amedeo PERRI

*Tecniche e misure preliminari di ISS (Ion Scattering Spectroscopy).*

Relatore: Prof.ssa Assunta BONANNO

Rosanna CARNEVALE

*Equilibri cinetici self-consistenti per plasmi astrofisici.*

Relatore: Prof. Gaetano ZIMBARDO

Francesca TEOCOLI

*Studio del rilassamento dello "Switching" Elettro-Ottico in cristalli liquidi nematici."*

Relatore: Prof. Nicola SCARAMUZZA

Isabella MARTIRE

*L'oscillatore armonico unidimensionale con termine perturbativo quartico nella formulazione dell'integrale sui cammini di Feynman.*

Relatore: Prof. Alessandro PAPA

Davide Remo GROSSO

*Catodoluminescenza: apparato strumentale e misure preliminari*

Relatore: Prof. Antonino OLIVA

#### **PhD THESIS' in 2004 (XVI Cycle)**

Enrico MACCALLINI

*Studio delle proprietà vibrazionali ed elettroniche di nanotubi di carbonio*

Supervisore: Prof. Gennaro CHIARELLO

Francesco VALENTINI

*Kinetic numerical simulation for collisionless plasma*

Supervisore: Prof. Pierluigi VELTRI

Manuela PANTUSA



*Liposomi stabilizzati stericamente ed interazione con l'albumina umana*

*Supervisore: Prof. Luigi SPORTELLI*

Andrea STIRPE

*Caratterizzazione calorimetrica e spettroscopia di metallo-proteine monomeriche e multimeriche*

*Supervisore: Prof. Luigi SPORTELLI*

Evelin MEONI

*Search for the standard model HIGGS in the channel  $H \rightarrow LL \rightarrow 4\mu$  with the ATLAS experiment at LHC*

*Supervisore: Prof.ssa Laura LA ROTONDA*

Antonio DE LUCA

*Non linear optical propagation in liquid crystals spatial solitoni and organic micro-lasers*

*Supervisore: Prof. Cesare UMETON*

Marco ONOFRI

*Three-dimensional simulations of magnetic reconnection in a current sheet in slabs geometry and of a reversed field pinch in cylindrical geometry.*

*Supervisore: Prof. Pierluigi VELTRI*

### **PhD Thesis' in Earth Sciences**

Anna. GERVASI

*Tomografia sismica per la definizione di strutture litosferiche in Italia Meridionale*

*Supervisore: Ignazio GUERRA*

## 1 ASTROPHYSICS

### *Professors and*

*Researchers:* Pierluigi Veltri  
Francesco Malara  
Vincenzo Carbone  
Gaetano Zimbardo  
Leonardo Primavera

*Contract owners* Pierre Pommois  
Antonella Greco  
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*PhD students* Marco Onofri  
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### *Post-Doc Researcher*

### *Research Training*

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F. Berrilli (*Università «Tor Vergata», Roma*)  
G. Consolini (*IFSI - CNR, Frascati*)  
V. Antoni et al. (*Consorzio RFX - CNR, Padova*)  
A. Vulpiani (*Università «La Sapienza», Roma*)  
G. Boffetta (*Università di Torino*)  
S. Savaglio (*Osservatorio Astronomico di Monteporzio, Roma*)  
A. Taktakishvili (*Abastumani Observatory, Tbilisi, Georgia, e University of Texas at El Paso, USA*)  
A. Milovanov (*Space Research Institute, Mosca, Russia*)  
L. Zelenyi (*Space Research Institute, Mosca, Russia*)  
V. Abramenko (*Crimean Astrophysical Observatory, Ukraina*)  
V. Yurchyshyn (*Big Bear Observatory, Big Bear City, CA, USA*)

### **Introduction**

The research in Astrophysics in the Physics Department of University of Calabria is mainly devoted to study plasmas. 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 various Italian universities (Florence, Rome) and with Italian Institutions (IFSI - CNR of Frascati, RFX - CNR of Padova) and foreign Institutions (Observatoire de Paris-Meudon, Space Research Institute, Moscow, Crimean Astrophysical Observatory, Ukraina, Abastumani Astrophysical Observatory, Tbilisi, Georgia). The specific research themes under study during the years 2003 and 2004 are indicated in the following.

### 1.1 PLASMA ASTROPHYSICS

### **1.1.1 Magnetohydrodynamic waves and turbulence in the solar atmosphere and in the solar wind**

#### ***Turbulence generation at photospheric level***

There are several indications that the MHD turbulence observed in-situ in solar wind high-speed streams is originated and mainly evolved in the atmosphere of the Sun. It is natural to think that the source of such fluctuations is related to photospheric motions. Measures of 2D photospheric velocity fields, performed by the IPM instrument, on the THEMIS telescope, has allowed to characterize a multifractal behaviour, typical of turbulence, at different altitudes in the photosphere, and thus to follow its dynamical evolution. This has been done using the Proper Orthogonal Decomposition (POD), an analysis technique of spatial and temporal datasets, which has allowed us to identify spatial structures associated with turbulence, thus representing a novel method in this research field.

#### ***Alfvén wave dissipation in 3D coronal structures***

The dissipation of Alfvén waves is one of the physical mechanisms proposed to explain the heating of the solar corona. The presence of Alfvénic fluctuations in the corona is supported by the resonance of coronal loops. Because of the very high values of the effective Reynolds/Lundquist number, the problem is how to move the wave energy on sufficiently small scales to be dissipated. Since the corona is very structured, one possibility is the interaction between waves and inhomogeneities of the background medium. In three-dimensional structures dissipative mechanisms are particularly efficient, since small scales can be generated exponentially (“fast dissipation” regime). Such a regime has been studied using WKB models for incompressible and compressible plasmas. It has been shown that for high Reynolds number the fast dissipation regime prevails. A quantitative evaluation has been obtained by using more realistic models of the coronal magnetic field, and by including the effects of energy leakage through the coronal base, as well as the effect of open magnetic lines and conversion into magnetosonic waves.

#### ***Turbulence in closed coronal structures***

In regions with closed magnetic lines in corona photospheric motions gives origin to an energy input in form of Alfvénic fluctuations propagating along the magnetic field, in both directions. Nonlinear interactions between such propagating modes give rise to an energy cascade to small scales, which finally leads to energy dissipation. Energy release events observed in corona can be then associated with dissipative events of turbulence. We have set up a new model (hybrid shell model), based on the RMHD equations, which employs the shell technique to describe nonlinear effects and includes wave propagation along the magnetic field. This model allows to describe turbulence in a wide range of spatial scales, and it includes the effects of photospheric motions by suitable boundary conditions. Distributions of energy, peak power, durations and waiting time observed in coronal energetic events are reproduced by the model. The model indicates that the dynamics of the system is determined by the combined effect of photospheric motions, loop resonance and nonlinear interactions. Moreover, it has shown the key role played by intermittency in coronal turbulence.

#### ***Turbulence and particle acceleration in solar flares***

Particle acceleration during solar flares is an extremely relevant phenomenon, but of difficult comprehension, due to the very short characteristic times and to the large number of involved particles. Observations suggest the presence of several acceleration sites within a given flare. The study of test particle acceleration in electric and magnetic fields within a MHD turbulence obtained by direct MHD simulations is limited by the small range of accessible spatial scales. This fact does not allow to evaluate the effects of intermittency in the simulation. We built up a synthetic turbulence model, based on the p-model technique, which includes an adequate range of scales. This model has allowed us to relate dissipative events in turbulence with particle acceleration, reproducing the spectra of high energy particles. Moreover, the effects of intermittency in the acceleration phenomenon has been studied.

### ***Turbulence and scale laws in the solar wind***

The scale laws of turbulent low-frequency fluctuations in the solar wind have been studied in the past, mainly for the velocity field, and it has been shown that they are not different from those measured in ordinary fluids. The magnetic field presents characteristic scale laws which are similar to those of passive scalars measured in laboratory experiments. Such scale laws are also different from those of magnetic field observed in fusion plasmas. We have used spacecraft data to study problems related to the active or passive role that magnetic field plays in the solar wind. We have performed a series of statistical data analyses, using wavelet transform and based on: a) identification of intermittent events at all the scales; b) statistical properties as quiet times, Poissonian statistics, etc.; c) the possible interconnection between intermittent events in the velocity and magnetic field. We have studied the scale laws of fluctuations of the angle between magnetic and velocity field, at different scales and at different distances from the Sun. Hence, from MHD equations we have phenomenologically obtained the scale laws of the defined quantities. These comparisons can be used as a further test to verify to which extent MHD describes solar wind turbulence.

### ***Dynamical evolution of Alfvénic fluctuations in solar wind fast-speed streams***

Spatial observations performed by both Ulysses spacecraft and by Helios in the inner heliosphere show that fluctuations gradually lose their Alfvénicity with increasing distance from the Sun, while their spectrum evolves. In collaboration with researchers from the IFSI (Institute of Interplanetary Space Physics) of INAF in Tor Vergata, we have studied the evolution of other properties of magnetic turbulence fluctuations with increasing the distance from the Sun. These properties have been successfully compared with the dynamical evolution obtained by simulating the development and nonlinear saturation of a parametric instability in a turbulent Alfvénic state.

### ***Spectrum and structure of the turbulence generated by magnetic reconnection instability***

In the Earth magnetotail current sheet, as well as in the current sheet of a plasma device as the RFX, a turbulence level has been identified, which is higher than in nearby regions. The origin of such a turbulence is probably the tearing instability which develops in the presence of a polarity inversion of the magnetic field. Using a 3D incompressible MHD numerical code we studied the nonlinear evolution of the reconnection instability of a current sheet, as well as its saturation. We have studied the spectral properties of the resulting turbulence, as spectral index and anisotropy, at different locations within the current sheet. Such properties can be compared with measures in the magnetotail current sheet.

## **1.1.2 Normal and anomalous transport processes in the heliosphere**

### ***High energy charged particle diffusion in the solar wind***

Particle transport in the solar wind strongly depends both on the magnetic structure and on the turbulence of the solar wind. The presence of magnetic turbulence in the heliosphere has the effect of a non-collisional charged particle diffusion; such a mechanism has a crucial importance for the cosmic ray transport and for the propagation to the Earth of energetic particles generated by solar events through the solar wind. Many uncertainties remain on the transport regime (Gaussian or non-Gaussian), as well as on the effective value of transport coefficients. Numerical results obtained by using models of synthetic turbulence have shown that different diffusion regimes are possible. Moreover, the anisotropy of turbulence gives origin to a strong anisotropy of diffusion coefficients.

### ***Anomalous diffusion in the Earth magnetopause and magnetotail***

The transport processes in the magnetotail and through the magnetopause require a particular attention because often anomalous diffusion phenomena are present, in which the properties of the random path are described by a Levy statistic, instead of a Gaussian statistic. The plasma transport across the magnetopause has been studied by a test particle simulation in which a sheared background magnetic field is included, as well as a model turbulence similar to that observed in the Earth magnetopause. This model has allowed us to calculate the plasma flux across the magnetopause. Moreover, we have developed a numerical model of the far magnetotail. Studying the test particle behaviour in this model we have shown that the current can break in two separate sheets, in accordance with some observations of the CLUSTER spacecraft. This study have been carried out in collaboration with researchers of the Space Research Institute of Moscow and of the Abastumani Astrophysical Observatory of Tbilisi.

### ***Anomalous transport processes in the transition region of the Sun***

The solar transition region represents the border between a region dominated by a collisional transport (photosphere) and a non-collisional region (the corona). In order to study the transport processes in these conditions we have developed a new Montecarlo numerical code which iteratively solves the Boltzmann equations. It allows us to calculate the evolution of electron distribution function and to evaluate the departures from a Maxwellian. The code has allowed us to build a new model of the solar transition region.

## **1.2 LABORATORY PLASMAS**

### **1.2.1 Characteristics of the turbulence generated by magnetic reconnection**

The nonlinear evolution of resistive instabilities which have origin within a current sheet generate a turbulence by a mechanism of energy transfer from large to small scales. Moreover, it is also responsible for the formation of large scale structures in consequence of magnetic island coalescence. A magnetic configuration has been studied in which both a magnetic field component which reverts its sign and a constant perpendicular component (guide field) are present. It has been shown that the presence of the guide field has a relevant effect on the evolution of the resistive instability: unstable modes with different wavevector have different resonance surfaces and then they are localized in different locations. In this case, the nonlinear evolution is characterized not only by mode coalescence on a single resonant surface but also by a direct energy cascade to resonant surfaces increasingly distant from the current sheet center, with the consequent formation of small scale structures on the sides. The study of the same physical processes in cylindrical geometry could allow to compare numerical results with measures obtained in laboratory devices, as the RFP.

## **A PUBLICATIONS ON SCIENTIFIC JOURNALS**

### **A.1 Publications on international journals**

#### **A.1.1 Publications on international journals printed in 2004**

1. Carbone V., Bruno R., Sorriso-Valvo L., Lepreti F., *Intermittency of magnetic turbulence in slow solar wind*, Planetary Space Science **52**, 953-956 (2004)
2. Zimbardo G., Pommois P., Veltri P., *Magnetic flux tube evolution in solar wind anisotropic turbulence*, Journal of Geophysical Research - Space Physics **109**, A02113-A02122 (2004)
3. Carbone V., Lepreti F., Veltri P., *Confining turbulence in plasmas*, Physics of Plasmas **11**, 103-109 (2004)
4. Bruno R., Sorriso-Valvo L., Carbone V., Bavassano B., *A possible truncated-Levy-flight statistics recovered from interplanetary solar-wind velocity and magnetic fluctuations*, Europhysics Letters **66**, 146-152 (2004)
5. Sorriso-Valvo L., Carbone V. and Bruno R., *One-point statistics and intermittency of induced electric field in the solar wind*, Europhysics Letters **67**, 504-510 (2004)
6. Nigro G., Malara F., Carbone V., Veltri P., *Nanoflares and MHD Turbulence in Coronal Loop: a Hybrid Shell Model*, Phys. Rev. Lett. **92**, 194501-1-194501-4 (2004)
7. Onofri M., Primavera L., Malara F., Veltri P., *Three-dimensional simulations of magnetic reconnection in slab geometry*, Phys. Plasmas **11**, 4837-4846 (2004)
8. Bruno R., Carbone V., Primavera L., Malara F., Sorriso-Valvo L., Bavassano B., Veltri P., *On the probability distribution function of small scale interplanetary magnetic field fluctuations*, Annales Geophysicae **22**, 3751-3769 (2004)
9. Sorriso-Valvo L., Abramenko V., Carbone V., Noullez A., Politano H., Pouquet A., Veltri P. and Yurchyshyn V., *Topological changes of the photospheric magnetic field inside active regions: a prelude to flares*, Planetary Space Science **52**, 937-943 (2004)
10. Lepreti F., Carbone V., Giuliani P., Sorriso-Valvo L. and Veltri P., *Statistical properties of dissipation bursts within turbulence: solar flares and geomagnetic activity*, Planetary Space Science **52**, 957-962 (2004)
11. Zimbardo G., Greco A., Veltri P., Taktakishvili A.L., and Zelenyi L.M., *Double peak structure and diamagnetic wings of the magnetotail current sheet*, Annales Geophysicae **22**, 2541-2546 (2004)

#### **A.1.2 Publications on international journals accepted during 2004**

1. Alfonsi G., Primavera L., *Proper orthogonal decomposition of moderately turbulent channel flow*, Fluid dynamics research - (2004)
2. Gaudio R., De Bartolo S. G., Primavera L., Gabriele S., Veltri M., *Lithologic control on the multifractal spectrum of river networks*, Journal of Hydrology - (2004)
3. Pommois P., Zimbardo G., Veltri P., *Energetic particle transport in anisotropic magnetic turbulence*, Adv. Space Res. - (2004)
4. Malara F., De Franceschis M. F., Veltri P. - *Dissipation of Alfvén waves in complex 3D coronal force-free structures* - Astron. Astrophys. - (2004).
5. Nigro G., Malara F., Veltri P. - *Large Amplitude Velocity Fluctuations in Coronal Loops: Flare Drivers?* - Astrophys. J. Lett. - (2004).

## **B MEMORIES (Extended proceedings of conferences or book chapters)**

### **B.1 International Memories**

#### **B.1.1 Memories published on International Conference Proceedings in 2004**

1. Nigro G., Malara F., Carbone V., Veltri P., *A Coronal Loop RMHD Shell Model for Turbulence generated Nanoflares*, in *Plasmas in the laboratory and in the Universe - New Insights and New Challenges*, Bertin G., Farina D., Pozzoli R., American Institute of Physics, Melville, New York, pp. 219-222 (2004)
2. Gaudio R., De Bartolo S. G., Primavera L., Veltri M., Gabriele S., *Procedures in multifractal analysis of river networks: a state of the art review*, in *Proceedings of the UNESCO/IAHS/TWHA symposium "The Basis of Civilization - Water Science?"*, Rome, Italy, December 2003, IAHS Redbook vol. 286, pp. 228-237 (2004)
3. De Bartolo S., Gaudio R., Primavera L., Gabriele S., Veltri M., *A new method for the assessment of river network fractal dimensions: introduction, computation and comparison*, in *Proceedings of the second international conference on fluvial hydraulics "River Flow 2004"*, Naples, Italy, 23-25 June 2004, M. Greco, A. Carravetta, R. Della Morte, Balkema, Leiden, The Netherlands, pp. 75-81 (2004)
4. De Bartolo S. G., Gaudio R., Primavera L., Gabriele S., Veltri M., *Probability distribution of Strahler stream lengths extracted from blue lines*, in *Proceedings of the International Scientific Seminar "Analysis and Stochastic modelling of Extreme Runoff in Euroasian Rivers under Conditions of Climate change"*, Irkutsk, Russia, 16-23 June 2003, L. M. Korytny and W. M. Luxemburg, Publishing house of the institute of geography SB RAS, Irkutsk, Russia, pp. 109-123 (2004)

#### **B.1.2 Memories accepted in International Conference Proceedings in 2004**

1. De Bartolo S. G., Veltri M., Primavera L., *Estimated Generalized Dimensions of River Networks*, in *Proceedings of "Hydrofractals 2003: an international conference on fractals in hydrosociences"*, Monte Verita', Ascona, Switzerland, 24th-29th August, 2003 (2004)

## **C INVITED PRESENTATIONS**

### **C.1 Invited presentations at International Conferences in 2003-2004**

1. Nigro G., Malara F., Carbone V., Veltri P., *Large Amplitude Velocity Fluctuations as Precursor of nanoflares in the Solar Coronal Loops*, *Solar Coronal Loops and Solar-B discussion*, Mondello (Palermo), 01/09-03/09 2004

### **C.2 Invited presentations at National Conferences in 2003-2004**

1. A. Vecchio, V. Carbone, L. Primavera, L. Sorriso Valvo, F. Lepreti, P. Veltri, T. Straus, *Solar oscillation observed in photosphere: the role of turbulent convection*, IV congresso italiano di fisica del plasma, Firenze (Italy), 12/01-14/01 2004

2. Zimbardo G., *Proprietà di trasporto anomalo in turbolenza magnetica anisotropa e barriere al trasporto*, Giornata Italiana su "Teoria della turbolenza e del trasporto nei plasmi magnetizzati", Milano, 17 maggio 2004-17 maggio 2004
3. Zimbardo G., *L'attività solare e le tempeste spaziali*, Convegno Liceo Scientifico 'L. da Vinci' e 'A. Volta': "Scienza e Tecnica negli Albori del Nuovo Millennio", Reggio di Calabria, 13 dicembre-14 dicembre 2004

## **D PRESENTATIONS AT CONFERENCES**

### **D.1 Presentations at International Conferences in 2003-2004**

1. Malara F., Nigro G., Veltri P., *Intermittency in MHD Turbulence and Coronal Nanoflares Modelling*, Alfvén 2004 Workshop on Space Environment Turbulence, Beaulieu - Francia, 19 Aprile-23 Aprile 2004
2. Malara F., De Franceschis M. F., Veltri P., *Dissipation of Alfvén waves in complex coronal magnetic fields*, Alfvén 2004 Workshop on Space Environment Turbulence, Beaulieu - Francia, 19 Aprile-23 Aprile 2004
3. Zimbardo G., Pommois P., Veltri P., *Anisotropy of magnetic turbulence in the solar wind deduced from magnetic flux tube evolution and energetic particle observations*, European Geosciences Union 1st General Assembly, Nizza, 25 aprile-30 aprile 2004
4. Zimbardo G., Greco A., Veltri P., Taktakishvili A.L., Zelenyi L.M., *Double peak and diamagnetic wings of the magnetotail current sheet*, European Geosciences Union 1st General Assembly, Nizza, 25 aprile-30 aprile 2004
5. Pommois P., Ippolito A., Zimbardo G., Veltri P., *Particle transport in the solar wind turbulence: comparison between numerical simulations and solar energetic particle observations*, European Geosciences Union 1st General Assembly, Nizza, 25 aprile-30 aprile 2004
6. Pommois P., Zimbardo G., Veltri P., *Energetic particle transport in anisotropic turbulence*, 35th Cospar scientific Assembly, Paris (France), July 19-July 24 2004

### **D.2 Presentations at National Conferences in 2003-2004**

1. M. Onofri, L. Primavera, P. Veltri, F. Malara, P. Londrillo, *Three-dimensional numerical simulations of magnetohydrodynamics equations*, IV congresso italiano di fisica del plasma, firenze, 12 gennaio-14 gennaio 2004
2. Zimbardo G., Pommois P., Veltri P., *Struttura delle superfici magnetiche nella turbolenza anisotropa del vento solare*, IV Convegno Nazionale sulla Fisica del Plasma in Italia, Firenze, 11 gennaio-13 gennaio 2004
3. Pommois P., Ippolito A., Zimbardo G., Veltri P., *Trasporto di particelle nella turbolenza del vento solare: confronto tra simulazione numerica e osservazioni*, IV Convegno Nazionale sulla Fisica del Plasma in Italia, Firenze, 11 gennaio-13 gennaio 2004
4. Nigro G., Malara F., Carbone V., Veltri P., *RMHD coronal loop model: comparison with velocity observations*, IV convegno nazionale di Fisica del Plasma in Italia, Firenze, Italy, 12/01-14/01 2004

## **ORGANIZATION OF CONFERENCES**

1. The Plasma Astrophysics Group has organized the *Summer School on Analysis Techniques for Turbulent Plasmas*, which has been held in Copanello (CZ), from September 28 to October 2, 2004.





## 2 THEORETICAL PARTICLE PHYSICS

The research activity during 2004 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;
- kaon-nucleon interaction at low energy;
- field theory of correlated systems.

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 computational facilities of the Physics Department and of the Istituto Nazionale di Fisica Nucleare (INFN) – Gruppo Collegato di Cosenza.

### 2.1 HADRON PHENOMENOLOGY AND QCD

#### 2.1.1 QCD

*Researchers :* R. Fiore, A. Papa, I.P. Ivanov

*Collaborators:* V.S. Fadin (*Budker Institute for Nuclear Physics, Novosibirsk, Russia*);  
D.Yu. Ivanov (*Sobolev Institute of Mathematics, Novosibirsk, Russia*).

The research activity along this line is concerned with the determination of the amplitude of hard scattering processes within perturbative QCD for asymptotic values of the squared center-of-mass energy ( $s$ ) and for values of the squared momentum transfer ( $t$ ) not growing with  $s$ . In this limit, called “Regge limit”, the so-called Balitskii-Fadin-Kuraev-Lipatov (BFKL) approach for the description of scattering amplitudes holds. Here is a list of the main results obtained.

1. The impact factor for the virtual photon ( $\gamma^*$ ) to light vector meson ( $V=\rho, \omega, \phi, \dots$ ) forward transition has been calculated in the next-to-leading order. In the “hard” kinematical domain, both at leading and next-to-leading order, the expression for the impact factor factorizes, up to power suppressed contributions, in the convolution of a hard perturbative amplitude and a twist-2 meson distribution amplitude. This impact factor can be used, together with the known Green’s function for the diffusion of two Reggeized gluons, to build up the scattering amplitude for the  $\gamma^* \gamma^* \rightarrow V V$  process completely within the BFKL approach in the next-to-leading order. This would be the first amplitude for a scattering process to be written completely in perturbative QCD in the next-to-leading order. In addition to the possibility to compare this amplitude with possible experimental results, this result can allow to understand the role played by the different energy scales entering the BFKL approach and to compare the BFKL approach with the DGLAP one.
2. It has been shown that the positive signature octet color state in the  $t$ -channel of the BFKL equation becomes Reggeized in the leading and in the next-to-leading order. In the latter case, this holds only for pure gluodynamics.
3. The kernel of the BFKL equation has been determined in the non-forward case at the next-to-leading order. The form in which it can be presented depends on the regularization of the infrared singularities in the “virtual” and in the “real” parts of the kernel. A form has been suggested for the total kernel free of singularities.

#### 2.1.2 Hadron phenomenology

*Researchers:* R. Fiore, A. Papa, I.P. Ivanov, F. Caporale

*Collaborators:* A. Flachi (Tsukuba University, Japan);  
F. Paccanoni (Università di Padova, Italy);  
L.L. Jenkovszky (Bogolyubov Institute of Theoretical Physics, Kiev, Ukraine);  
A. Kotikov (Joint Institute of Nuclear Research, Dubna, Russia);  
A.I. Lengyel (Institute of Electron Physics, Uzhgorod, Hungary)  
W. Magas (Universidad Valencia, Spain)  
N.N. Nikolaev (Forschungszentrum Juelich, Germany),  
A.A. Savin (DESY Hamburg, Germany),

I.F. Ginzburg (Budker Institute for Nuclear Physics, Novosibirsk, Russia).

1. The inclusive electron-proton cross section in the nucleon resonance region, recently measured at the Thomas Jefferson Laboratory, provided new data for the nucleon structure function  $F_2$ , with unprecedented precision. A new description of these experimental data has been proposed, based on a dual Regge model for  $F_2$ . The main ingredient of the model is given by complex non-linear Regge trajectories, which are responsible both for the isobaric resonances and for the background. The model has been compared with experimental data and the dependence from  $Q^2$  of the moments has been determined. The model for the structure function, with the parameters coming out from the fit, is a limiting case of the more general scattering amplitude applicable to the deeply virtual Compton scattering.
2. A model has been suggested for baryonic Regge trajectories compatible with the threshold behavior required by unitarity and asymptotics, in agreement with the unitarity constraints. The widths and the masses of the baryonic resonances of the neutron and of the  $\Delta$  has been reproduced by the model.
3. The cross section for the neutrino-nucleon interaction has been considered in the limit of ultra-high neutrino energy. The ingredients of the calculation have been (a)  $Q^2$  evolution of the structure functions for the neutrino-nucleon interaction, analytically determined in the twist-2 approximation and for small values of the  $x$  Bjorken variable, starting from a “soft” non-perturbative input; (b) recombination corrections, given by a twist-4 term, included in the DGLAP evolution equations and analytically handled in the particular case of “flat” initial conditions. The charged-current neutrino-nucleon cross section has been analytically estimated and its behavior for ultra-high neutrino energy has been discussed.
4. The dipion diffractive production has been proposed as a new method for the determination of the phase of the Pomeron amplitude.
5. In a review paper the recent HERA data on vector meson diffractive production have been considered and their theoretical interpretation has been given in the  $k_T$ -factorization and color dipole models.
6. In the deep inelastic diffractive scattering the production of excited states of vector mesons and of spin-3 mesons has been considered in the  $k_T$ -factorization model. Predictions for the current and future experiments have been put forth.

## 2.2 LATTICE GAUGE THEORIES

*Researchers:* R. Fiore, A. Papa, D. Giuliano, D. Marmottini, P. Giudice  
*Collaborators:* C. Vena (Università della Calabria, Italy);  
P. Sodano (Università di Perugia, Italy)

1. The critical exponent  $\nu$  for the correlation length in SU(2) gauge theory in (3+1) dimensions at finite temperature has been determined by a method inspired by the Svetitsky-Yaffe conjecture and based on the study of the finite-size scaling of simple lattice operators, such as the plaquette. The result is in excellent agreement with the corresponding value in the 3-dimensional Ising model, according to the predictions of universality.
2. The phase diagram of the (3+1)-dimensional SU(2) gauge theory in presence of dynamical quarks for non-zero temperature and baryon density has been studied on the lattice by numerical Monte Carlo simulations. The case of SU(2) gauge theory is interesting because numerical simulations are feasible both for real and imaginary chemical potential, this allowing to test the method of analytical continuation from imaginary to real chemical potential adopted in the physically interesting case of SU(3), where only simulations with imaginary chemical potential are possible.
3. The so-called Polyakov loop effective model for the deconfined phase of SU(N) gauge theories has been studied in the case of the (3+1)-dimensional SU(2) pure gauge theory. According to this model, the deconfined phase can be described by a *mean field* effective theory of the Polyakov loop. It has been shown that this is indeed the case in a certain interval of temperatures above the deconfinement.
4. The (3+1)-dimensional Quantum Electrodynamics (QED<sub>3</sub>) with dynamical matter fields is being studied by numerical Monte Carlo on the lattice. This theory is a candidate for the description of the pseudo-gap phase in high-temperature

superconductors. The aim of this study is to understand the nature of the transition from the superconductive phase to the anti-ferromagnetic one in planar systems. On the other side, QED<sub>3</sub> can be used to understand the mechanisms of confinement in presence of fermionic matter fields, with special attention to the role played by magnetic monopoles.

### 2.3 PHYSICS OF KAON-NUCLEON INTERACTIONS

*Researcher:* G. Violini  
*Collaborator:* P. Gensini (*Università di Perugia, Italy*)

The first Dafne results, which solved the puzzle of kaonic atoms, and the perspective of J-Parc in Japan, which should start to work in 2008, as well as the debate on the pentaquark have reopened after many years the interest in this field of physics. A talk has been given in collaboration with P. Gensini at the Workshop on the proton driver (Fermilab, October 2004) and other ones have been planned for the beginning of 2005 at TRIUMF and the INFN Frascati Laboratories. The short-term perspectives include the possibility to collaborate with Frascati experimental groups (in particular with DEAR/SIDDHARTA and KLOE) and the revision of the old Kbar-nucleon low-energy data, using the constrains already given by DEAR on the *s*-wave at threshold and those which could come from SIDDHARTA for the *p*-wave.

### 2.4 FIELD THEORY OF CORRELATED SYSTEMS

#### Quantum criticality

*Researcher:* D. Giuliano  
*Collaborators:* R.B. Laughlin, B.A. Bernevig (*Stanford University, USA*)

The analysis of relevant aspects of quantum numbers fractionalization as critical phenomenon has been carried ahead.

#### 2.4.1 Correlated systems and states of matter different from the Fermi liquid

*Researcher:* D. Giuliano  
*Collaborators:* A. Tagliacozzo (*Università di Napoli, Italy*)

A Hamiltonian theory for the dynamics of a two-channel Kondo system near the zero-temperature fixed point has been formulated. The regularization scheme introduced by P. Coleman has been used, which allows to treat the overscreened fixed point with the approach à la Nozieres, in combination with techniques of chiral bosonization and lattice fermions. The Hamiltonian theory allows for exactly calculating the zero-temperature scattering matrix and constructing the operators describing the irrelevant perturbations of the critical theory, which made it possible to calculate the finite-temperature corrections to the scattering matrix.

#### 2.4.2 Effective theories of Josephson junctions networks

*Researcher:* D. Giuliano  
*Collaborator:* P. Sodano (*Università di Perugia, Italy*)

The phases of a chain of Josephson junctions have been studied using conformal theory techniques and integrable models. In particular, a link of the chain has been assumed to be “weaker” than the others, while the chain itself is linked to two superconductors with fixed phase difference. The theory for a such system turns out to correspond to a particular limit of the double boundary Sine –Gordon theory. By an accurate renormalization group analysis, the entire phase diagram of the system has been determined. The existence of a repulsive Luttinger liquid has been verified, as originally suggested by Glazman and Larkin. The transition from sinusoidal to sawtooth behavior in the Josephson current along the chain has been derived, corresponding to the transition from repulsive to attractive Luttinger phase.

## **A PUBLICATIONS ON SCIENTIFIC JOURNALS**

### **A.1 Publications on international journals**

#### **A.1.1 Publications on international journals printed in 2004**

1. D.Yu. Ivanov, M.I. Kotsky, A. Papa, "*The impact factor for the virtual photon to light vector meson transition*", Eur. Phys. J. C38 (2004) 195.
2. R. Fiore, A. Flachi, L.L. Jenkovszky, A.I. Lengyel, V.K. Magas, "*A kinematically complete analysis of the CLAS data on the proton structure function  $F_2$  in a Regge dual model*", Phys. Rev. D69 (2004) 014004.
3. R. Fiore, L.L. Jenkovszky, F. Paccanoni, A. Prokudin, "*Baryonic Regge trajectories with analyticity constraints*", Phys. Rev. D70 (2004) 054003.
4. A. Papa, C. Vena, "*Finite-size scaling and deconfinement transition: the case of 4d SU(2) pure gauge theory*", Int. J. Mod. Phys. A 19 (2004) 3209.
5. P. Giudice and A. Papa, "*Real and imaginary chemical potential in 2-color QCD*", Phys. Rev. D 69 (2004) 094509.
6. B.A. Bernevig, D. Giuliano, R.B. Laughlin, "*Spectroscopy of matter near criticality*", Annals of Physics, 311 – 1 (2004) 182 – 190, ed. Elsevier (Holland).
7. D. Giuliano, A. Tagliacozzo, "*Hamiltonian theory of the strongly-coupled limit of the Kondo problem in the overscreened case*", J. Phys. C: Condensed Matter 16, 6075 (2004).
8. D. Giuliano, A. Naddeo, A. Tagliacozzo, "*Linear Kondo conductance in a quantum dot*", J. Phys. C: condensed matter, 16, S1453 (2004).
9. G. Campagnano, D. Giuliano, A. Naddeo, A. Tagliacozzo, "*Josephson versus Kondo coupling at a quantum dot with superconducting contacts*", Physica C 406 (2004) 1-8.

#### **A.1.2 Publications on international journals accepted during 2004**

1. V. Fadin, R. Fiore, "*Non-forward BFKL Pomeron at the next-to-leading order*", hep-ph/0412386, to appear on Phys. Lett. B.
2. R. Fiore, L.L. Jenkovszky, A.V. Kotikov, F. Paccanoni, A. Papa, E. Predazzi, "*Analytical evolution of nucleon structure functions with power corrections at twist-4 and predictions for ultra-high energy neutrino-nucleon cross section*", hep-ph/0412003, to appear on Phys. Rev. D.
3. D. Giuliano, P. Sodano, "*Effective boundary field theory for a Josephson junction chain with a weak link*", to appear on Nucl. Phys. B.

#### **A.1.3 Papers submitted for publication during 2004**

1. I.F. Ginzburg and I.P. Ivanov, "*How to measure the Pomeron phase in diffractive dipion photoproduction*", hep-ph/0401180.
2. I.P. Ivanov, N.N. Nikolaev, A.A. Savin, "*Diffractive vector meson production at HERA: from soft to hard QCD*", 178 pp., preprint DESY-04-243, eprint: hep-ph/0501034, submitted to "Physics of Elementary Particles and Atomic Nuclei".

## **B MEMORIES (Extended proceedings of conferences or book chapters)**

## **B.1 International Memories**

### **B.1.1 Memories published on International Conference Proceedings in 2004**

1. I.P. Ivanov, N.N. Nikolaev, W. Schafer, "*Saturation and s-channel helicity nonconservation in diffractive DIS*", Phys. Part. Nucl. 35 (2004) S30-S37.
2. I.F. Ginzburg, I.P. Ivanov, "*The use of the charge asymmetry of pions in  $e p \rightarrow e \pi^+ \pi^- p'$  at HERA for the discovery of the Odderon and measurements of Pomeron phase*", Phys. Part. Nucl. 35 (2004) S14-S23.

## **D PRESENTATIONS AT CONFERENCES**

### **D.1 Presentations at International Conferences in 2004**

1. D.Yu. Ivanov, M.I. Kotsky, A. Papa, "*The virtual photon to light vector meson impact factor in the next-to-leading order*", talk given by A. Papa at "Diffraction 2004", International Workshop on Diffraction in High-Energy Physics, Cala Gonone (Nuoro, Italy), Sept. 18-23, 2004; to appear on Nucl. Phys. B [Proc. Suppl.].
2. I.P. Ivanov, "*On the Reggeization of the positive-signature color-octet in BFKL*", talk given by I.P. Ivanov at "Diffraction 2004", International Workshop on Diffraction in High-Energy Physics, Cala Gonone (Nuoro, Italy), Sept. 18-23, 2004; to appear on Nucl. Phys. B [Proc. Suppl.].
3. R. Fiore, L.L. Jenkovszky and V.K. Magas, "*Generalized Parton Distributions, Analyticity and Crossing*", talk given by L.L. Jenkovszky at "Diffraction 2004", International Workshop on Diffraction in High-Energy Physics, Cala Gonone (Nuoro, Italy), Sept. 18-23, 2004; to appear on Nucl. Phys. B [Proc. Suppl.].
4. P. Giudice and A. Papa, "*Finite temperature 2-color QCD for real and imaginary chemical potential*", poster presented by P. Giudice at "Lattice 2004", International Symposium on Lattice Field Theory, Fermilab, Batavia, June 21 - 26, 2004, to appear on Nucl. Phys. B [Proc. Suppl.].
5. R. Fiore, P. Giudice, A. Papa, "*Numerical test of Polyakov loop models in high temperature  $SU(2)$* ", poster presented by A. Papa at "Lattice 2004", International Symposium on Lattice Field Theory, Fermilab, Batavia, June 21 - 26, 2004, to appear on Nucl. Phys. B [Proc. Suppl.].
6. R. Fiore, P. Giudice, D. Giuliano, D. Marmottini, A. Papa, P. Sodano, "*QED<sub>3</sub> on a space-time lattice: compact versus non-compact formulation*", talk given by P. Giudice at "SMFT-2004", XII Workshop on Statistical Mechanics and non-perturbative Field Theory, Bari (Italy), September 29 - October 1, 2004.
7. D. Giuliano, "*Spectroscopy of Matter at a Quantum Critical Point*", talk given at the "Workshop on Novel States and Phase Transitions in Highly Correlated Matter", Trieste (Italy), July 2004.
8. D. Giuliano, "*Deconfinement of Spinons as a Quantum Critical Phenomenon*", talk given at "SMFT-2004", XII Workshop on Statistical Mechanics and non-perturbative Field Theory, Bari (Italy), September 29 - October 1, 2004.
9. D. Giuliano, "*Two-channel Kondo Effect in a Quantum Dot*", talk given at the International Conference "CMME-2004", Poznan (Poland), September 2004.
10. D. Giuliano, "*Two-boundary Sine-Gordon theory for a Josephson-junction chain with a weak link*", talk given at the International Conference "From Bohr atomic scale to Planck's scale", Capri (Italy), September 2004.

## **ORGANIZATION OF CONFERENCES**

The Theoretical Particle Physics Group has organized **Diffraction 2004 – International Workshop on Diffraction in High-Energy Physics**, held in Cala Gonone (Sardinia, Italy) in the period September 18-23, 2004.

### 3 EXPERIMENTAL PARTICLE PHYSICS

The experimental particle physics studies the most fundamental constituents of matter and the forces that cause their mutual interactions. The researches 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 some TeV) and allow them to collide against a target that can be fixed or a second beam. The detectors are designed to reconstruct the particles produced as a consequence of the beam-target particle interactions.

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

1. Study of the proton structure by means of deep inelastic scattering at electron-proton accelerator HERA of DESY laboratory (Hamburg, Germany) with the experiment ZEUS.
2. Study of proton-proton interactions at LHC accelerator of CERN laboratory (Geneva, Switzerland) with the experiment ATLAS.

#### 3.1 ZEUS EXPERIMENT AT HERA E-P COLLIDER (HAMBURG-GERMANY)

*Physicists:* M. Capua  
S. Fazio  
A. Mastroberardino  
M. Schioppa  
G. Susinno  
E. Tassi  
*Technicians:* F. Pellegrino  
*International collaboration*

Scattering experiments have been a huge success in revealing the complex world of structure of matter. The basic concept is quite simple: a point-like and energetic test particle (i.e. electron) is scattered on a target (i.e. proton) and its angular and energy distribution are measured. The first time that this technique was employed (1911) revealed that the atom has a positively charged core with a radius of less than 30 fm (Rutherford-Geiger-Marsden). Since 1911 many scattering experiments have been performed to explore the structure of nucleus on scale smaller and smaller. The "object" size  $\Delta$  that can be resolved in the scattering process is determined by the four momentum  $Q$  transferred from the test particle to the target one. From the uncertainty relation it follows that  $\Delta \approx 1/Q$ , therefore to increase the resolution it is required larger momentum transfer and hence higher beam energies. This is best achieved in the storage rings where the test and the target particle collide head-on. In the HERA collider two separate magnet systems guide the e and 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 820GeV energy respectively. The electrons meet protons in a head-on collision in four points along the ring where are located as many detectors always ready to record any interesting event coming from the interaction point. The four experiments are known as H1, ZEUS, HERMES and HERA-B.

At the maximum beam energies the centre of mass energy is  $(4 \cdot E_e \cdot E_p)^{1/2} \cong 314\text{GeV}$ , much larger than previously achieved in such collisions, and the exploring distance scale  $10^{-18}\text{m}$  of the proton structure can be reached. At large momentum transfers (the kinematical limit at HERA is  $10^5 \text{ GeV}^2/c^2$ ) there is a direct interaction of the electron with one of the proton quarks, while the "remnants" of the proton are only slightly involved. For this reason HERA is often addressed as the world's only electron-quark collider.

The Cosenza HEP group has been involved, since 1988, in the design, construction, testing, calibration, alignment, running and maintenance of three sub-detectors of ZEUS experiment: Forward Muon Spectrometer, Leading Proton Spectrometer and Vertex Detector. Furthermore the Cosenza researchers participate, since 1991 when the detector start to operate, the data taking as well as the physics analysis. During this last year there are new ZEUS results on the total neutral and charged differential cross sections, structure functions and their QCD fits. Analysis of the hadronic final states in these data have produced several precision measurements of the  $\alpha_s$  and have been used to test the NLO QCD calculations. Zeus data show evidence of the pentaquark baryons with strangeness. Electroproduction of  $\phi$  and  $J/\psi$  mesons show consistency with VMD and Regge phenomenology as well as with pQCD.

#### 3.2 ATLAS EXPERIMENT AT LHC P-P COLLIDER (GENEVA-SWITZERLAND)

*Physicists:* G. Avolio  
C. Adorisio  
G. Crosetti

E. Lamanna  
L. La Rotonda  
E. Meoni  
A. Polocicchio  
D. Salvatore  
M. Schioppa  
G. Susinno  
P. F. Zema  
F. Pellegrino

*Technicians:*

*International collaboration*

Nature has given us more than one elementary particle (6 fermions, 6 quarks and the carriers of the four fundamental interactions), whose masses ranges in a wide interval of values from the mass-less gauge bosons to the top quark  $M_t=100 \text{ GeV}/c^2$ . With this variety of particles and masses we should have an answer about the mechanism that determines the particle masses. Many experiments with particle accelerators are looking into the mechanism that gives rise to mass.

In 1964 Peter Higgs first proposed a very clever and very elegant solution to this problem: the whole of space is permeated by an undetectable field, similar in some ways to the electromagnetic field. As particles move through space they travel through this field, and if they interact with it they acquire what appears to be mass. This is similar to the action of viscous forces felt by particles moving through any thick liquid: the larger the interaction of the particles with the field, the more mass they appear to have. Thus the existence of this field is essential in Higg's hypothesis for the production of the mass of particles. Moreover from quantum theory follows that fields have particles associated with them (i.e. the photon is associated with the electromagnetic field). So the Higg's field should has a particle associated with, the Higgs boson. Finding the Higgs boson is thus the key to discovering whether the Higgs field does exist and whether our best hypothesis for the origin of mass is indeed correct.

The Standard Model of particle physics predicts that the Higgs boson is a hypothetical, massive subatomic neutral particle whose existence would explain the masses of the elementary particles. Up to now, no experiment definitively detected the existence of the Higgs bosons. The Higgs field is perceived the same from every direction (scalar field) and is mostly indistinguishable from empty space. The Higgs boson, sometimes called the **God particle**, itself has a characteristic rest-mass. The best estimate value for this mass is  $117 \text{ GeV}$ , with a theoretical upper limit of  $251 \text{ GeV}$ . Particle accelerators have probed energies up to about  $115 \text{ GeV}$ , and have recorded a small number of events that could be interpreted as resulting from Higgs bosons, but the evidence is as yet inconclusive. It is expected that LHC, the multi-TeV p-p collider currently under construction at CERN, will be able to confirm or disprove the existence of the God particle. LHC will provide 10 times higher centre of mass energy and 100 times higher p-p collision rates than previous colliders. This opens up a new frontier of physics and ATLAS detector will explore this great potential.

ATLAS is a general purpose detector designed to detect clean signal and perform accurate measurements of: charged leptons, photons, non-interactive particles such as neutrinos through missing energy measurements, hadronic jets, bottom quarks. The basic design concept to achieve these goals includes three detector systems:

1. a **tracker** with semi-conductor pixel and strip detectors for very high accuracy measurements of the charged particle trajectories, followed by straw tubes detector giving a bubble chamber like image of the event and independent electron identification. The tracker is confined to a cylinder  $6,8\text{m}$  long and  $1,1\text{m}$  radius in a  $2\text{T}$  magnetic field provided by a superconductive solenoid.
2. a **calorimeter** with an inner cylinder in highly granular liquid argon technology with Pb absorber, followed at large radius by an iron-scintillator calorimeter providing good resolution in a very cost-effective manner.
3. a high precision stand-alone **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 Cosenza HEP group are actively involved in various aspects of the design, construction and installation of the muon spectrometer detector system since 1994. During this decade the hardware projects in which the group participated have employed and trained many undergraduates and doctorates student in the process.

During this year the Cosenza group has participated to the following ATLAS activities:

1. construction and test of the drift tubes of the inner most high precision tracking chambers of the barrel region (BIL), concluded on December.
2. rewiring of damaged MDT chambers using a no-invasive technique
3. commissioning and test of the BIL chambers at CERN.
4. ATLAS MDT ageing studies at the Gamma Irradiation Facility of CERN.
5. realization of a low level, real time data acquisition software for the ATLAS sub-detector to monitoring the data during test beam and the first period of ATLAS data taking.



6. Monte Carlo simulation of muon spectrometer performances with GEANT 4.
7. study of Higgs and bottom signals using the muon spectrometer.

## A PUBLICATIONS ON SCIENTIFIC JOURNALS

### A.1 Publications on international journals

#### A.1.1 Publications on international journals printed in 2004

1. ZEUS Collaboration; M. Capua, A. Mastroberardino, M. Schioppa, G. Susinno, et al.  
*Search for a narrow charmed baryonic state decaying to  $D^{*+}p^{+-}$  in ep collisions at HERA*  
European Physical Journal C 38 (2004) 29-41
2. ZEUS Collaboration; M. Capua, A. Mastroberardino, M. Schioppa, G. Susinno, et al.  
*Dissociation of virtual photons in events with a leading proton at HERA*  
European Physical Journal C 38 (2004) 43-67
3. ZEUS Collaboration; M. Capua, A. Mastroberardino, M. Schioppa, G. Susinno, et al.  
*Substructure dependence of jet cross sections at HERA and determination of  $\alpha_s$*   
Nuclear Physics B 700 (2004) 3-50
4. ZEUS Collaboration; M. Capua, A. Mastroberardino, M. Schioppa, G. Susinno, et al.  
*Measurement of beauty production in deep inelastic scattering at HERA*  
Physics Letters B 599 (2004) 173-189
5. ZEUS Collaboration; M. Capua, A. Mastroberardino, M. Schioppa, G. Susinno, et al.  
*Evidence for a narrow baryonic state decaying to  $K0s$ -(anti)proton in deep inelastic scattering at HERA*  
Physics Letters B 591 (2004) 7-22
6. ZEUS Collaboration; M. Capua, A. Mastroberardino, M. Schioppa, G. Susinno, et al.  
*The dependence of dijet production on photon virtuality in ep collisions at HERA*  
European Physical Journal C 35 (2004) 487-500
7. ZEUS Collaboration; M. Capua, A. Mastroberardino, M. Schioppa, G. Susinno, et al.  
*Exclusive electroproduction of  $J/\psi$  mesons at HERA*  
Nuclear Physics B 695 (2004) 3-37
8. ZEUS Collaboration; M. Capua, A. Mastroberardino, M. Schioppa, G. Susinno, et al.  
*Observation of isolated high- $E_T$  photons in deep inelastic scattering*  
Physics Letters B 595 (2004) 86-100
9. ZEUS Collaboration; M. Capua, A. Mastroberardino, M. Schioppa, G. Susinno, et al.  
*Photoproduction of  $D^{*+}$  Mesons Associated with a Leading Neutron*  
Physics Letters B 590 (2004) 143-160
10. ZEUS Collaboration; M. Capua, A. Mastroberardino, M. Schioppa, G. Susinno, et al.  
*Search for contact interaction, large extra dimensions and finite quark radius in ep collisions at HERA*  
Physics Letters B 591 (2004) 23-41
11. ZEUS Collaboration; M. Capua, A. Mastroberardino, M. Schioppa, G. Susinno, et al.  
*High- $Q^2$  neutral current cross section in  $e^+p$  deep inelastic scattering at  $\sqrt{s}=318$  GeV*  
Physical Review D 70 (2004) 052001
12. ZEUS Collaboration; M. Capua, A. Mastroberardino, M. Schioppa, G. Susinno, et al.  
*Bottom photoproduction measured using decays into muons in dijet events in ep collisions at  $\sqrt{s}=318$  GeV*  
Physical Review D 70 (2004) 012008
13. ZEUS Collaboration; M. Capua, A. Mastroberardino, M. Schioppa, G. Susinno, et al.  
*Search for QCD-instanton induced events in deep inelastic ep scattering at HERA*  
European Physical Journal C 34 (2004) 255-265

14. ZEUS Collaboration; M. Capua, A. Mastroberardino, M. Schioppa, G. Susinno, et al. *Isolated tau leptons in events with large missing transverse momentum at HERA* Physics Letters B 583 (2004) 41-58
15. ZEUS Collaboration; M. Capua, A. Mastroberardino, M. Schioppa, G. Susinno, et al. *Bose-Einstein correlations in one and two dimensions in deep inelastic scattering* Physics Letters B 583 (2004) 231-246
16. ZEUS Collaboration; M. Capua, A. Mastroberardino, M. Schioppa, G. Susinno, et al. *Measurement of  $D^{*\pm}$  production in deep inelastic  $e^\pm p$  scattering at HERA* Physical Review D 69 (2004) 012004
17. ZEUS Collaboration; M. Capua, A. Mastroberardino, M. Schioppa, G. Susinno, et al. *Observation of  $K_s^0, K_s^0$  resonances in deep inelastic scattering at HERA* Physics Letters B 578 (2004) 33-44
18. La Rotonda et al. NOMAD Collaboration, *A study of strange particles produced in neutrino neutral current interactions in the nomad experiment.* Nucl.Phys.B700:51-68,2004
19. La Rotonda et. al., *Test of the first bil tracking chamber for the atlas muon spectrometer.* Nucl.Instrum.Meth.A523:309-322,2004
20. La Rotonda et al., *Bose-einstein correlations in charged current muon-neutrino interactions in the nomad experiment at CERN. NOMAD Collaboration,* Nucl.Phys.B686:3-28,2004

## 4 MEDICAL PHYSICS

*Professor :* Lamanna Ernesto -  
*PhD Student:* Bruno Carlo, Cucè Daniela  
*Researcher :* Castrovillari Francesca -  
*Graduate Student:* De Bartolo Maria Luisa , Sinopoli Ivan  
*Researcher:* Santaniello Anna

### Research area

Radioprotection, Dosimetry, Radiotherapy, Nuclear Medicine, New educational approach in health physics.

The most relevant activity in the 2003-2004 period has been devoted to:

1. Dosimetry and treatment planning in IORT (AO Cs);
2. Optimization of the methodology in clinical practice (AO Cs);
3. Master level for the training of experts in radioprotection and dosimetry;
4. Feasibility study of the proton therapy centre at Germaneto Campus (Cz);

1. The compact and movable LINAC IORT1 has been recently installed in Cosenza Hospital. It will be used for radiation therapy during a surgical operation. The system produces an electron beam of high and tuneable intensity to deliver a high dose on a tumoral bed, relapse of a tumour surgically extracted.

The dose is delivered directly to the tumoral bed excluding the radiation protection problems coming using the standard radiation therapy in the crossing of healthy tissues.

Our project fits that research line with the use of the IORT1 system developed by ENEA in collaboration with the Hythesis and High Tech Spa.. In the setting-up of the system we have studied the dose distribution inside the tissues and particularly the beam line geometries. The effects of the principal elements (applicators geometry, scattering filters) were simulated through the simulation of the system implemented using the toolkit Geant4. The study will follow through the search of the most appropriate detector to measure the high dose.

2. Thyroid pathologies are cured efficiently through the administration of  $^{131}\text{I}$ . This element is efficaciously absorbed inside the thyroid and the beta decays destroy the host cells. The damages induced on the health cells are reduced with a personal approach of the treatment. In the clinical practise the radioisotope is administrated taking into account some parameters of the patients which are measured experimentally: the target mass, the absorption rate of the thyroid, the effective decay rate. In most of the cases the dose to deliver is estimated using the average values for the parameters. This approach can cause the start of the opposite pathology: the ipo-thyroidism.

This project characterizes a clinical methodology for personal treatment in therapy radio metabolic, pointing in particular to the more efficient way to measure or evaluate the needed parameters in the clinical context where the therapy will be applied.

The first step was the measurement of the absorption rate of the thyroid. This was achieved by measuring the neck activity in the 24 hours following the administration of the  $^{131}\text{I}$ . The measures are done by means of a probe setting-up implemented in the context of the collaboration between the Physics Dep. of the University of Calabria and the Hospital "Annunziata" of Cosenza.

The mass of the pathological tissue of the thyroid is evaluated through the determination of the connected volume in SPECT images, processed by a dedicated software tool that we have implemented. The improvement of this approach will be our future job.

3. Experts in Radioprotection are needed in numerous areas: health, security, management and transport of radioactive materials in any sector. The investigation of the utilization of ionizing radiation in Calabria has shown that about 150 centres, distributed uniformly on the territory, utilize the radiation in medicine. It was pointed out the demand of a great number of professional person to monitor the environment and the people.

We proposed a first level of MASTER (2 years) on Radioprotection and Dosimetry, approved by the MIUR (2002) and financed with the European Funds within the *Programma Operativo Nazionale "Ricerca Scientifica, Sviluppo Tecnologico, Alta Formazione 2000-2006"* – *Avviso n. 4391 del 31 Luglio 2001, Mis. III. 4.*

The project was designed with a high level of training, inviting teacher and speaker qualified at local and national level within the collaboration between the University of Calabria, University "Magna Græcia" of Catanzaro, INFN, INFM, AO of Cosenza and Catanzaro, ASL n. 4 of Cosenza, ENEA, Sogin, Istituto "Regina Elena" of Rome. The partnership gave hospitality to the students in the training period.

The Master ended in the 2004 with good results. A student was employed by the Sogin, other three students appreciated the clinical experience during the training and decided to continue the formation with the Medical Physics School, other are utilizing the skills acquired in the environment sectors. This experience (especially the second year) was appreciated greatly by all the participants, students, teachers, manager and it tracks a good road for the formation of experts in radioprotection.

## **A PUBLICATIONS ON SCIENTIFIC JOURNALS**

### **A.1 Publications on international journals**

#### **A.1.1 Publications on international journals printed in 2004**

1. EAS-TOP& MACRO Collaborations (M. Aglietta et al.) *The cosmic ray proton, helium and CNO fluxes in the 100 TeV energy region from TeV muons and EAS atmospheric Cherenkov light observations of MACRO and EAS-TOP.* Astropart. Phys. 21 (2004) 223-240.
2. EAS-TOP and MACRO Collaborations (M. Aglietta et al.) *The cosmic ray primary composition between  $10^{15}$  and  $10^{16}$  eV from Extensive Air Showers electromagnetic and TeV muon data.* Astropart. Phys. 20 (2004) 641-652.
3. *Measurementg of atmospheric muon neutrino oscillations, global analysis of the data collected with MACRO detector.* By MACRO Collaboration (M. Ambrosio et al.). 2004. 17pp; Eur. Phys. J. C36 (2004) 323-339.

## **D PRESENTATIONS AT CONFERENCES**

### **D.1 Presentations at International Conferences in 2004**

1. E. Lamanna, R. Agostino, F. Castrovillari, E. Colavita, V. Formoso, G. Pecora, A. Santaniello, L. Sciommarella, S. Vivona, G. Barca & M. Veltri. *On the formation of experts in Radiation Protection and Dose Measurement: our Master course experience. GIREP 2004 Conference "Teaching and Learning Physics in new contexts" - Ostrava, 19-23 July 2004.*

## 5 SURFACE PHYSICS

### 5.1.1 SURFACE ELECTRON SPECTROSCOPY (SPES)

#### 5.1.2 Chemisorption on metal surfaces and Carbon nanostructures spectroscopic studies

*Group leader:* Prof. E. Colavita

*Collaborators :* Prof. G. Cannelli, Prof. G. Chiarello, Prof. R. Agostino, Dr V. Formoso (*Senior Researcher*), Dr T. Caruso (*Junior Scientist*), Dr S. Abate (*Graduated in Material Science*), Dr G. Desiderio (*Graduated in Material Science*), Dr E. Maccallini (*PhD Fellowship*), Dr. A. Policchio (*PhD student*), Dr. E. Infusino (*Graduated*), Dr. A. Marino (*Graduated*), Antonio Napolitano (*Student*).

#### Scientific program

The scientific activity of the SPES Group has developed essentially along two distinct branches, i.e. a) **Chemisorption on metal surfaces** and b) **Carbon nanostructures spectroscopic studies**.

The former topics deal with the interaction of simple metals with Ni single crystals and, moreover, with their catalyzing promotion of chemical surface reactions.

The latter branch deals with the vibrational and electronic properties of single wall carbon nanotubes as well as with the Synchrotron photoemission yield of nanostructured carbon films containing transition metal nanocrystals. The aim is the study of their strategic importance for applications in several technological fields such as energy conversion and storage.

#### a) Chemisorption on metal surfaces

A1) Spectroscopic investigations of the co-adsorption of potassium and oxygen on Ni(111) at room temperature . (ref.1).

The electronic and vibrational properties of oxygen and potassium co-adsorbed on the Ni(111) surface at room temperature were studied by high resolution electron energy loss and x-ray photoelectron spectroscopies. The sample surface was prepared by means of two different procedures, namely by adsorbing oxygen on a pre-dosed potassium ad-layer and by reversing this sequential order. In both experiments we observed that a K coverage as high as 0.25 ML ( i.e.  $p(2 \times 2)$  phase) is the condition necessary for measuring a weak K-O bond, while a K coverage greater than 0.30 ML ( almost full layer), gives rise to a strong K-O bond which is evidenced by the loss feature at 27 meV. The loss spectrum of the K-O- $c(4 \times 2)$  phase shows that both species interact mainly with the substrate.

A2) CO dissociation and CO<sub>2</sub> formation catalysed by Na atoms adsorbed on Ni (111). (ref.2).

The co-adsorption of CO and Na on Ni (111) was investigated by High-Resolution-Electron Energy-Loss-Spectroscopy (HREELS). The measurements were performed at room temperature and 160 K and for several Na coverages from sub-monolayer up to almost two monolayers. The evidence of the CO dissociation promoted by Na atoms is unambiguous occurring above a critical Na coverage and at room temperature. Unexpectedly, the CO dissociation takes place also at 160 K. Low Na coverages induce a direct CO-CO reaction whose products, CO<sub>2</sub> molecules and C atoms, remain adsorbed on the Ni surface at low temperature.

A3) A comparison between Auger and photoelectron emission detection in an X-ray standing –waves analysis of adsorbates. (ref.3)

We studied the contribution of secondary electrons emission to the Auger intensity when the adsorption edge is low compared to the photon energy. We performed a Normal Incidence X-ray Standing Wave experiment comparing photoemission K 2s and Auger K-LVV yields of Ni(111)- $p(2 \times 2)$ K system. The analysis of both profiles permits us to estimate that 5% of the total secondary electrons contributes to the K-L<sub>23</sub>VV excitation strongly modifying the line-shape of the potassium Auger profile. In this case the use of the Auger peak intensity profile as a monitor during an X-ray Standing Wave experiment for surface structural studies gives completely unreliable results.

#### b) Carbon nanostructures spectroscopic studies

B1) Vibrational and electronic properties of hydrogen adsorbed on single wall carbon nanotubes. (ref.4)

The vibrational and electronic properties of hydrogen molecules adsorbed on single wall carbon nanotubes were investigated by high-resolution electron energy loss spectroscopy. We found that at room temperature and  $2.6 \times 10^{-2}$  Pa, the

adsorption of  $H_2$  molecules is dissociative. The energy of the C-H vibrational mode is 360 meV, in agreement with the expected  $sp^2$ - $sp^3$  local re-hybridization induced by H chemisorption. The hydrogenation of carbon nanotubes gives also rise to significant changes for both the line shape and the excitation energy of the  $\pi$  plasmon. Upon H adsorption, the plasmon shifts by 0.8 eV towards lower energies and, moreover, a weak feature rises up at 3.5 eV.

B2) Spatially resolved valence band study of nanostructured carbon films containing transition metal nanocrystals. (ref.5)

We studied the electronic structure of nanostructured C films produced by ultrasonic cluster beam deposition with the intention to find out the bonding configuration of the C network and to determine the modification induced by transition metal cluster inclusion in the film. Exploiting the energy and spatial resolution of the Spectromicroscopy beamline at Elettra Synchrotron, we were able to follow the valence band features depicted in 95.0 eV-excited photoemission spectra with a 0.5  $\mu$ m lateral resolution. The spectroscopic results allowed to conclude that nanostructured C films have a mixed  $sp^2/sp^3$  bond configuration and an amorphous-like structure and that those features are uniformly distributed in the film. The inclusion of metal cluster (Ni, Ti and Mo) in the film strongly modifies the valence band spectra. The surface stoichiometry of the embedded metal clusters and the keeping of their metallic nature are determined by a detailed analysis of the spatial dependence of the ultraviolet photoemission spectroscopy (UPS) spectra and by a comparison with previous studies on metal-carbide and -oxide surfaces.

B3) Writing submicrometric metallic patterns by ultraviolet synchrotron irradiation of nanostructured carbon and  $TiO_x$ -carbon films. (ref.6).

Nanostructured carbon and carbon- $TiO_x$  films produced by supersonic cluster beam deposition have been characterized by spatially resolved  $\sim 0.5$   $\mu$ m lateral resolution photoemission spectroscopy with synchrotron light. We have found that pure and  $TiO_x$ -containing nanostructured carbon is modified under high flux UV exposure showing the onset of a metallic character near the Fermi level. We have studied the spectroscopic features, the spatial confinement, and the kinetics of this metallization process of the irradiated regions. This effect allows one to write metallic patterns in the  $TiO_x$ -containing films with a submicrometric resolution and with a fast kinetic.



## **A PUBLICATIONS ON SCIENTIFIC JOURNALS**

### **A.1 Publications on international journals**

#### **A.1.1 Publications on international journals printed in 2004**

1. D. Pacilè, M. Papagno, G. Chiarello, L. Papagno, E. Colavita, *Spectroscopic investigations of the co-adsorption of potassium and oxygen on Ni(111) at room temperature*, Surface Science 558, 58 (2004) .
2. A.Cupolillo, G.Chiarello, F.Veltri, D.Pacilè, M.Papagno, V.Formoso, E.Colavita,L. Papagno, *CO dissociation and CO<sub>2</sub> formation catalysed by Na atoms adsorbed on Ni (111)*, Chemical Physics Letters 398/1-3,118 (2004) .
3. D. Pacilè, M. Papagno, A. Cupolillo, G. Chiarello, L. Papagno, *A comparison between Auger and photoelectron emission detection in an X-ray standing –waves analysis of adsorbates*, Journal of electronic Spectroscopy and Related Phenomena 135, 201 (2004).
4. G. Chiarello, E. Maccallini, R.G. Agostino, T. Caruso, V. Formoso, L. Papagno, E. Colavita, L.Petaccia, R. Larciprete and S. Lizzit, A. Goldoni, *Vibrational and electronic properties of hydrogen adsorbed on single wall carbon nanotubes*, Physical Review B69,153409( 2004). Selected for the May 3, 2004 issue of Virtual Journal of Nanoscale Science and Technology.
5. R.G. Agostino, T. Caruso, G. Chiarello, R. Filosa, V. Formoso, E. Colavita, E. Barborini, C. Lenardi, P. Piseri P. Milani, S. La Rosa, M. Bertolo, *Spatially resolved valence band study of nanostructured carbon films containing transition metal nanocrystals*, Carbon 42 , 923-929 (2004).
6. T. Caruso, R. G. Agostino, G. Bongiorno, E. Barborini, P. Piseri, and P. Milani, C. Lenardi, S. La Rosa, M. Bertolo. *Writing submicrometric metallic patterns by ultraviolet synchrotron irradiation of nanostructured carbon and TiO<sub>x</sub>–carbon films*, Applied Physics Letters 84, 3412 (2004).
7. F. Trequattrini, F. Cordero, G. Cannelli, R. Cantelli, *Anelastic Relaxation Processes Due to Hopping of Interstitial Oxygen in Scandium.*, Solid State Commun. 129, 217 (2004).
8. F. Trequattrini, F. Cordero, G. Cannelli, R. Cantelli. *Hydrogen and Deuterium Tunnelling in Scandium* Materials Science and Engineering A370, 118-122 (2004).
9. F. Trequattrini, F. Cordero, G. Cannelli, R. Cantelli. *Anelastic Relaxation Processes Due to Hopping of Interstitial Oxygen* , in Scandium Materials Science and Engineering A370, 93-95 (2004).

## 6 SURFACE ION INTERACTIONS (IIS)

*Researchers:* A. Oliva  
A. Bonanno  
M. Camarca  
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F. Xu  
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Laboratory for Atomic and Surface Physics, University of Virginia, Charlottesville USA.  
Fujitsu Laboratories Ltd., Akashi, Hyogo, JAPAN.  
Dipartimento di Fisica, Facoltà di Ingegneria, Università di Catania  
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The 2004 research activity achieved the following results :

a. Observations of electron emission from MgO surfaces induced by impact of 100 eV–4 keV He<sup>+</sup>, Na<sup>+</sup>, Ne<sup>+</sup>, Ar<sup>+</sup> ions have been studied. The energy distribution of emitted electrons is nearly independent of ion type and energy, showing that it is caused by the decay of an intrinsic electronic state of the solid excited by the ions. The similar yields and energy distributions for incident Na<sup>+</sup> and Ne<sup>+</sup> ions rule out the potential mechanism of electron emission. The results are consistent with a novel model in which excitation occurs when electrons centered at the oxygen anions are promoted during a collision with the projectile (kinetic mechanism), and transferred to a surface exciton that can autoionize since it lies above the vacuum level, as determined by combining measurements of electron energy loss and photoelectric threshold.

b. Electronic transitions in molecular solids revealed many similarities and differences with gas phase single molecule spectra. For some weakly bound solids as condensed N<sub>2</sub> and CO, very narrow peaks with line width in the order of meV were observed while for others like water ice the electronic levels broaden significantly to form bands and no distinct transition features can be discerned. We performed an electron energy loss study on electronic transitions of condensed amorphous ethylene. C<sub>2</sub>H<sub>4</sub> was chosen because it is a simple organic molecule and because a large number of molecular spectroscopic data is available. Our results show that transitions from valence levels into Rydberg ones are not necessarily quenched in solids and these orbitals may still be well separated from the ionization continuum. The experiment was performed in a UHV chamber equipped for standard surface analysis. The chamber base pressure was  $5 \cdot 10^{-10}$  Torr. A close cycled liquid He cold finger was mounted on a sample manipulator which could be rotated to vary the electron incidence angle. A copper rod was attached to the head of the cold finger and ice was formed on the flat part at the end of this extension rod. The temperature was measured with a Au–0.17% Fe–Chromel thermocouple mounted on the sample surface. Pure C<sub>2</sub>H<sub>4</sub> gas was introduced into the chamber through a precision leak valve. 200 eV primary electrons were used in this study and the scattered electrons and we present energy loss spectra for 75 LC<sub>2</sub>H<sub>4</sub> condensed at T = 19 K (1 L =  $1 \cdot 10^{-6}$  Torr s). No contribution from the Cu substrate was detected, as also verified by the total absence of signal in the energy band gap region. Deposition of more C<sub>2</sub>H<sub>4</sub>, changing the detection angle, or varying exposure to the electron beam resulted in no changes in the spectral shape indicating the bulk nature of the amorphous solid ethylene. Im and minimal electron damage.

c. In the field of multimedial education a Java applet has been presented which helps a better understanding of numerical integration with the scope of supplying a simpler use of computational tools in order to stimulate in the student a greater attention to the physical contents of the problem. Moreover other Java applets have been developed to supply learning support concerning: relative motion, harmonic oscillators, static and dynamic friction, parabolic motion of a projectile.

### A PUBLICATIONS ON SCIENTIFIC JOURNALS

#### A.1 Publications on international journals

##### A.1.1 Publications on international journals printed in 2004

1. P. Riccardi, M. Ishimoto and R.A. Baragiola, *Ion-Induced Electron Emission from MgO by Exciton Decay into Vacuum*, Surf. Sci. 571 (2004) L305-L310.
2. F. Xu, G. Manico, A. Bonanno, P. Barone, P. Riccardi, A. Oliva, A. Cupolillo, L. Papagno, *Electron energy loss spectrum of solid ethylene*, Chem. Phys. Lett. 394 (2004) 280-282.

#### **A.1.2 Publications on international journals accepted during 2004**

1. A. Sindona, R. A. Baragiola, S. Maletta, G. Falcone, A. Oliva, P. Riccardi, *Broadening effects in Auger Neutralization of 130-430 eV Ar<sup>+</sup> ions at Al surfaces.*, Nucl. Instr. and Meth. in press
2. P. Riccardi, P. Barone, A. Bonanno, A. Oliva, P. Vetrò, M. Ishimoto, R.A. Baragiola, *Kinetic Electron Emission in the Interactions of Slow ions with MgO Surfaces*. Nucl. Instr. and Meth. in press
3. M. Commisso, A. Bonanno, A. Oliva, M. Camarca, F. Xu and P. Riccardi, *Plasmon Excitation and Electron Promotion in the Interaction of Slow Na<sup>+</sup> Ions with Al Surfaces.*, Nucl. Instr. and Meth. in press
4. P. Sapia, A. Milazzo, A. Bonanno, *Approccio Visuale all'Integrazione Numerica delle Equazioni del Moto: un'Applet Java sul Moto Parabolico con Attrito Viscoso*. Didattica e Didattiche Disciplinari, in press.
5. Sapia P., Milazzo A., Bonanno A. *Un'applet Java per lo studio dei moti relativi*. La Fisica nella Scuola, **in press**.
6. A. Milazzo, A. Bonanno, *Un Laboratorio Virtuale di Cinematica per visualizzare e rendere interattivo il moto del proiettile*. Scienzaonline , in press

#### **A.1.3 Papers submitted for publication during 2004**

1. A. Sindona, R.A. Baragiola, G. Falcone, A. Oliva, P. Riccardi, *Many-body shake-up in Auger neutralization of slow Ar<sup>+</sup> ions at Al surfaces*. Physical Review A, submitted
2. A. Bonanno, P. Sapia, *Java Applets as a Visual Tool for Teaching the Numerical Integration of the Equation of Motion*. The Physics Teacher , submitted.

### **D PRESENTATIONS AT CONFERENCES**

#### **D.1 Presentations at International Conferences in 2004**

1. Bonanno A., Milazzo A., Sapia P., *A Java Kinematics Laboratory: early results*. XC Congresso della S.I.F. - Brescia 20-25 settembre 2004.
2. Bonanno A., Milazzo A., Sapia P. *A on-line Java Kinematics Laboratory to make projectile motion visual and interactive*. 9th Workshop on Multimedia in Physics Teaching and Learning (MPTL9) - Graz , 2004.
3. Sapia P., Milazzo A., Bonanno A. *Un'applet Java per lo studio dei moti relativi*. XLIII Congresso dell' A.I.F. - Salice (PV) 18-21 ottobre 2004.
4. Sapia P., Milazzo A., Bonanno A. *Approccio Visuale all'Integrazione Numerica delle Equazioni del Moto: un'applet Java sul moto parabolico con attrito viscoso*. VI Congresso Nazionale dell' Associazione per la Didattica con le nuove Tecnologie (ADT) – Vietri, 2004.

## 7 THEORETICAL MATTER PHYSICS

*Researchers:* Prof. G. Falcone, prof. F. Piperno, Dr. F. Plastina, Dr. A. Sindona, Dr. A. Tallarico

*Research Fields:* Surface effects induced by ion bombardment, Quantum information theory

### 7.1 Study of Surface Effects and Collective Excitations Induced at Metal and Semiconducting Surfaces Probed by Low Energy Atomic Projectiles.

Electron and energy exchange processes between an atom or a molecule and a surface play an important role in gas surface interactions and are of interest in various branches of physics and chemistry. In fact, slow ions reflecting at some Angstroms from (or within) a solid target provide a unique probe for electronic excitations confined just to the surface region, making the related spectroscopies very surface sensitive tools to study solids; Moreover, ion probes may be used in the study of the electronic states of nanostructural material.

In atomic collisions, several questions of both fundamental and practical interest are involved, concerning the ionization/neutralization of projectiles, the mechanisms of electron and photon emission, and the characteristics of sputtered particles from the surface. The many existing experimental techniques yield structural information on both the projectile and the solid, together with the complicated dynamical aspects of the collision.

The interaction of an ion with a solid surface presents a highly dynamic many-body problem. A theoretical description of the motion of the impinging ion should treat the trajectory followed by the projectile taking into account the geometric structure of the target surface, the (multi-) electron exchange between target and projectile as well as the accompanying excitation of both collision partners. At present, most models handle the trajectories followed by the projectile classically while they combine both classical and quantum mechanical concepts in the treatment of the electronic ion-surface system. The classical treatments of ion trajectories make extensive use of Monte Carlo based simulation codes in which the paths followed by the projectiles are in principle made up of sequences of trajectory-changing binary projectile-target collisions. The electronic ion-surface system is mostly treated in terms of a model Hamiltonian formalizing the interaction between the discrete electronic projectile levels and the target conduction or valence bands. In this, the target electrons are often treated as a non-interacting, free electron gas and the interaction with the ion is described in terms of charge exchange probabilities.

Electron transfer occurs usually either by one electron processes, such as in resonant electron tunnelling, or by two electron Auger-type processes, such as Auger neutralization or Resonant neutralization followed by Auger De-excitations. In recent years, considerable progress has been achieved in the theoretical description of resonant electron exchanges for which non-perturbation methods have been developed and applied to the description of many-electron atoms on simple metallic surfaces, generally using a jellium model. Excellent agreement with experiments on negative ion formation on various surfaces was achieved.

A very cumbersome problem is positive/negative ionization of secondary atoms sputtered from solid surfaces, because of the complicated physical and chemical reactions occurring during ejection. In some previous papers, we have proposed a generalized time dependent Anderson-Newns Hamiltonian, obtained from first principles, to describe the interaction of secondary  $\text{Cu}^{\pm}$  atoms ejected from clean Cu surfaces. Surface effects were explained in terms of quasi-molecular interactions between secondary emitted and their nearest-neighbor substrate atoms that, in the collision cascade generated by the primary ion beam, provide the initial impulse to emitted particles. We used a Jellium surface and modelled the motion of ejected atoms with simple analytical trajectories. We developed a parameter-free theory whose numerical solution produced excellent agreement with the studied experiments, especially at very low emission energy of the order of some electronvolts.

Another active and alive field is secondary electron emission from positive atomic ion impacts, because of the huge number of applications to solid, clusters and biomolecules and water. From a theoretical point of view, the ejection of an electron from a solid can be described by the following three mechanisms: excitation of the electron, transport of the excited electron to the surface, and finally, emission from the surface. The minimum energy which a bound electron must gain in order to be emitted from a conductor equals the excitation energy to the conduction band of the solid, plus the energy which is needed to overcome the work function of the target-vacuum interface. However, if the electron is excited at some depth below the surface, it may lose energy during the transport to the surface. This means that an initial energy even higher than the minimum energy is required to transport electrons from the depth of the solid to outside the surface.

Particle-induced secondary electron emission is normally divided into two different mechanisms, in which either the translational kinetic energy or the internal potential energy of the incident projectile is transferred to a target electron. The requirement for potential electron emission from a conductor is that energy which is released when an incident ion is either neutralized, or else relaxes to a lower excited state, is larger than twice the work function of the surface. Potential emission occurs for most multiply-charged atomic ions, but only for a few singly-charged atomic ions such as ions of hydrogen and noble gases. Kinetic electron emission can occur when kinetic energy from the incident particle is transferred to target electrons.

The detailed mechanism for kinetic emission is not well understood, which is reflected in poor predictions of the threshold velocity below which kinetic emission should not be observed. On the other hand, potential electron emission has been long discussed in terms of two-electron, Auger type processes, such as Auger neutralization and resonant neutralization followed by interatomic Auger de-excitation. In Auger Neutralization, the electrostatic repulsion between two target electrons leads to one of the electrons tunnelling to neutralize the incoming ion, and the other being excited. Recent experimental studies have shown that the energy released by ion neutralization at metal targets can also produce collective excitations in the conduction band, such as surface plasmons, whose decay occurs predominantly by excitation of a single conduction electron. Although some models have been proposed to describe the creation of plasmon excitations, a theory of this processes is still lacking as well as with theoretical results to be compared with experimental data.

Another collective excitation has recently been proposed: the sudden change of charge of the projectile leads to a rearrangement of the ground state of conduction electrons on a long time-scale; this final-state effect parallels the sudden creation of a core hole by absorption of a soft x-ray photon, known as Fermi edge singularity, and reflects in the broadening of the kinetic energy distributions of ejected electrons, for a given incident ion velocity.

Finally, a collaboration with the research institute on membrane technology (ITMCNR) lead to the construction of a model for quantitative analysis of membrane emulsification, including both the permeation of the disperse phase through the membrane pores and the mechanism of droplet detachment.

## 7.2 Research on quantum information theory

The main theme of the research work performed in 2003-2004 has been the characterization of static and dynamical properties of quantum correlations in some model system amenable to an exact or approximate analytical solution. Pure quantum correlations (entanglement) is at the heart of many counter intuitive quantum mechanical effects and is also a basic resource for quantum information processing and computation. Furthermore, it has become more and more clear recently, that entanglement plays a key role in some condensed matter phenomena such as magnetic phase transitions.

In collaboration with researchers from the universities of Catania, Milano and Pisa (SNS), we studied the dynamics of quantum correlations in a class of exactly solvable Ising-type models. We analyzed, in particular, the time evolution of initial Bell states created in a fully polarized background and on the ground state of spin systems. We found that the pairwise entanglement propagates with a velocity proportional to the reduced interaction for all the four Bell states. Singlet-like states are favored during the propagation, contrary to triplet-like states that change their character with time under certain circumstances. In the presence of anisotropy in the spin interaction, pairwise entanglement is quickly created from a fully polarized state (i.e., even from an initially uncorrelated system); furthermore, the propagation of pairwise entanglement is suppressed in favor of creation of different types of multipartite correlations and of entanglement sharing. The "entanglement wave" evolving from a Bell state on the ground state turns out to be very localized in space time.

We also analyzed entanglement propagation in terms of spin waves. This approximate approach gives the possibility of studying more complicated models with spins residing on any kind of lattice structure. We found that, indeed, spin waves are responsible for entanglement transmission throughout the lattice and that interaction among spin waves is the main cause of entanglement sharing. We also used this method to investigate the critical properties of entanglement. In particular, we analyzed the ordered to canted phase transition occurring in the so called bi-dimensional X-Y model and found that entanglement (as quantified by the concurrence) has quite different spatial behaviors in the two phases, thus signalling the occurrence of the phase transition. In our approach, this difference in the

structure of entanglement of the ground state is a direct consequence of the modification of the magnon excitation spectrum in the two phases, leading to remarkable differences in the Bose occupation factors and, thus, to a different behavior of the correlation functions.

### **7.3 Geophysics**

In collaboration with researchers from CNR-IRPI we studied the radon anomalies in seismotectonic and tectonic-gravitational settings in the south-eastern Crati graben. The studies has confirmed that radon anomalies correspond to neotectonic features (quaternary recent and active normal faults) and deep-seated gravitational phenomena. In particular, the highest radon values match well the macroseismic zones of the main historical earthquakes.

## **A PUBLICATIONS ON SCIENTIFIC JOURNALS**

### **A.1 Publications on international journals**

#### **A.1.1 Publications on international journals printed in 2004**

1. G. De Luca, A. Sindona, L. Giorno, E. Drioli, *Quantitative Analysis of coupling effects in cross-flow membrane emulsification*, Jour. of Membr. Sci. 229, 199 (2004).
2. Amico L., A. Osterloh, F. Plastina, R. Fazio and G. M. Palma “*Dynamics of entanglement in one-dimensional spin systems*” Phys. Rev. A 69, 022304 (2004).
3. Plastina F., Amico L., A. Osterloh and R. Fazio “*Spin wave contribution to entanglement in Heisenberg systems*”, New J. Phys. 6, 124 (2004).

#### **A.1.2 Publications on international journals accepted during 2004**

1. A. Sindona, R.A. Baragiola, S. Maletta, G. Falcone, A. Oliva, P. Riccardi, *Broadening effects in Auger Neutralization of 130-430 eV Ar<sup>+</sup> ions at Al surfaces*, Nucl. Instr. & Meth. in Phys. Res. B, in press
2. A. Sindona, P. Riccardi, G. Falcone, *Resonant mechanisms for negative ionization of secondary emitted atoms from sputtered metals*, Nuclear Instruments and Methods in Physics Research B
3. Tansi C., Tallarico A., Iovine G., Folino-Gallo M. & Falcone G. *Interpretation of radon anomalies in seismotectonic and tectono-gravitational analyses: the SE portion of the Crati graben (Northern Calabria, Italy)*. Tectonophysics, in press.

## **8 MOLECULAR PHYSICS**

Bartolino Roberto  
Blinov Lev M.  
Umeton Cesare  
Barberi Riccardo  
Cazzanelli Enzo  
Cipparrone Gabriella  
Scaramuzza Nicola  
Versace Carlo  
De Santo Maria Penelope  
Pagliusi Pasquale  
Strangi Giuseppe  
Ciuchi Federica  
Giocondo Michele  
Lombardo Giuseppe  
Mazzulla Alfredo  
Bruno Vincenzo  
De Luca Antonio  
Caputo Roberto  
Veltri Alessandro  
Carbone Gianni  
Zappone Bruno  
Vena Carlo  
Barna Valentin  
Castriota Marco  
Pane Alfredo  
Barone Tiziana  
De Santo Giuseppe  
Ferjani Sameh  
Ayeb Habib  
Marino Salvatore  
De Nardo Bruno  
Prete Carmine  
De Sio Luciano,  
Pezzi Luigia

### **8.1 Vibrational spectroscopy**

Vibrational spectroscopy has been widely used in the last years to characterize the materials developed for electrochromic devices, in particular thin solid films for active electrodes and counterelectrodes, and polymeric ion conductors for the electrolyte layer and in asymmetric liquid crystal cells. Combined with other bulk and surface techniques it allows to get information on the chemical composition of the films (oxidation states, degree of hydration, etc.) grown both via sputtering techniques, as well as via sol-gel routes, after dip-coating or spin-coating deposition, on the presence of various phases of the same compound as well as on the degree of structural order. The confocality of the micro-Raman spectrometer allows a good discrimination of thin films spectroscopic contributions, obtainable via the Z-scan option, as in the case of Ru-doped  $\text{WO}_3$  films. In addition, the mapping option implemented in the micro-Raman equipment allows a more extensive and statistically reliable analysis on the various local structural configurations of the materials, as demonstrated by previous measurements on thin film samples of mixed titania-vanadia grown by sol-gel techniques. A particular mention deserves the combined study of magnetic and vibrational excitations in mixed magnesium-nickel oxides, where different degrees of disordered antiferromagnetism are present. However, the most recognized relevance of the Raman technique holds for the characterization of the carbon systems; in fact extensive investigations on the carbon nanotubes obtained by a great variety of metal and oxide catalysts are on going in this laboratory, also in collaboration with the other Italian and foreign groups. Finally, novel characterizations have been obtained on compounds of a new class, the ionic liquids, and some preliminary work started on archeological ceramic manufactures.

#### **8.1.2 Fast electro-optic switching in nematic liquid crystals**



The switching between on and off states of nematic liquid crystal pixels can be controlled with the well-known electro-optic effect. This effect however presents a fast response at switching on the electric field but a slow response at switching it off. Here we show a suitable choice of materials, cell geometries, surface preparations, and time dependence of the applied voltage that leads to a switch off response as fast as that at switch on. This is due to the particular conductivity mechanism in polymers with aromatic rings leading to rectifying properties when deposited on top of indium tin oxide surface. A transient negative charge at polymer–liquid crystal interface favors a faster and stronger planar orientation of the nematic molecules diminishing drastically the switch off time and increasing the contrast ratio. These facts, interesting enough from a fundamental point of view, could also lead to important technological consequences.

### 8.1.3 Different conduction zones in a NLC sample

Current vs voltage measurements have revealed two different conduction zones in a NLC sample. A standard sandwich type sample was filled with K18 (6CB) which was aligned (approximately) homeotropically by the two ITO surfaces previously cleaned in orthochromic mixture. On two opposite sides of the cell, the NLC was limited by two Mylar stripes acting as spacers. The other two sides were left open, and the liquid crystal had two free surfaces (limited only by air) in the form of a cylindrical meniscus. The overall conductivity of the cell depended strongly on the length of the free surface. For the same area, samples with a larger free surface experienced a higher overall conductivity. In the absence of an electric field, we considered the order in the free surface zone to be planar with  $n$  being normal to LC-air interface. For small electric fields the conduction along director  $n$  in the bulk is less than the conduction perpendicular to  $n$  on the free zone. At higher fields, the Freedericksz transition which operates on the free zone reduces the overall conductivity. This reduced conductivity was practically equal to that obtained when ITO electrodes were completely immersed in liquid crystal; that is, the free surfaces do not contribute to the conduction. Considering the measured values, we have concluded that the order in the free surface zone was planar for a depth of about 50  $\mu\text{m}$ . Moreover, current vs voltage measurements have revealed a nonstandard behavior of the electric conductivity within some nematic liquid crystals (NLC) samples, and the results have been associated with the local orientational order at the free surfaces of the liquid crystal. We have used Monte Carlo simulation of a liquid crystal in a cell with two free surfaces at the opposite sides to understand how a local director imposed by free surfaces competes with the homeotropic alignment imposed by electrodes of the nematic cell. Applying an electric field across a nematic liquid crystal display changes the texture of the thin nematic film. When the field is switched off, the texture relaxes to the initial one within seconds.

### 8.1.4 Plasma polymerized aniline

A thin film of plasma polymerized aniline induces a stronger planar anchoring of cyanobiphenyl liquid crystals. This strong anchoring appears when, due to an asymmetric conduction of the liquid crystal cell, alternating voltages create a transient electrically charged layer at the polyaniline/liquid crystal interface. This layer favors an expansion of anchoring toward the bulk, thus lowering dramatically the relaxation time and increasing the contrast ratio.

### 8.1.5 Electrochromic devices and asymmetric liquid crystal cells

In the search of new materials for electrodes in electrochromic devices and in asymmetric liquid crystal cells, some modified vanadium oxide thin films has been investigated. The new gels have been generated by the addition of 10% of bismuth (atomic ratio) to the precursors mixture. The sol–gel route started from metal alkoxides, vanadium oxo isopropoxide and  $\text{BiCl}_3$  dissolved in ethanol (99%), to give the atomic ratio  $\text{Bi/V} = 1:10$ . The crystallization temperature of such bulk gels has been found by DTA analysis to occur at 320  $^{\circ}\text{C}$ , while only seeds of a crystal phase are found after annealing the dip-coated films at 400  $^{\circ}\text{C}$ , identified as  $\text{Bi}_4\text{V}_6\text{O}_{21}$ . Microscopic visual investigation and micro-Raman analysis were performed on the deposited films, “as grown” and “400  $^{\circ}\text{C}$  annealed”. Finally, the films have been tested as electrodes in asymmetric nematic liquid crystal (NLC) cells, to investigate the rectification effect. The electro-optic measurements were performed in modified nematic liquid crystal cells for both “as deposited” and annealed films. The voltage dependence of the electro-optical response and the current flow have been analyzed at the same time in the voltage range  $-10/ + 10$  V. A model based on the electrical interaction between both the indium tin oxide (ITO)-Bi/V oxide films and Bi/V oxide films–liquid crystal interfaces was proposed, to explain the electric and electro-optic asymmetric responses of the cells

### 8.1.6 Transmission ellipsometry of both nematic and smectic liquid crystals (LCs) confined by mixed conductor substrates

We studied transmission ellipsometry of both nematic and smectic liquid crystals (LCs) confined by mixed conductor substrates. By simultaneously measuring the Stokes parameters of transmitted light, we follow the modification of the polarization state of the monochromatic light propagating through the LC cells. The analysis of the polarization states of the probe beam during the application of a specific voltage waveform at the LC samples allows obtaining important physical information on the investigated systems. The weakening of the anchoring energy in nematic LC samples and the experimental evidence of the Goldstone mode during the switching process of smectic LCs are highlighted.

#### **8.1.7 Influence of the bias-voltage on the anisotropic part of the nematic surface energy**

The influence of the bias-voltage on the anisotropic part of the nematic surface energy has been analyzed. The experimental data show a strong dependence of the anchoring strength on the bias-voltage when the electrodes of the nematic cell are covered with WO<sub>3</sub>. The observed dependence can be interpreted taking into account the ions dissolved in the liquid crystal. We propose a model in which the effect of the bias-voltage is to collect the ions near the electrodes, in a surface layer whose thickness is of the order of the Debye's screening length. The surplus of electric field due to this ions confinement gives rise to an electrostatic contribution to the total energy that can be considered as a surface energy. The proposed model is in good agreement with the experimental data. The model is used to interpret the observed independence of the anchoring strength on the bias-voltage when the indium-tin-oxide electrode is covered with a film of polyimide, or it is without any covering.

#### **8.1.8 Optically induced nonlinear dynamics and control in liquid crystal film**

The nonlinear response of a LC to an intense optical field represents an example of radiation(laser)-matter interaction in which nonlinear phenomena can be easily investigated. Recently, we observe that due to the symmetry of the system, the cascade of successive homoclinic gluing bifurcations is responsible for the transition towards stochastic regime. The interest is that our system is not ad hoc experiment to reproduce the homoclinic chaos, but the route to chaos through gluing bifurcation happens in a natural way, due to the symmetry of the NLC system. The obtained results shown that LC are systems in which complex dynamics can be studied with very simple experiments, and suggest to use them for the control of the chaos. The possibility of controlling chaos or, generally, to control nonlinear dynamics in complex systems has attracted many scientists both from a theoretical point of view and for applications. The activity has been focused on the development of a technique to control nonlinear dynamics: different methods has been tested, but particular attention has been devoted to achieve an all optical control. A large investigation of the dynamical regimes reached by the system through the control has been realised starting from different initial regimes.

#### **8.1.9 Surface induced photorefractive effect in pure liquid crystal cells**

Highly sensitive photo-electrical reorientation effects have been observed in pure LC cell. These effects occur under the combined application of DC electrical field and low power illumination (microW). The observed nonlinear behaviour is characterized by very large nonlinear coefficients ( $>10 \text{ cm}^2/\text{W}$ ). Results of wave mixing experiments suggest PR-like effect induced by photoelectric activation of polymer-LC interface in pure LC. Beam coupling measurements confirmed the PR nature of the gratings. The hypothesis made are that DC field works as charges accumulator at the LC-substrate interface, the light intensity pattern locally modifies the surface charge density, through recombination processes leading to a modulated charge field, which produces refractive index grating via molecular reorientation in the bulk. Several experimental geometries in the TBC experiments have been performed that support the hypothesis. The electrical behaviour of the cell was characterized from both experimental and theoretical point of view.

#### **8.1.10 Polarization holography in molecular materials**

LC polymers composite materials and azo-benzene based systems have been investigated for holographic recording. Several experimental techniques related to intensity and polarization holography have been used. Interesting results have been obtained for polarization holography. In the case of polymer liquid crystals composite systems, materials with oriented liquid crystal domains and uniform morphology have been obtained. Formation of the surface relief grating has been reported for the first time with polarization holography in systems without azo-based systems. The manipulation of the topography in thin films of azo-benzene based dyes and polymers has been achieved by controlling the intensity and polarization states of the interference beams.

### **8.1.11 Tunable lasing in dye doped cholesteric liquid crystals**

The study of dye doped cholesteric liquid crystal devices with the purpose of developing low threshold and widely tunable laser has been performed. Several strategies have been investigated obtaining lasing from a cascade of CLC laser systems and tunability of the same laser device in the wavelength range 350nm-700nm.

### **8.1.12 Self-assembly of organosilane**

Highly ordered thin PTFE (polytetrafluoroethylene) films have been deposited on glass substrates by the sliding on technique. The thickness of the films have been ellipsometrically determined to vary in the interval 10Å-100Å as function of the temperature, the pressure applied during the deposition and the speed of the sliding PTFE tip. These coated surfaces have been used as substrates for the assembly of organosilane molecular films (n-octadecyldimethyl[3-(trimethoxy-silyl)-propyl]ammoniumchloride). Finally nematic liquid crystal cells have been assembled by the coated substrates. The insertion of a PTFE film allows the control of the pretilt angle of the NLC molecules at the surface. The results of the study have been presented at the Conference of the Italian Liquid Crystal Society (Ischia 2004) and at the 2<sup>nd</sup> International Conference of Spectroscopic Ellipsometry held in Vienna (2003).

### **8.1.13 Electroconvective instabilities and anchoring breaking in nematic liquid crystals**

The two turbulent regimes (dynamic scattering modes), which characterize the electroconvection in nematics, have been studied by photopolarimetry. The analysis of the degree of polarization of the light transmitted by the LCV cells allowed further insight of the phenomenon and the formulation of a better model for the DSM1 $\leftrightarrow$ DSM2 transition. These results have been presented at the 2<sup>nd</sup> Japanese-Italian Liquid Crystal Societies Meeting (Tsu 2004) and they will be published on the Molecular Crystal Liquid Crystal issue devoted to the meeting.

### **8.1.14 Lasing in Microcavity**

Liquid crystals with a helicoidal supermolecular order act as photonic crystals allowing distributed feedback process. Laser emission tuned at different wavelength can be achieved by the dispersion of a fluorescent dye in to the liquid crystal structure.

Recently laser emission has been observed at pumping energies one order of magnitude lower with respect to conventional system by confining the LC-dye mixture in light sculptured polymeric microchannel (Policryps). This system implement an intrinsically "phase locked" array of microlasers, whom emitted intensity can be controlled applying an external electric field. The high level of integration of these systems can be produce a new architecture of photonic devices. The results this study have been presented at the Conference of the Italian Liquid Crystal Society (Ischia 2004) and submitted for publication on Physical Review Letters.

### **8.1.15 Characterization of POLICRYPS diffraction gratings**

We have performed a first characterization of the diffraction efficiency of POLICRYPS gratings, written in liquid - crystalline composite materials by the interference pattern of two curing beams. Fringes consist of polymer slices separated by films of a continuous nematic phase. The temperature dependence of the diffraction efficiency reveals a non-monotonous behavior, with several maxima and minima. The shape of curves is also dependent on slight changes in the initial concentration of the nematic component of the mixture, the number of extrema increasing with the increase of this concentration. The dependence on an applied external voltage also appears to be non-monotonous, the particular shape depending on the sample temperature. Both "switch-on" and "switch-off" dependences have been observed. We have also investigated the POLICRYPS diffraction properties both at wavelength of 632.8 nm and 1550 nm. Diffraction efficiency of 98% was measured and an electric field as low as 5 V/ $\mu$ m switches off the phase grating. Measured angular spectra are fitted by using the modified coupled mode theory including the effects of the grating birefringence.

### **8.1.16 Microcavity Laser Array Using Distributed Feedback**

Distributed feedback microstructures play a fundamental role in confining and manipulating light to obtain lasing in media with gain. We have fabricated an innovative array of organic, color-tunable microlasers which are intrinsically phase locked. Dye-doped helixed liquid crystals were embedded within periodic, polymeric microchannels sculptured by light through a single-step process. The helical superstructure was oriented along the microchannels; the lasing was observed along the same direction at the red edge of the stop band. Several physical and technological advantages arise from this

engineered heterostructure: a high quality factor of the cavity, ultralow lasing threshold, and thermal and electric control of the lasing wavelength and emission intensity. This level of integration of guest-host systems, embedded in artificially patterned small sized structures, might lead to new photonic chip architectures.

### 8.1.17 Routing of anisotropic spatial solitons and modulational instability in liquid crystals

In certain materials, the spontaneous spreading of a laser beam can be compensated for by the interplay of optical intensity and material nonlinearity. The resulting nondiffracting beams are called ‘spatial solitons’, and they have been observed in various bulk media. In nematic liquid crystals, solitons can be produced at milliwatt power levels and have been investigated for both practical applications and as a means of exploring fundamental aspects of light interactions with soft matter. Spatial solitons effectively operate as waveguides, and can be, therefore, considered as a means of channelling optical information along the self-sustaining filament. Actual steering of these solitons within the medium has proved more problematic, being limited to tilts of just a fraction of a degree. We have performed an experimental and theoretical investigation of voltage-controlled ‘walk-off’ and steering of self-localized light in nematic liquid crystals. We have found not only that the propagation direction of individual spatial solitons can be tuned by several degrees, but also that an array of direction-tunable solitons can be generated by modulation instability. Such control capabilities might find application in reconfigurable optical interconnects, optical tweezers and optical surgical techniques.

## 8.2 SOFT MATTER NANOSCIENCE

The thrust toward the nanoscience has affected many areas of matter physics, including Liquid Crystals (LC). Indeed, fundamental issues in the LC research since its very beginning are the LC interactions with surfaces and the potential of these materials for a large variety of topological defects. Surface properties and topology, with their underlying topic of elasticity, become crucial when LC either nanoconfined or facing nanopatterned surfaces are considered. More recently, the evidence of order reconstruction in bulk has been provided, which makes the typical defect structure to be unfolded dynamically in a sequence of states that reproduces in time what is traditionally observed in space. Indeed, the self organization of liquid crystalline order at the nanoscale, where simple continuum descriptions are challenged, involves a host of crucial issues in the condensed matter physics, such as the role of the various interactions (steric, electric, van der Waals, structural, hydrophobic) in the structuring process, ordering in reduced dimensionality, competition bi- and tri-dimensional, uniaxial and biaxial ordering in the very same system, the role of interfaces.

Besides the usual optical and electro-optical experimental investigations, we are at present developing new experimental techniques, based on SPM observations. In the period 2003-2004, the main research objectives were: surface properties of thin organic thin films, the bulk order reconstruction in nematics and the development of novel mirror-less lasers.

## A PUBLICATIONS ON SCIENTIFIC JOURNALS

### A.1 Publications on international journals

#### A.1.1 Publications on international journals printed in 2004

1. G. Strangi, C. Versace, N. Scaramuzza, E. Cazzanelli, V. Bruno, C. Vena, S. D’Elia, R. Bartolino, “*Photopolarimetric investigations of liquid crystals–electrochromic oxides interface*”, Thin Solid Films, 455–456, pp. 513–518 (2004)
2. Anca-Luiza Alexe-Ionescu, Andrei Th. Ionescu, Emil S. Barna, Valentin Barna and Nicola Scaramuzza: “*Fast electro-optic switching in nematic liquid crystals*”. Applied Physics Letters 84 (1) (2004) 40-42
3. G. Barbero, D. Olivero, N. Scaramuzza, G. Strangi, C. Versace: “*Influence of the bias-voltage on the anchoring energy for nematic liquid crystals*”. Physical Review E 69, (2004) 021713-1 – 02173-8
4. Nicola Scaramuzza, Catalin Berlic, Emil S. Barna, Giuseppe Strangi, Valentin Barna, Andrei Th. Ionescu: “*Molecular simulation of the free surface order in NLC samples*”. J. of Physical Chemistry B 108 (2004) 3207-3210

5. Anca-Luiza Alexe-Ionescu, Andrei Th. Ionescu, Emil S. Barna, Valentin Barna, Nicola Scaramuzza: "Role Of Delocalized Electrons In Polyaniline - Nematogen Cyanobiphenyls Interaction". J. of Physical Chemistry B 108 (2004) 8894-8899
6. G. Russo V. Carbone, G. Cipparrone "Optical control of photoinduced nonlinear dynamics in nematic liquid crystal films" JOSA B, 21, 599-604 (2004).
7. P. Pagliusi and G. Cipparrone "Dynamic grating features for surface induced photorefractive effect in undoped nematics " , JOSA B, 21, 996 (2004)
8. A. Chanishvili, G. Chilaya, G. Petriashvili, R. Barberi, R. Bartolino, G. Cipparrone, A. Mazzulla, Luis Oriol "Lasing in dye-doped cholesteric liquid crystals: two new strategies of tuning" Advanced Materials, 16, 791, (2004).
9. P. Pagliusi and G. Cipparrone . "Photorefractive effect due to a photo-induced surface-charge modulation in undoped liquid crystals" Phys. Rev. E, 69, 061708, (2004)
10. P. Pagliusi , B. Zappone, G. Cipparrone, G. Barbero, "Molecular reorientation dynamics due to DC-Voltage- induced ion redistribution in undoped nematic planar cell" , Journal of Applied Physics, 96, 218, (2004).
11. M. Scalerandi, P. Pagliusi, G. Cipparrone, G. Barbero, "Influence of the ions on the dynamical response of a nematic cell submitted to a dc voltage", Phys. Rev. E, 69, 051708, (2004)
12. A. Mazzulla, P. Pagliusi, C. Provenzano, G. Russo, G. Carbone, G. Cipparrone, "Surface relief gratings on polymer dispersed liquid crystals by polarization holography", Applied Physics Letters, 85, 2505 (2004)
13. A. Chanishvili, G. Chilaya, G. Petriashvili, R. Barberi, R. Bartolino, G. Cipparrone, A. Mazzulla, "Laser emission from dye doped cholesteric liquid crystal pumped by another cholesteric liquid crystal laser", Applied Physics Letters, 85, 3378 (2004).
14. A. Chanishvili, G. Chilaya, G. Petriashvili, R. Barberi, R. Bartolino, G. Cipparrone, A. Mazzulla, L. Oriol, "Lasing in dye-doped cholesteric liquid crystals: two new tuning strategies", Advanced Materials, 16 (2004) 791
15. A. Chanishvili, G. Chilaya, G. Petriashvili, R. Barberi, R. Bartolino, G. Cipparrone, A. Mazzulla, "Laser emission from a dye-doped cholesteric liquid crystal pumped by another cholesteric liquid crystal", Appl. Phys. Lett., 85 (2004) 3378-3380
16. M. Talarico, G. Carbone, R. Barberi, A. Golemme, "Fullerenes surface gratings for liquid crystal slignment", Appl. Phys. Lett., 85 (2004) 528-530
17. R. Barberi, F. Ciuchi, G. E. Durand, M. Iovane, D. Sikharulidze, A. M. Sonnet, E.G. Virga, "Electric Field Induced Order Reconstruction in a Nematic Cell", Eur. Phys. J. E, 13 (2004) 61-71
18. R. Barberi, F. Ciuchi, G. Lombardo, R. Bartolino, G. E. Durand, "Time resolved experimental analysis of the electric field induced biaxial order reconstruction in nematics", Phys. Rev. Lett., 93 (2004) 137801
19. G. Lombardo, M. Malara, R. Barberi, J. C. Rudin, "32-channel arbitrary waveform generator for bistable nematic devices", Rev. of Sci. Instrum., 75 (2004) 2008-2012
20. A. Chanishvili, G. Chilaya, G. Petriashvili, R. Barberi, R. Bartolino, M. P. De Santo, "Luminescent dichroic-dye-doped cholesteric liquid crystal displays", J. Soc. Inf. Display - SID, 12/3 (2004) 341
21. A. Veltri, R. Caputo, A.V. Sukhov, C. Umeton: "Model for the photoinduced formation of diffraction gratings in liquid-crystalline composite materials", Appl. Phys. Lett., 84, 3492 (2004).
22. R. Caputo, L. De Sio, A.V. Sukhov, A. Veltri, C. Umeton: "Development of a new kind of holographic grating made of liquid crystal films separated by slices of polymeric material", Opt. Lett., 29, 1261 (2004).

23. R. Asquini, A. d'Alessandro, C. Gizzi, R. Caputo, A.V. Sukhov, C. Umeton, A. Veltri: "*Electro optic properties of switchable gratings made of polymer and nematic liquid crystal slices*", Opt. Lett., 29, 1405 (2004).
24. A. Marino, F. Vita, V. Tkachenko, R. Caputo, C. Umeton, A. Veltri, G. Abbate: "*Dynamical behaviour of holographic gratings with a nematic film -Polymer slice sequence structure*", Euro. Phys. J. E, 15, 47 (2004).
25. R. Caputo, A.V. Sukhov, C. Umeton, A. Veltri: "*Characterization of the Diffraction Efficiency of New Holographic Gratings with a Nematic Film-Polymer Slice Sequence Structure (POLICRYPS)*", Journal of Optical Society of America B, 21, 1939 (2004).
26. M. Peccianti, C. Conti, G. Assanto, A. De Luca and C. Umeton: "Routing of anisotropic spatial solitons and modulational instability in liquid crystals", Nature, 432, 733 (2004).

#### **A.1.2 Publications on international journals accepted during 2004**

1. V. Bruno, M. Castriota, S. Marino, C. Versace, G. Strangi, E. Cazzanelli, N. Scaramuzza , "*Asymmetric Response to Electric Field in Nematic Liquid Crystal Cells Containing Vanadium Oxide Thin Films Prepared by Sol-Gel Synthesis*", accepted by Molecular Crystals & Liquid Crystals.

#### **A.1.3 Papers submitted for publication during 2004**

1. M. Castriota, C. Dewan, E. Cazzanelli, D. Teeters, "*Characterization of V2O5 Confined in Nanoscale Pores*", submitted to Solid State Ionics.
2. Nicotera, L. Coppola, C. Oliviero, M. Castriota, E. Cazzanelli, "*Investigation of ionic conduction and mechanical properties of PMMA-PVdF blend based polymer electrolytes*", submitted to Journal of Physical Chemistry A
3. M. Castriota , N. Epervrier , E. Cazzanelli, "*Raman spectroscopic monitoring of the sol-gel synthesis, spin coating deposition and thermal treatments of vanadium pentoxide films*". Inviato a Journal of Raman Spectroscopy

### **B MEMORIES** (*Extended proceedings of conferences or book chapters*)

#### **B.1 International Memories**

##### **B.1.1 Memories published on International Conference Proceedings in 2004**

1. G. Carbone, B. Zappone, R. Barberi: "AFM force measurements in the smectic phase", in "*Surface and interfaces of liquid crystals*", Ed. Th Rasing and I. Musevic, Springer, 2004, ISBN 3-540-20789-9
2. M.P. De Santo, R. Barberi, L. Blinov: "*Electric force microscope observations of electric surface potentials*", in "*Surface and interfaces of liquid crystals*", Ed. Th Rasing and I. Musevic, Springer, 2004, ISBN 3-540-20789-9
3. M. P. De Santo, M. Lombardo, S. Serrao, G. Lombardo, R. Barberi, "*Atomic force microscopy in ophthalmic surgery*", Proceedings in *IEEE NANO 2004, 4th Conference on Nanotechnology*, Munich, Germany (2004) 562-564
4. M. Castriota , E. Cazzanelli , L. Palermo , R. Ceccato , D. Teeters, "*Comparative Micro-Raman Study on Vanadium Pentoxide Samples Obtained via Sol-Gel Routes: Pure, Confined in a Porous Membranes and Mixed with Titania*", XVIII Congress GNSR, Perugia, Settembre 2003, ed. by A. Morresi and P. Sassi, Morlacchi Editore, Perugia, 2004, p. 177-186

### **D PRESENTATIONS AT CONFERENCES**

#### **D.1 Presentations at International Conferences in 2003-2004**

1. M. Castriota, N. Epervrier, E. Cazzanelli, “*Raman spectroscopic monitoring of the sol-gel synthesis, spin coating deposition and thermal treatments of Vanadium Pentoxide films*”, International Conference IME-6, Brno (Czech Rep.), August 29 – September 2004
2. E. Cazzanelli, L. Palermo, R. Ceccato, “*Comparative spectroscopic characterization of powders and films of V<sub>2</sub>O<sub>5</sub>, grown via sol-gel, method and undergoing thermal treatments and laser irradiation.*”, International Conference IME-6, Brno (Czech Rep.), August 29 – September 2004
3. R. Ceccato, S. Dirè, E. Cazzanelli, M. Castriota, L. Palermo, “*Thermal evolution of Vanadium oxide based gels and thin films*”. “IV WorkShop Italiano Sol-Gel” Monteponi, Iglesias Cagliari. 17-18/06/2004
4. M. Castriota, T. Caruso, R.G. Agostino, W.A. Henderson, S. Passerini, E. Cazzanelli, “*Temperature Evolution of Ionic Liquid Solvent and its Solution with Lithium Salt: a Raman, Spectroscopic Investigation*” Patras Conference on "Solid-State Ionics - Transport Properties" September 14 - 18, 2004, University of Patras, Hellas
5. Marino G., Cazzanelli E., Bruno V., Castriota M., Strangi G., Versace C. C., Scaramuzza N., "Characterizations of both mixed Bi/V and Ti/V oxide films, deposited via sol gel route, used as electrodes in asymmetric liquid crystal cells". Atti del convegno "20th International Liquid Crystal Conference", Ljubljana, Slovenia, 03-09 Luglio, 2004, 2004
6. Bruno V., Marino S., Castriota M., Cazzanelli E., Strangi G., Versace C. C., Scaramuzza N. "Direct and Inverse Electrooptical Response in Liquid Crystal Cells Containing Oxide Thin Films". Atti del convegno "The 2nd Japanese-Italian Workshop on Liquid Crystals", UST Tsu Hall, Tsu City, Mie Prefecture (Japan), 05-08 Settembre, 2004, 2004
7. G. Strangi, V. Barna, R. Caputo, A. De Luca, C. Versace, N. Scaramuzza, C. Umeton, R. Bartolino, G. Price - “*Distributed Feedback Organic Microcavity Laser*” 20th International Liquid Crystal Conference, Ljubljana, Slovenia, July 4 - 9, 2004
8. V. Barna, N. Scaramuzza, G. Strangi, E. S. Barna, A. Th. Ionescu, A.L. Alexe-Ionescu, “*Fast Electro-Optic Switching in NLC Cells Due to the Delocalized Electrons in Polyaniline-Nematogen Cyanobiphenyls Interaction*”, 20th International Liquid Crystal Conference, Ljubljana, Slovenia, July 4 - 9, 2004
9. G. Cipparrone, P. Pagliusi, “*Surface induced photorefractive effect in undoped liquid crystals*”, (oral presentation), 20<sup>th</sup> International Liquid Crystal Conference, Ljubljana, Slovenia, Luglio 2004
10. A. Chanishvili, G. Chilaya, G. Petriashvili, R. Barberi, R. Bartolino, G. Cipparrone, A. Mazzulla L. Oriol, “*New strategies of laser tuning in dye doped cholesteric liquid crystals*”, 20<sup>th</sup> International Liquid Crystal Conference, Ljubljana, Slovenia, Luglio 2004.
11. R. Caputo, L. De Sio, A.V. Sukhov, A. Veltri, C. Umeton: “*Experimental and Theoretical Aspects of POLICRYPS Gratings*”, International School of Liquid Crystals, 11th Workshop, Erice, Italy, 10-17 Luglio, Abstracts (2004).
12. R. Caputo, A.V.Sukhov, C. Umeton, A Veltri: “*Realization of POLICRYPS gratings - Optical and electro-optical properties*”, The 2nd Japanese-Italian Workshop on Liquid Crystals, Tsu, JAPAN September 5-8, Abstracts (2004).
13. G. Strangi, V. Barna, R. Caputo, A. De Luca, C. Versace, N. Scaramuzza, C. Umeton and R. Bartolino – “*Color Tunable Distributed Feedback Organic Micro-Cavity Laser*”- 11th Course of International School Liquid Crystals on “Phase Transitions in Liquid Crystals Effects of Surfaces and Ferroelectric Subphases - Erice, 10-17 July (2004).
14. M. Peccianti, C. Conti, G. Assanto, A. De Luca and C. P. Umeton – “*Nonlinear light beam propagation in nematic liquid crystals: nematicons and modulational instability*”- 6th National Meeting - (SICL) - Ischia, Hotel Continental Terme, 2-5 Giugno (2004)

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16. A. Veltri, L. Pezzi, A. De Luca, C. Umeton – “*A model for enforced unperturbed states and critical reorientation of liquid crystal acted on by two competing light beams*”- 6th National Meeting - (SICL) - Ischia, Hotel Continental Terme , 2-5 Giugno (2004)



## 9 BIOPHYSICS

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The research activity in year 2004 has essentially concerned two main topics in the field of Molecular Biophysics. In particular, the first has regarded self assembled supramolecular lipid structures, their dynamic properties and interaction with active biomolecules, while the second topic has concerned the thermal and spectroscopic properties of Metal-Proteins with oxidase activity. Molecular Dynamics Simulation of a Metal-Protein, Azurin, has also been considered. In the following the main results obtained in each field are reported.

### 9.1 SELF ASSEMBLED SUPRAMOLECULAR LIPID STRUCTURES: DYNAMICS PROPERTIES AND INTERACTIONS

#### 9.1.1 Transfer of stearic acids from Albumin to polymer-grafted lipid containing membranes probed by spin-label Electron Spin Resonance

Human serum albumin (HSA) has been spin labelled with stearic acids having the nitroxide moiety attached to the hydrocarbon chain either at the 5<sup>th</sup> or at the 16<sup>th</sup> carbon atom (n-SASL, n = 5 and 16, respectively) with respect to the carboxyl groups. Its interaction with sterically stabilized liposomes (SSL) composed of dipalmitoylphosphatidylcholine (DPPC) mixed with submicellar content of poly(ethylene glycol:2000)-grafted dipalmitoyl phosphatidylethanolamine (PEG:2000-DPPE) has been studied by conventional electron spin resonance (ESR) spectroscopy. In the absence of bilayer membranes, the ESR spectra of nitroxide stearic acids non-covalently bound to HSA are single component powder patterns, indicative of spin labels undergoing temperature dependent anisotropic motion in the slow motional regime on the conventional ESR timescale. The adsorption of HSA to DPPC bilayers results in two components ESR spectra. Indeed, superimposed to an anisotropic protein-signal appears a more isotropic signal due to the labels in the lipid environment. This accounts for the transfer of fatty acids from the protein to DPPC bilayers. Two spectral components with different rotational mobility are also singled out in the spectra of n-SASL bound to HSA when DPPC/PEG:2000-DPPE mixtures are present in the dispersion medium. The fraction,  $f_L(16-SASL)$ , of spin labels transferred from the protein to lipid/polymer-lipid lamellar membranes has been quantified performing spectral subtraction. It is found that  $f_L(16-SASL)$  decreases on increasing the content of the polymer-lipid mixed with DPPC. It is strongly reduced in the low-density mushroom regime and levels off in the high-density brush regime of the polymer-lipid content as a result of the steric stabilization exerted by the PEG-lipids. Moreover, the fraction of transferred fatty acids from HSA to SSL is dependent on the physical state of the lipid bilayers. It progressively increases with increasing the temperature from the gel to the liquid-crystalline lamellar phases of the mixed lipid/polymer-lipid membranes, although such a dependence is much weaker in the brush regime.

#### 9.1.2 Paclitaxel interaction with phospholipid bilayers: high-sensitivity differential scanning calorimetric study

High-sensitivity differential scanning calorimetry (DSC) has been used to study the interaction of the low water soluble anticancer agent Paclitaxel with multilamellar (MLVs) and unilamellar (ULVs) phospholipid vesicles. Three

different lipid matrices have been investigated: pure di-palmitoyl-phosphatidyl-choline (DPPC), a mixture of DPPC with 3 mol % of the polymer-lipid poly(ethylene glycol:2000)-dipalmitoyl-phosphatidyl-ethanolamine (PEG:2000-DPPE) and a mixture of DPPC with 10 mol % of dipalmitoyl-phosphatidyl-glycerol (DPPG). Each lipid matrix has been investigated with a Paclitaxel concentration ranging from 0 to 5 mol %.

For MLVs dispersions, irrespective of the lipid matrix, the presence of Paclitaxel from 1 to 3 mol % causes the down shift of both pre- ( $T_p$ ) and main ( $T_m$ ) phase transition temperatures and the broadening of the thermograms. The effects are, however, more pronounced on the pre-transition. The interaction of the drug with the lipid multilamellar vesicles is reduced at 5 mol % of Paclitaxel. In ULVs containing charged lipids, i.e., DPPC/PEG:2000-DPPE and DPPC/DPPG mixtures, the presence of Paclitaxel at concentrations  $\geq 3$  mol % affects significantly the main transition endothermic scans, with the appearance of side shoulders. The results suggest that the interaction of Paclitaxel is favoured with bilayer vesicles of low radius of curvature and with those containing lipids bearing a net negative charge on the polar heads.

### 9.1.3 Echo-Detected EPR Spectra of Spin-Labelled Lipids in Membrane Model Systems

The dynamics of spin-labelled lipid chains in the low-temperature phases of dipalmitoyl phosphatidylcholine (DPPC) membranes, with and without equimolar cholesterol, have been investigated by pulsed electron paramagnetic resonance (EPR) spectroscopy. Echo-detected spectra from the two-pulse, primary spin echo (pulse sequence:  $\pi/2 - \tau - \pi - \tau - \text{echo}$ ) are used to detect rapid angular motions, on the timescale of the phase memory time (T2M) that is in the nanosecond regime. Echo-detected spectra from the three-pulse, stimulated spin echo (pulse sequence:  $\pi/2 - \tau - \pi/2 - T - \pi/2 - \tau - \text{echo}$ ) are used to detect slow angular motions, on the timescale of the spin-lattice relaxation time (T1) that is in the microsecond regime. Spectra recorded at very low temperature (77 K) are used to correct the two-pulse echo spectra for instantaneous diffusion that arises from dipolar spin-spin interactions between different spin labels. Echo-detected inversion recovery spectra are used to correct the three-pulse echo spectra for intrinsic spin-lattice relaxation and large-scale spectral diffusion induced by nitrogen nuclear spin flips. The dependence of the echo-detected spectral lineshapes on the two time delays,  $\tau$  and T, can be simulated adequately by using a simple two-state model to represent the small-amplitude librational motions in the low-temperature membrane phases. The fast librational motion has isotropic character, no singly defined direction of the librational axis, and is segmental in nature, depending on chain position and also on the presence of cholesterol. The slow librational motion is of a more global, cooperative nature, being independent of chain position and cholesterol content.

### 9.1.4 Water concentration profiles in membranes measured by ESEEM of spin-labeled lipids

Electron spin echo envelope modulation (ESEEM) spectroscopy of phospholipids spin-labelled systematically down the *sn*-2 chain was used to detect the penetration of water ( $D_2O$ ) into bilayer membranes of dipalmitoyl phosphatidylcholine with and without 50 mol% cholesterol. Three-pulse stimulated echoes allow the resolution of two superimposed  $^2H$ -ESEEM spectral components of different widths, for spin labels located in the upper part of the lipid chains. Quantum-chemical calculations (DFT) and ESEEM simulations assign the broad spectral component to one or two  $D_2O$  molecules that are directly hydrogen-bonded to the N-O group of the spin label. Classical ESEEM simulations establish that the narrow spectral component arises from non-bonded water ( $D_2O$ ) molecules that are free in the hydrocarbon-chain region of the bilayer membrane. The amplitudes of the broad  $^2H$ -ESEEM spectral component correlate directly with those of the narrow component, for spin labels at different positions down the lipid chain, reflecting the local H-bonding equilibria. The  $D_2O$ -ESEEM amplitudes decrease with position down the chain towards the bilayer center, displaying a sigmoidal dependence on position that is characteristic of transmembrane polarity profiles established by other, less direct, spin-label methods. The midpoint of the sigmoidal profile is shifted towards the membrane center for membranes without cholesterol, relative to those with cholesterol, and the  $D_2O$ -ESEEM amplitude in the outer regions of the chain is greater in the presence of cholesterol than in its absence. For both membrane types, the  $D_2O$  amplitude is almost vanishingly small at the bilayer center. The water-penetration profiles reverse-correlate with the lipid-chain packing density, as reflected by  $^1H$ -ESEEM intensities from protons of the membrane matrix. Analysis of the H-bonding equilibria provides essential information on the binding of water molecules to H-bond acceptors within the hydrophobic interior of membranes. For membranes containing cholesterol, approximately 40% of the nitroxides in the region adjacent to the lipid headgroups are H-bonded to water, of which ca. 15% are doubly H-bonded. Corresponding H-bonded populations in membranes without cholesterol are ca. 20%, of which ca. 6% are doubly bonded.

### 9.1.5 Librational Motion of Spin-labelled Lipids in High-Cholesterol containing Membranes from Echo-Detected EPR Spectra

Two-pulse, echo-detected (ED) EPR spectroscopy was used to study the librational motions of spin-labelled lipids in membranes of dipalmitoyl phosphatidylcholine +50 mol% cholesterol. The temperature dependence, over the range 77-240 K, and the dependence on position of spin-labelling in the *sn*-2 chain ( $n = 5, 7, 10, 12$  and  $14$ ) of the phospholipid, were characterised in detail. The experimental ED-spectra were corrected for instantaneous spin diffusion arising from static spin-spin interactions, by using spectra recorded at 77 K, where motional contributions are negligible. Simulations according to a model of rapid, small-amplitude librations about an axis whose direction is randomly distributed are able to describe the experimental spectra. Calibrations, in terms of the amplitude-correlation time product,  $\langle \alpha^2 \rangle \tau_c$ , were constructed for diagnostic spectral lineheight ratios at different echo delay times, and for relaxation spectra obtained from the ratio of ED-spectra recorded at two different echo delays. The librational amplitude,  $\langle \alpha^2 \rangle$ , was determined for a spin label at the 14-C position of the lipid chain from the partially motionally averaged hyperfine splitting in the conventional EPR spectra. The librational correlation time,  $\tau_c$ , which is deduced from combination of the conventional and ED-EPR results, lies in the sub-nanosecond regime and depends only weakly on temperature. The temperature dependence of the ED-EPR spectra arises mainly from an increase in librational amplitude with increasing temperature, and position down the lipid chain. A gradual transition takes place at higher temperatures, from a situation in which segmental torsional librations are cumulative, i.e., the contributions of the individual segments add-up progressively on going down the chain, to one of concerted motion only weakly dependent on chain position. Such librational motions are important for glass-like states and are generally relevant to high lipid packing densities, e.g., in cholesterol-containing raft domains and condensed complexes.

## 9.2 THERMAL STABILITY AND MOLECULAR DYNAMICS SIMULATION OF METAL-PROTEIN WITH ELECTRON-TRANSFER PROPERTIES

### 9.2.1 Thermal stability of wild type and disulfide bridge containing mutant of poplar plastocyanin.

A comparative study of the thermal stability of wild type poplar plastocyanin and of a mutant form containing a disulfide bridge between residues 21 and 25 was performed using differential scanning calorimetry and optical spectroscopic techniques.

For wild type plastocyanin the transition temperature, determined from the calorimetric profiles, is 62.7 °C at the scan rate of 60 °C/h, whereas for the mutant it is reduced to 58.0 °C. In both cases the endothermic peak is followed by an exothermic one at higher temperatures.

The unfolding process monitored by optical absorption at 596 nm also reveals a reduced thermal stability of the mutated plastocyanin compared to the wild type protein, with transition temperatures of 54.8 and 58.0 °C, respectively. For both proteins, the denaturation process was found to be irreversible and dependent on the scan rate preventing the thermodynamic analysis of the unfolding process.

In parallel, small conformational changes between wild type and mutant plastocyanin emerge from fluorescence spectroscopy measurements. Here, a difference in the interaction of the two proteins between the microenvironment surrounding the fluorophores and the solvent was proposed.

The destabilization observed in the disulfide containing mutant of plastocyanin suggests that the double mutation, Ile21Cys and Glu25Cys, introduces strain into the protein which offsets the stabilizing effect expected from the formation of a covalent crosslink.

### 9.2.2 Calorimetric and spectroscopic investigations of the thermal denaturation of wild type Nitrite Reductase

Nitrite reductase (NiR) is a multicopper protein, with a trimeric structure containing two types of copper site: type 1 is present in each subunit whereas type 2 is localized at the subunits interface. The paper reports on the thermal behaviour of wild type NiR from *Alcaligenes faecalis* S-6. The temperature-induced changes of the copper centres are characterized by optical spectroscopy and electron paramagnetic resonance spectroscopy, and by establishing the thermal stability by differential scanning calorimetry. The calorimetric profile of the enzyme shows a single endothermic peak with maximum heat absorption at  $T_m \approx 100$  °C, revealing an exceptional thermal stability. The thermal transition is irreversible and the scan rate dependence of the calorimetric trace indicates that the denaturation of NiR is kinetically controlled. The divergence of the activation energy values determined by different methods is used as a criterion for the inapplicability of the one-step irreversible model. The best fit of the DSC profiles is obtained when the classical Lumry-Eyring model,  $N \leftrightarrow U \Rightarrow F$ , is considered. The simulation results indicate that the irreversible step prevails on the reversible one. Moreover, it is found that the conformational changes within the type-1 copper environments precede the denaturation of the whole protein. No evidence of protein dissociation within the temperature range investigated was observed.

### **9.2.3 The early steps in the unfolding of azurin**

High temperature molecular dynamics simulations were used to gain insight into the early steps in the unfolding pathway of azurin, a blue copper protein with a  $\beta$ -barrel structure formed by two sheets arranged in a Greek-key folding topology. The results reveal that unfolding of the  $\beta$ -barrel in azurin is associated with dislocation of its unique  $\alpha$ -helix with respect to the protein scaffold. Exposure of the hydrophobic core to solvent precedes complete disruption of secondary and tertiary structure, and modifications in the region around the active site are directly connected with this event. Denaturation of the protein initiates from the sheet coordinating the copper ion and the other sheet maintains its topology. Results derived from the simulation were compared with experimental data obtained with different techniques, showing excellent agreement and providing a framework to understand the process of disruption and formation of the  $\beta$ -barrel in azurin.

### **9.2.4 Selective analysis of protein inner motions at increasing time scale**

Different intramolecular motions activate at increasing timescale in atomic simulations of proteins. Essential dynamics as well as other techniques can be used to analyze principal components in search of coordinated motions of amino acid residues, but long enough protein simulation times are required. In this work, essential dynamics was applied to dissect out the internal motions of the blue-copper protein azurin in molecular dynamics simulation. The results show that simulations in the range of a few nanoseconds are not sufficient to assess global collective motions, but do give several indication on the dynamics on a longer timescale for this intrinsically rigid protein. Convergence of sampling for coordinate displacements of residues is obtained by leaving out of the analysis a small region of the protein structure selected by using the information achieved on the nanosecond scale. Selective filtering of the motions of uninteresting protein regions with high conformational freedom is suggested to be a suitable method to study the collective inner motions of proteins in the timescale currently accessible to molecular dynamics simulations.

## **A PUBLICATIONS ON SCIENTIFIC JOURNALS**

### **A.1 Publications on international journals**

#### **A.1.1 Publications on international journals printed in 2004**

1. B. Rizzuti, M. Swart, R. Guzzi, L. Sportelli, *Active site modeling in copper azurin molecular dynamics simulations* J. Mol. Modeling 10, 25-31 (2004)
2. D.A. Erilov, R. Bartucci, R. Guzzi, D. Marsh, S.A. Dzuba, L. Sportelli, *Echo-Detected EPR spectra of spin-labelled lipids in membrane model systems.*, J. Phys. Chem. B 108, 4501-4507 (2004)
3. R. Guzzi, L. Andolfi, S. Cannistraro, M. Ph. Verbeet, G. W. Canters, L. Sportelli, *Thermal stability of wild type and disulfide bridge containing mutant of poplar plastocyanin*, Biophysical Chem. 112, 35-43 (2004)
4. D.A. Erilov, R. Bartucci, R. Guzzi, D. Marsh, A.A. Dzuba, L. Sportelli, *Librational motion of spin-labelled lipids in high-cholesterol Containing membranes from echo-detected EPR spectra*. Biophysical Journal 87, 3873-3881 (2004)
5. B. Rizzuti, V. Daggett, L. Sportelli, R. Guzzi, *The early steps in the unfolding of azurin*, Biochemistry 43,15604-15609 (2004)

#### **A.1.2 Publications accepted on international journals during 2004**

1. S. Belsito, R. Bartucci, L. Sportelli, *Paclitaxel interaction with phospholipids bilayers: High-sensitivity differential scanning calorimetry investigation.*, Thermochemica Acta, (2004), Accepted
2. M. Pantusa, L. Sportelli, R. Bartucci, *Transfer of stearic acids from albumin to polymer-grafted lipid containing membranes probed by spin-label electron spin resonance*. Biophysical Chem. (2004), Accepted
3. M. Arca, G. Azimi, F. Demartin, F. A. Devillanova, L. Eschriche, A. Garau, F. Isaia, R. Kivelas V. Lippolis, V. Muns, A. Perra, M. Shamsipur, L. Sportelli, A. Yari, *Complexes of Cu(II) with mixed-donor phenantroline-containing macrocycles: analysis of their structural, redox and spectral properties in the context of type-I blue copper proteins biomimetic models*. Inorg. Chim. Acta (2004), Accepted

#### **A.1.3 Papers submitted for publication during 2004**

1. D.A. Erilov, R. Bartucci, R. Guzzi, A.A. Shubin, A.G. Marysov, D. Marsh, S.A. Dzuba, L. Sportelli, *Water concentration profile in membrane measured by ESEEM of spin labelled lipids*, J. Phys. Chem. (2004) submitted
2. B. Rizzuti, L. Sportelli, G. Guzzi, *Selective analysis of protein inner motion at increasing time scale*. Phys. Rev. E (2004) submitted

## **D PRESENTATIONS AT CONFERENCES**

### **D.1 Presentations at International Conferences in 2004**

1. Bartucci R., *Time resolved studies in spin labeled biosystems*, Workshop on "Lipid-Protein Interactions", Szeged, Hungary, 23-25/07/2004

### **D.2 Presentations at National Conferences in 2004**

1. G. Di Santo, R. Bartucci, L. Sportelli, *Interaction of Beta-Amyloid peptide(25-35) and lipid bilayers probed by spin-label ESR*. XVII Congresso Nazionale della Società Italiana di Biofisica Pura ed Applicata, Pisa, 23-25 Sett. 2004.
2. A. Stirpe, R. Guzzi, H. Wijma, M. Ph. Verbeet, G. W. Canters and L. Sportelli, *Calorimetric and spectroscopic investigations of the thermal unfolding of wild type and type-2 copper depleted Nitrite Reductase*. XVII Congresso Nazionale della Società Italiana di Biofisica Pura ed Applicata, Pisa, 23-25 Sett. 2004.

3. B. Rizzuti, V. Daggett, L. Sportelli and R. Guzzi, *Molecular Dynamics of Early Unfolding Events in Azurin*, XVII Congresso Nazionale della Società Italiana di Biofisica Pura ed Applicata, Pisa, 23-25 Sett.2004
4. F. Scarpelli, R. Guzzi, R. Bartucci, L. Sportelli, *Pulsed ESR study of spin labeled hemoglobin*, Contributo a MDM CNR-INFM Meeting, Italian conference on matter, devices and materials Genova, 8-10 Giugno 2004
- 5.** B. Rizzuti, R. Guzzi, L. Sportelli, *Unfolding Events in Azurin as Evidenced with Experiments and Simulation* MDM CNR-INFM Meeting, Italian Conference on Physics of Matter, Genova, 8-10 Giugno 2004
6. B. Rizzuti, L. Sportelli, R. Guzzi, *Molecular dynamics of early unfolding events in azurin* (Invited ), XVII Congresso Nazionale della Società Italiana di Biofisica Pura ed Applicata, Pisa, 23-25 Sett.2004
7. G. Di Santo, R. Bartucci, L. Sportelli, *Perturbation of lipid bilayers by beta-amyloid peptide(25-35). Spin-label ESR studies*, MDM CNR-INFM Meeting, Italian conference on matter, devices and materials, Genova, 8-10 Giugno 2004
8. B. Rizzuti, L. Sportelli, R. Guzzi, *Sampling of protein inner motions in molecular dynamics simulations*, MDM CNR-INFM Meeting, Italian conference on matter, devices and materials, Genova, 8-10 Giugno 2004.

## 10 GEOPHYSICS, APPLIED GEOPHYSICS, ENVIRONMENTAL GEOPHYSICS

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### 10.1 Seismotectonics

Seismotectonics is the branch of seismology that deals with the complex relations between earthquakes and geological structures. 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 map of seismicity that results 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 non 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, Rom (INGV); the second is the basic instrument to conduct seismotectonic investigations.

In 2004, the greatest effort has been the *CAT/SCAN* project designed by a research group in the Lamont-Doherty Earth Observatory (Columbia University, New York). Its main aim is the better understanding of the structure and tectonic relationship between Northern Calabria and the neighbouring areas. Since Winter 2003 about 40 seismographic stations have been installed in Campania, Basilicata, Puglia and Calabria. The program has developed in a joint effort of Lamont, INGV and University of Calabria. In particular this research group was entrusted with the management of 20 seismographic stations installed in Northern Calabria.

A first workshop held in Camigliatello Silano (near Arcavacata) in the Summer 2004 has been attended by about 80 scientists from Italy and USA.

### 10.2 Statistical Seismology

A new line of research has been recently developed as a result of a joint effort between this group and the Astrophysics Group of the Physics Department.

The main interest has been in modelling the pattern of seismic occurrence. The main result is the retrieval of a relation that describes the pattern of both of main events and seismic sequences. A fall-out of this investigation is the observation that world wide distributed main events have a pattern of occurrence that shows a weak correlation of every event with those preceding it.

The most recent line of investigation is related to eventual links between Sun free oscillations and earthquakes activity. This investigation seems very promising but is still at an initial stage.

A consequence of this activity has been the organization of a meeting in Cetraro (near Arcavacata) in the Spring 2004. This meeting has been attended by all the most known researchers in the field in Italy.

### **10.3 Site effects**

One of the problems in seismic risk assessment arises from the frequent empirical observation that different sites at very short distances one from the other can behave very differently under the effects of an earthquake. This is due to differential amplifications and polarizations of the elastic waves due to very local conditions. Identification, characterization and detailed mapping of small-sized homogeneous are the phases of the so-called “seismic microzonation”. This knowledge will then be transferred in the construction of the seismic risk maps.

In 2004, the research group has been involved in the “Urban Project” of the city of Crotona, devoted to analyze the present situation and provide scientific and technical basis for the future development of the inhabited area. In this activity collaboration exists with research groups in urban-planning and earthquake engineering active in the Calabria University. Specific task of the geophysical group was to provide for the seismotectonic framework of the city by analyzing the seismicity, both historical and instrumental, and the necessary information for the microzonation.

### **10.4 Applied Geophysics**

Several surveying techniques can be used to map buried geological bodies. Among these, the *magnetic survey* is one of the most interesting. It consists in measuring the intensity of the magnetic field within a closely spaced grid (about 1 km step). Then the main earth core source component of the signal is subtracted from the collected data. In a similar manner also the periodical variation are subtracted. The remaining portion of the signal, termed *magnetic anomaly*, can be attributed to variations in the magnetic susceptibility of the rocks that compose the Earth crust. The interpretation of this residual field consist in creating a geometrical model of the buried structures that causes a synthetic field as similar as possible to the observed one.

The research group is currently working on the construction of a detailed magnetic map of Calabria. The effort will obviously take several years.

### **10.5 Environmental geophysics**

This branch of geophysics deals with the investigation of very shallow phenomena that however most directly affects human activity.

Among the many possible techniques, the research group concentrates on the analysis of the content of  $Rn^{222}$  of gases flowing from soils. It is in fact well known that excessive Radon concentrations can be extremely dangerous to human health. This gas is naturally discharged in particular geodynamic areas. Since it is rather heavy, it has the tendency not to be dispersed in the atmosphere, particularly in closed and badly ventilated buildings.

Its interest is also linked to its association to seismic activity. In the frame of a CIPE Project completed in 2004, the prototype has been built of a continuous gas monitoring station. Data being acquired by this device will be analyzed by searching for correlations with seismic activity.



## **A PUBLICATIONS ON SCIENTIFIC JOURNALS**

### **A.1 Publications on international journals**

#### **A.1.1 Publications on international journals printed in 2004**

1. Barberi G., Cosentino M.T., Gervasi A., Guerra I., Neri G. e Orecchio B.: *Crustal seismic tomography in the Calabrian Arc region, South Italy* - Phys. Earth Plan. Inter., 147, 4, 297-314. (2004)

## **B MEMORIES** (Extended proceedings of conferences or book chapters)

### **B.1 International Memories**

#### **B.1.1 Memories published on International Conference Proceedings in 2004**

1. Carbone V., Cosentino M. T. e Guerra I.: *Departures from a local Poisson process in the distribution of aftershocks* – Atti 21° Conv. Ann. Gr. Naz. Geofis. Terra Solida, CD ROM, 2004
2. Guerra I., Harabaglia P., Cosentino M.T. e Gervasi A.: *La sequenza sismica del 21 ottobre 2001 nell'Alta Valle del Savuto (Calabria): un caso di migrazione di stress* – Atti 21° Conv. Ann. Gr. Naz. Geofis. Terra Solida, CD ROM, 2004
3. Guerra I., Cosentino M. T., Gervasi A., Harabaglia P. e Rosa A. B.: *The September, 9th, 1998, Pollino, Southern Italy, earthquake sequence : a case of sequential activity of multiple tectonic systems* - Atti 21° Conv. Ann. Gr. Naz. Geofis. Terra Solida, CD ROM, 2004
4. Carbone V., Cosentino M. T., Sorriso-Valvo L., Harabaglia P. and Guerra I.: *Multifractal Distribution of Seismic Moment* - Atti 22° Conv. Ann. Gr. Naz. Geofis. Terra Solida, Cd Rom, 2004
5. Carbone V., Cosentino M. T., Sorriso-Valvo L., Harabaglia P. and Guerra I.: *Scaling Law for Calm Intervals Between Seismic Events* – Atti 22° Conv. Ann. Gr. Naz. Geofis. Terra Solida, 2004

## **D PRESENTATIONS AT CONFERENCES**

### **D.1 Presentations at International Conferences in 2004**

1. G. Barberi, A. Gervasi, I. Guerra, P. Harabaglia, G. Neri, B. Orecchio: *Crustal structure and shallow seismicity in the Calabrian Arc region, South Italy* - EGS, Nice, 2004.
2. Guerra I.: *The seismicity of the Calabrian Arc region: an overview* – 1<sup>st</sup> CAT/SCAN Workshop, Camigliatello Silano.
3. Neri G., Oliva G., Orecchio B., Presti D., Barberi G., Guerra I.: *Seismogenic fault detection, a basic step towards the correct management of territory in the earthquake-prone area of Northeastern Sicily and Southern Calabria* – 1<sup>st</sup> International Conference of Applied Geophysics for Engineering – Messina, 2004
4. Pizzino L., Quattrocchi F., Guerra I., Moretti A., Cinti D., Galli G., Voltattorni N.: *Fluid geochemistry as a tool in the discrimination of fault systems and fault interaction areas and their stress-strain pathfinders parameters: case histories from Italy* – 1<sup>st</sup> International Conference of Applied Geophysics for Engineering – Messina, 2004
5. ATTOLICO A., CIORCIARI C., GALLIPOLI M.R., GUERRA I., HARABAGLIA P., MUCCIARELLI M. E ROSA A. B.: *IL SIGNIFICATO SISMOTETTONICO DELLA MICROSISMICITÀ IN BASILICATA* – 22° CONV. ANN. GR. NAZ. GEOFIS. TERRA SOLIDA, 2004
6. Gervasi A., Guerra I., Neri G., Orecchio B., Valensise G.: *Detailed identification of large seismogenic sources in Calabria, Southern Italy, based on recent shallow seismicity and crustal tomographic structure vs. local geology* – AGU Fall Meeting, S. Francisco, 2004.
7. Steckler M.S., Amato A., Guerra I., Di Luccio F., Lerner-Lam A., Persaud P., Seeber L., Armbruster J., Tolstoy M., Cimini G.B., Piomallo C., Di Maro R., D'Anna G., Gervasi A., De Rose C.: *CAT/SCAN, the Calabria-Apennine-Tyrrhenian/Subduction-Accretion-Collision Network* - AGU Fall Meeting, S. Francisco, 2004.

## ORGANIZATION OF CONFERENCES

1. *Modelli non lineari ed analisi statistiche in sismologia: caos, frattali e processi di auto-organizzazione*, Cetraro, May 12-14, 2004. (in collaboration with the group of Astrophysics)
2. *1<sup>st</sup> CAT/SCAN Workshop*, Camigliatello Silano (Cosenza, Italy), June 30 – July 2, 2004.