EMMS STUDENTS' WORKSHOP

"A look into the future of materials science"

BOOK OF ABSTRACTS

AAU
UA
TUHH

EMMS
European Master in Materials Science

Education and Culture
Erasmus Mundus

**AVEIRO,
JUNE 8-9, 2006**

WELCOME

Wherever we look, the materials are an important part of the every day life. The development of better sporting goods, medical devices, structures, and machines is only possible by deeply understanding the materials' properties. The students that choose to study materials science have the aim of pushing further the limits of the currently available materials and develop new ones.

We, the students of the first EMMS class, are about to conclude our course. Therefore, we are working now on the development of our master thesis. The aim of this workshop is precisely to present the progress obtained in these works. Furthermore, this workshop pretends to increase the interaction between the students of the three universities involved in the programme.

This book of abstracts contains the summary of the presentations carried out during the EMMS Students' Workshop *"A look into the future of materials science"* that took place at the University of Aveiro. It is divided in three sections:

1. Metals and Ceramics
2. Polymer Nanocomposites
3. Optoelectronics and Semiconductors

We would like to bid you the welcome in the different languages of the students of the first EMMS class and the partner universities involved.

English
Welcome to the EMMS Students' Workshop, *"A look into the future of Materials Science"*.

Danish
Velkommen til workshoppen for EMMS studerende, *"Et kig ind i materiale-fysikkens fremtid"*.

German
Herzlich Willkommen beim EMMS Studentenworkshop, *"Ein Augenblick in der Zukunft der Materialswissenschaft"*.

Portuguese
Bem-vindos ao Workshop dos estudantes do EMMS, "Um olhar no futuro da Ciência dos Materiais".

Chinese
EMMS 学生专题研讨会欢迎您! *"展望材料科学未来的天空".*
(EMMS xue sheng tao lun hui huan ying nin, " Zhan wang cai liao ke xue wei lai de tian kong")

Igbo
Ibiala na ogbako workshop nke Umu akwukwo EMMS, " Ileba anya na ubochi ndi di na ihu nke ihe omumu Materials Science".

Indonesian
Selamat datang di Workshop Mahasiswa EMMS, " Memandang masa depan ilmu bahan".

Russian
Добро пожаловать на студенческую конференцию "Взгляды на будущее материаловедения"
(Dabro pojalovat' na studencheskuyu konferenziyu "Vzglyad na buduschee materialovedeniya")

Spanish
Bienvenidos al EMMS Students' Workshop, *"Una Mirada al Futuro de la Ciencia de los Materiales"*.

EMMSSA 2004-2006

EMSSA

Ricardo Chavez

Sonia Pinho

Orley Ferri

Adhitya Trenggono

Kingsley Iwu

Ilya Peshekhodov

Nataliya Kalashnik

ACKNOWLEDGEMENTS

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Thanks to all the students who participated in this workshop with their presentations.

Thanks to Mr. Raul Chavez for helping during the edition of this book of abstracts and the development of the workshop's image.

Thanks to all our guest speakers for contributing with their presentations.

Thanks to Prof. Ana Barros, Prof. Vítor Amaral, and Prof. Elisabete Costa for helping us with the organization and providing ideas for this workshop.

Thanks to Mrs. Raquel Valz for assessing us during this workshop's organization.

Thanks to Mr. Rodrigo Pacher Fernandes for his comments and ideas.

Thanks to Região de Turismo de Aveiro for providing information about Aveiro.

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PROGRAMME

June 8 at “Sala de Actos Académicos” of Rectory

8:30-9:00: Register

9:00: Welcome message from EMMSSA

9:15: Opening by Prof. Isabel Martins, UA’s Vice-rector for Postgraduate studies

9:30: “Effect of periodic overloads on fatigue crack propagation in Ti-6Al-4V” by Orley Ferri

9:50: “BST Thin Films Prepared by a Modified Sol-Gel Processing at Low Annealing Temperature for Microelectronic Applications” by Jie Gao

10:10: Coffee break

10:25: “INEGI: Developing new composite materials” by Dr. Celeste Pereira and Dr. Nuno Correia, Guest speakers from Instituto de Engenharia Mecânica e Gestão Industrial (INEGI)

11:00: “Poly(meth)acrylates/Double-walled Carbon Nanotubes: grafting from” approach via ATRP” by Adhitya Trenggono

11:20: “Development of PA12 nanocomposites based on functionalized CNFs and CNTs” by Ricardo Chavez

11:40: Lunch

14:00: “Nanoparticles encapsulating lanthanide complexes for bio-application” by Kingsley Iwu

14:20: “Experimental characterization and ab-initio modeling of a Si (111) substrate and the growth of a thin film of Ag on this substrate” by Sonia Pinho

14:40-16:00: Poster session

16:00: “New trends” by Dr. Paulo Ventura, Guest speaker from Qimonda

16:30: “Dealing with complexity in the machines of the future” by Prof. Osvaldo Novais de Oliveira Júnior, Guest speaker from Instituto de Física de São Carlos.

17:30: “Understanding Fracture Behaviour of Thin Layers: Mechanical Characterization of Thin Film Resistors on LTCC Substrates” by Ilya Peshekhodov

18:00-18:30: Concert

20:00: Dinner

June 9 at "Anfiteatro de Engenharia Mecânica" of Mechanical Engineering Department

9:00: "Research activities in Materials Science at UA" by Dr. Tito Trindade and Dr. Paula Vilarinho

10:00: "Research activities in Materials Science at TUHH" by Dr. Hans Wittich

10:30: Coffee break

11:00: EMMSSA activities report

11:20: Closing

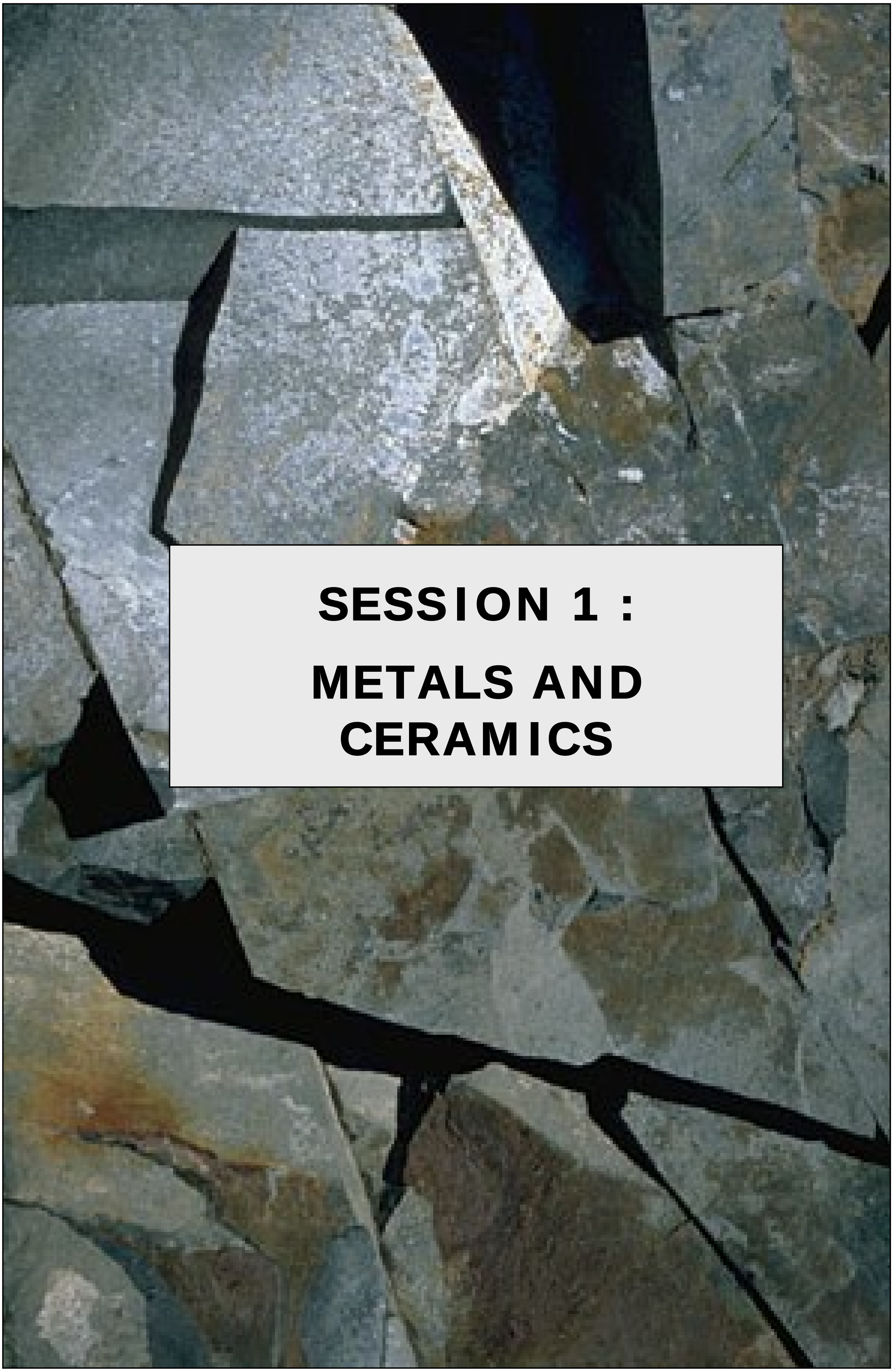
12:00-14:00: Lunch

14:00: "Presentation of UA" by Dr. Niall Power

14:20-16:30: Tour through UA's laboratories

SESSION 1 :

METALS AND CERAMICS



Effect of periodic overloads on fatigue crack propagation in Ti-6Al-4V

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The reliability of damage-tolerant structures subjected to variable amplitude loading during service depends on understanding the effect of the loading conditions on fatigue crack propagation. In this study, the influence of periodically applied tensile overloads on the crack propagation behavior of Ti-6Al-4V alloy was investigated. Former studies on aluminum alloys showed that such overloads caused acceleration or retardation of crack propagation rate depending on the microstructure, the number n of intermittent baseline cycles between consecutive overloads and the environment [1].

The influences of the microstructure on the crack propagation behavior in the $(\alpha + \beta)$ titanium alloy Ti-6Al-4V was studied by comparing a fine bi-modal and a coarse lamellar condition. The thermo mechanical treatment to achieve the two different microstructures involved cross-rolling (ϕ=-1.4) at 940°C using 15 passes with intermediate reheating for 2 minutes, and air cooling after the last pass. Recrystallization at 960°C for 1 hour and air cooling was performed in order to obtain the bi-modal microstructure. A lamellar microstructure is achieved by heat treatment at 1050°C for 1 hour in the β phase field, followed by controlled cooling (1K/min) to room temperature. Finally, the two different microstructures were age-hardened at 500°C for 24 hours to precipitate fine coherent Ti_3Al particles.

Fatigue crack propagation tests were performed using CT-specimens (B=8mm, W=32mm) with a computer controlled servo hydraulic testing machine, operating under load control at 30Hz (sine wave) and an R-ratio of 0.1. The experiments were performed at room temperature in air and in vacuum. Tests at constant amplitude and periodically superimposed single tensile overloads (overload ratio 1.5) were carried out. Intermittent baseline cycles of n=5,000 between consecutive overloads was applied. The crack closure effect was monitored using the conventional back-face strain gauge technique. The characterization of the overload effects has been accomplished by the comparative analysis of fracture surfaces and the measured resistance against fatigue crack propagation for the different testing conditions. Detailed investigations of the fracture surfaces have been carried out with a scanning electron microscope (SEM). Furthermore, crack front profiles in the through-thickness (S) direction were prepared for the investigation of the crack front geometry by light microscopy (LM).

The first results from tests performed in air revealed a retardation of the crack propagation rate due to periodic overloads for both microstructures, when compared to constant amplitude loading. The reduction of the crack propagation rate due to the overloads was more pronounced for bi-modal microstructure than for the lamellar one. The coarse lamellar microstructure showed higher resistance to fatigue crack propagation than the bi-modal microstructure. This superior behavior of lamellar microstructures is explained by crack branching, secondary cracking, and an overall tortuous crack path [2]. The most probable explanation for the retardation effect could be due to changes of the crack front roughness and the slip mechanism [3].

The experiments in vacuum will be performed and the results will be compared to the experiments in air. The differences in the fracture surfaces will be analyzed in order to identify the mechanism causing the fatigue crack growth retardation.

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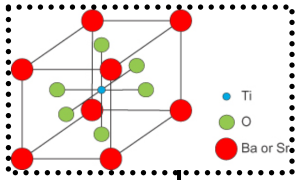

BST Thin Films Prepared by a Modified Sol-Gel Processing at Low Annealing Temperature for Microelectronic Applications

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$(Ba_{1-x}Sr_x)TiO_3$ (BST) materials have much potential application in microelectronic devices owing to its excellent dielectric properties, in terms of high dielectric constant, low loss tangent, low leakage current, and high dielectric breakdown strength [1-4]. In order to minimize thermal stress and interdiffusion between different layers, the temperature of the preparation process should be as low as possible. In the current work, sol-gel derived $(Ba_{0.8}Sr_{0.2})$ TiO_3 (BST80/20) thin films were fabricated on $Pt/Ti/SiO_2/Si$ substrate at a lower annealing temperature by using BST nano powders as seeds. The effect of seeds were investigated and analyzed on the crystallinity, microstructure and morphology of BST thin films. XRD analysis showed the crystallization temperature of BST thin films was decreased from 750 ºC to 600 ºC when using BST seeds. The crystallization kinetics of BST thin films were studied with respect to the effect of seeds. Scanning electron microscopy (SEM) and piezoforce microscopy (PFM) were employed to characterize the influence of seeds on the microstructure, morphology and ferroelectric domain structure of BST thin films. The dielectric properties of BST thin films, including permittivity, loss tangent, tunability and leakage current, were measured and studied as a function of seeds effect. The relationship between effect of seeds and dielectric properties of BST thin films was established and discussed.

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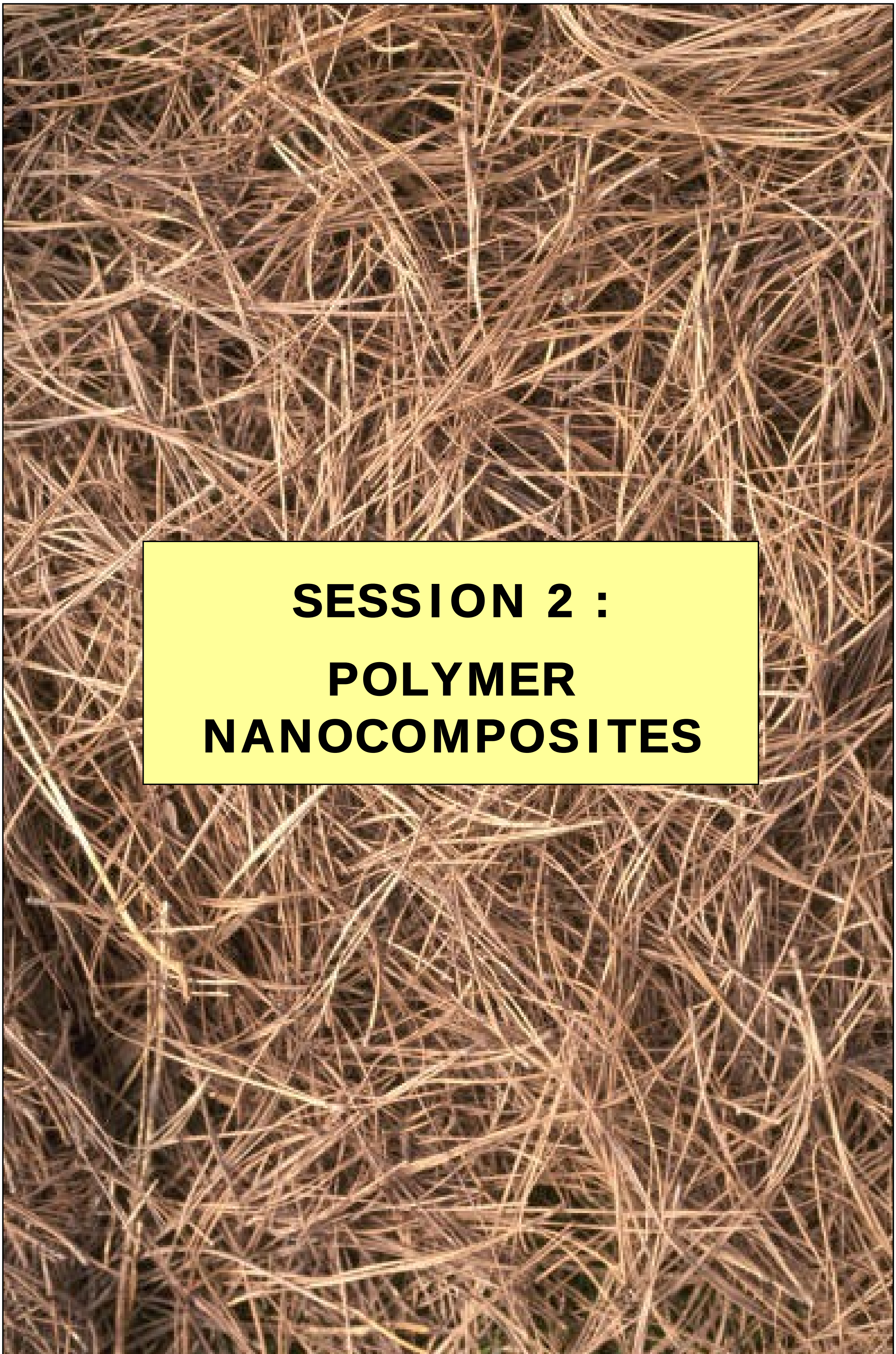
SESSION 2 :

POLYMER NANOCOMPOSITES



Poly(meth)acrylates/ Double-walled Carbon Nanotubes: "grafting from" approach via ATRP

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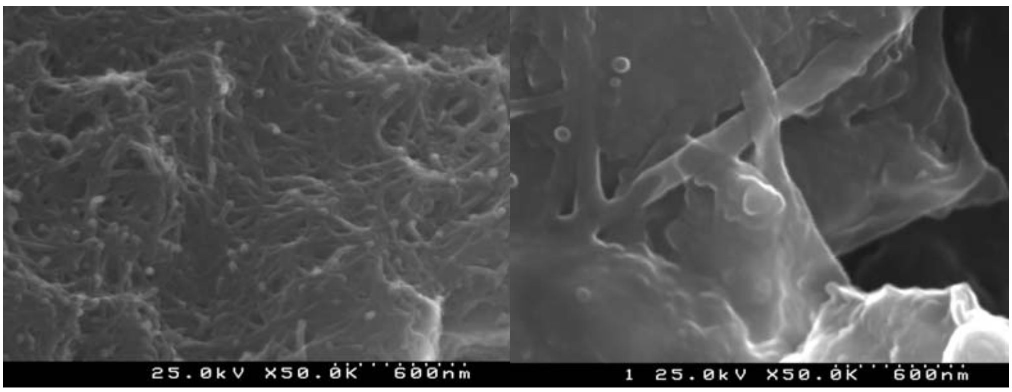
One of challenging aspects of carbon nanotubes/polymer composite is insufficient dispersion of carbon nanotubes in polymer matrices. Chemical functionalization of carbon nanotubes surfaces have been used to increase the dispersion [1, 2]. Atom Transfer Radical Polymerization (ATRP) is one type of controlled radical polymerization, which enables to increase the dispersion and grow well-defined polymer molecules from inorganic surfaces [3], including carbon nanotubes [4].

The objectives of this work are to improve the dispersion of double-walled carbon nanotubes (DWNT) in a poly(methyl methacrylate) (PMMA) matrix and to investigate the effect of interface structure of polymer functionalized DWNTs over the mechanical and thermal properties of DWNTs/PMMA composites. The surfaces of DWNTs have been functionalized by carboxylic acid, halogen acid, glycol, and ATRP initiator successively. Then, methyl methacrylate (MMA) and butyl acrylate (BA) - monomers were initiated and grown from the initiator functionalized DWNTs surfaces to yield DWNTs/PMMA and DWNTs/poly (BA-b-MMA).

The presence of the polymer molecules on the DWNTs surfaces has been confirmed by FTIR, Raman, TGA, and SEM. Studies regarding the morphology, thermal stability, and dynamic mechanical performance of polymer functionalized DWNTs/PMMA nanocomposites samples prepared via solution polymerization and then casting are presently being investigated.



a **b**

SEM image: pristine DWNTs (a) and polymer functionalized DWNT (b).

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Development of PA12 nanocomposites based on functionalized Carbon Nanofibres and Carbon Nanotubes

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Recently, carbon nanofibre (CNF) and carbon nanotube (CNT) composites gained attention due to their electrical and mechanical properties, which made them to be introduced in a great diversity of new applications [1, 2]. The development of carbon nanotube and carbon nanofibre reinforced polymer composites does not only offer unique opportunities to improve the physical and mechanical properties of a given matrix, but also allows the evaluation of the intrinsic properties of the reinforcing nanoscaled phase. The utilization of carbon nanotubes and vapour-grown carbon nanofibres as reinforcements already yielded in an improvement of the mechanical, electrical and thermal properties of various polymer matrix systems [1, 2]. The manufacture of CNT / CNF reinforced polymer composites depends mainly on two factors: a homogeneous dispersion of the CNT / CNF in the polymer matrix and a strong interfacial adhesion to enable a stress transfer from the matrix to the reinforcing element. However, the synergisms between the reinforcing element and the changes in morphology of the matrix are not totally understood.

In order to improve the interaction between a Polyamide 12 (PA12) matrix with the CNFs, the nanofibres were oxidized for 4hrs. using nitric acid at 80°C. Composites with different weight percentages of carbon nanofibres were produced: 0.1%, 0.2%, 0.5%, 1.0%, and 2.5%. The composites were obtained using two processes. First, the functionalized CNFs were mixed with the PA12 using a twin screw extruder. Thereafter, the obtained material was pelletized and injection moulded. All composites were characterized using dynamic mechanical analysis (DMA) and differential scanning calorimetry (DSC).

DMA results indicate that already 0.1% of CNFs lead to an increase in the storage modulus of the studied materials. This increase is about 30% at room temperature (RT). Further increases in the CNF weight percentage produce higher modulus. DMA results also show that the neat PA12 and all the nanocomposites present the same β- and glass transition temperatures.

The nanocomposite with 0.1% of oxidized CNFs present higher storage modulus than the one compounded using the same amount of non oxidized CNFs [3]. In comparison to neat PA12, this increase is about 30% and 17% for the nanocomposites containing oxidized and untreated fibres, respectively.

DSC studies point out changes of the PA12 because of the CNFs, which act as nucleating agents leading to a smaller crystal size. A CNF weight content of 0.1% produces an increase of around 3°C in the crystallization temperature in comparison to the neat PA12. Further increases in the CNF content do not lead to higher crystallization temperatures, but further decrease the crystal size.

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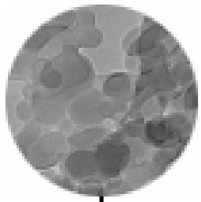
SESSION 3 :

OPTOELECTRONICS AND SEMICONDUCTORS



Nanoparticles encapsulating lanthanide complexes for bioapplication

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Silica and titania nanoparticles encapsulating lanthanide (Ln) complexes of 3-hydroxypicolinate (L3HP)) and picolinate (LP) were synthesized by the sol-gel method based hydrolysis of alkoxides in a reverse micelle medium-water in oil emulsion stabilized by a surface active agent (surfactant). The size of the water droplets or nano-reactor approximately determined the size of the nanoparticles formed. The size of the nano-reactor was varied by using distinct amount of water, maintaining constant the surfactant concentration.

The optical features of the as prepared nanocomposites were investigated and compared to those of the pure Ln complexes, having in mind their potential application as bio-labels. Transmission electron microscopy was chiefly employed to study the morphology of the nanocomposites. The results showed that the luminescence properties of the LP in the nanocomposites were severely affected by the synthetic process while those of the L3HP were markedly different from those of the pure L3HP. These optical properties will be correlated to the synthetic strategy employed and the implication for the envisaged bioapplications will be discussed.

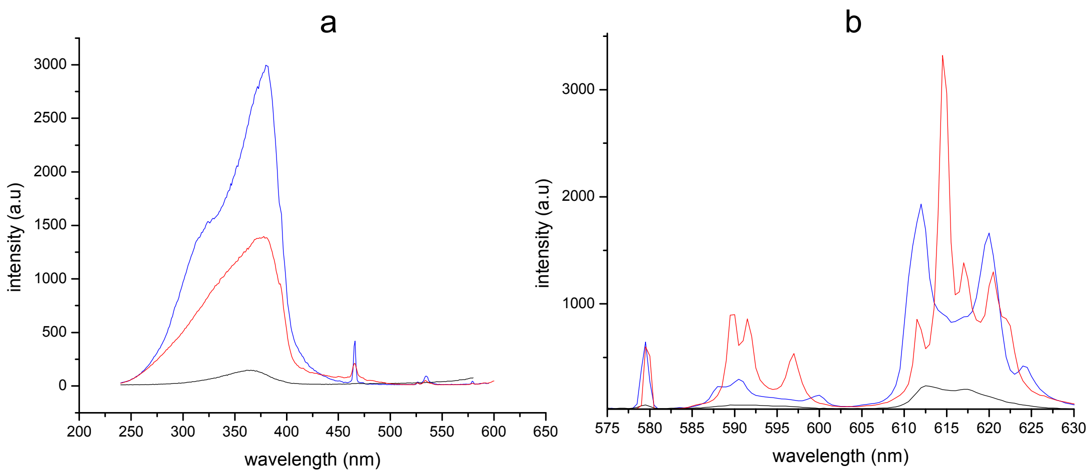

Fig. a. Photoluminescence excitation (PLE) spectra of pure L3HP (red), silica-L3HP nanocomposite (blue), and titania-L3HP nanocomposite (black). The broad excitation band centered around 370 nm represents absorption by the ligands (3-hydroxypicolinate), implying that energy was efficiently absorbed by the ligands and transferred to the europium for subsequent emission. The small, sharp peak at 465 nm represents direct europium excitation. b. Photoluminescence (PL) spectra of pure L3HP (red), silica-L3HP nanocomposite (blue), and titania-L3HP nanocomposite (black).

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Experimental characterization and ab-initio modelling of a Si (111) substrate and the growth of a thin film of Ag on this substrate

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The exploration of properties of semiconductor crystals has undergone a large development in decades past, provoking an intense impact on the technological industry, particularly in the area of information technology. Silicon plays a very important role in the technological world and there have therefore already been intensive studies carried out upon this semi-conductive crystal.

Miniaturization has become the primary goal of this industry; reducing in size while increasing in quality. An important part of the development of nanotechnology is the ability to implement it in society in a realistic commercial framework. From this perspective it is necessary to develop and improve the nanoscale production techniques.

A new innovative subject within this field is nanowires. A possible technique is the deposition of an adsorbate on the edges of regularly spaced, parallel steps on a substrate crystal. This requires the capability of characterising and producing substrate surfaces as well as experience with selection of substrate, adsorbate and preparation techniques. A deeper understanding of the mechanisms of such constructions could contribute to the development of more efficient methods to gain satisfactory results.

The bulk structure for Si were produced and investigated by *ab-initio* modelling, where a pseudopotential spin density-functional supercell code (AIMPRO) [1] was used. Lattice constant, Bulk Modulus, Total Energy, Gap Energy, Bandstructure, and Density of States were calculated and compared with previously published measurements. A reconstructed Si (111)-(7x7) surface structure was also produced and investigated by *ab-initio* modelling.

Experimental characterization of a surface of a Si-crystal was obtained. This surface was prepared in a planar orientation, some 3º degrees skew relative to the Si (111) plane. The characterization was achieved with the use of Auger Electron Spectroscopy (AES), Low Energy electron Diffraction (LEED), and Electron Energy Loss Spectroscopy (EELS). The achievement of a reconstructed Si (111)-(7x7) surface structure was confirmed as well as the $\sqrt{3} \times \sqrt{3}$-Ag superstructure.

In terms of applications, it is both very important and difficult to understand film growths especially since a variety of factors contribute to the growth process. The Ag growth on a Si (111) surface was studied by AES. A possible wetting-layer-island growth mode was verified by comparing the coverage predicted by different growth mode equations. The possibility of Ag deposition in the area between islands was detected based on the characteristics of the AES and the obtained growth curves.

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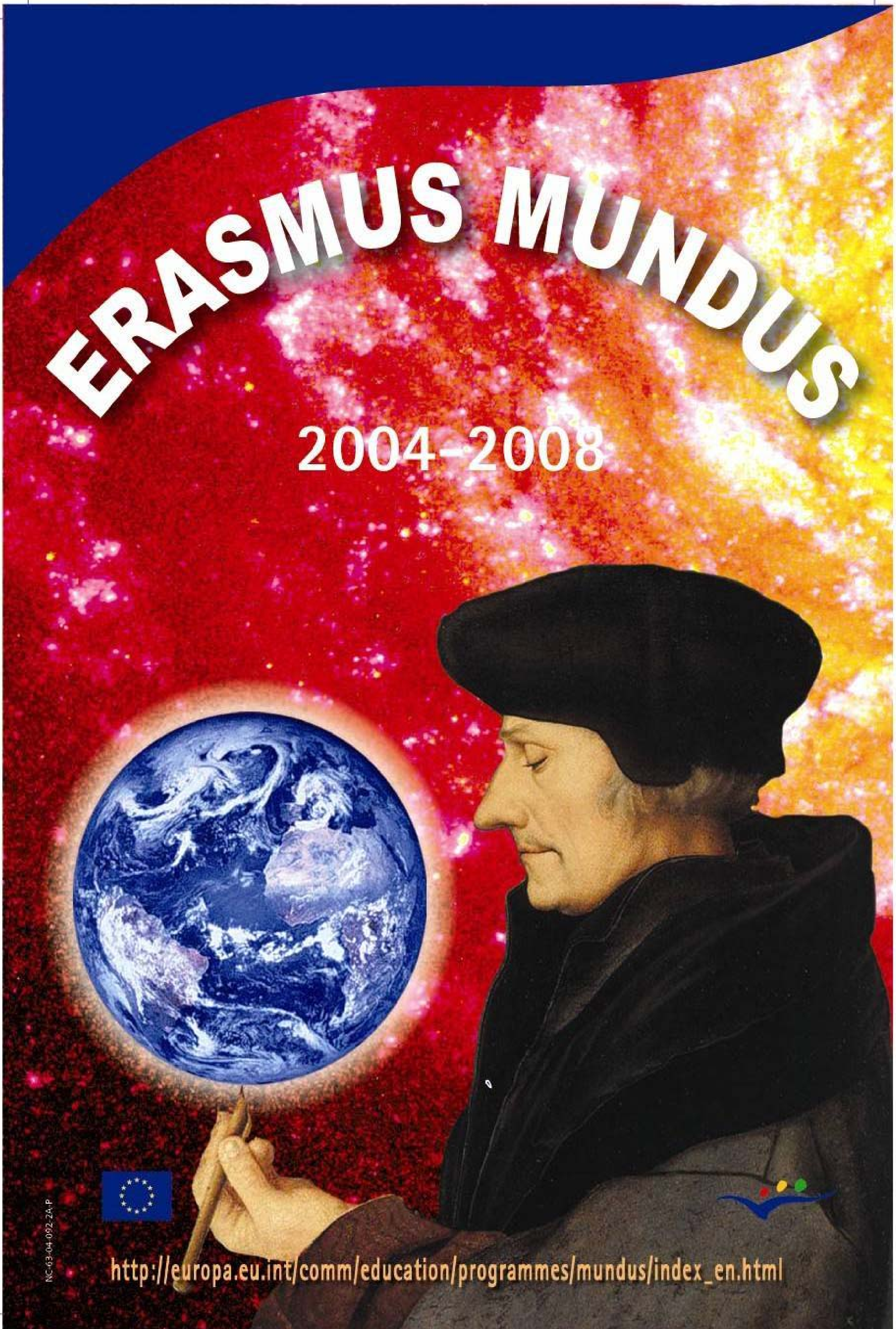
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