

Modern Methods of Materials Science Modelling

organizers:

Interdisciplinary Centre for Mathematical and Computational Modelling
in the frame of
Centre for Materials Modelling

Workshop will begin on Tuesday, September 6, 2005 at 11.00. The workshop will be held at the Warsaw University, ICM, Al. Zwirki i Wigury 93, 02-089 Warsaw, Poland (for more information about the workshop location - how to get to, see [www: http://www.icm.edu.pl/eng/about/](http://www.icm.edu.pl/eng/about/)).

1 Scope of the Workshop

The workshop is organized by Interdisciplinary Centre for Mathematical and Computational Modelling (Warsaw University) in the frame of Centre for Materials Modelling.

The workshop to be held at the Warsaw University is an international event, intended mostly for the postgraduate and PhD students as well as young scientist specialising in the modelling of materials.

The workshop will provide an opportunity for young scientists to learn structural and elastic properties investigations from first principles (ab initio) calculations and to introduce to methods of computer simulation in meso and macro scale.

All participants are welcome to discuss the research problems encountered in computational materials science.

2 Scientific Program

11.00-11.30 **Prof. Marek Niezgodka, Dr Maria Gokieli** *Meso and macro scale structure formation by means of phase separation mechanism*

We will expose some propositions of mathematical models for phase transformations mechanisms, expressed in the language of partial differential equations and of discrete lattices. The first of the phenomena is spinodal decomposition, which is a conservative process, observed in macroscale. The second one is an order-disorder transition, that might be observed only in microscale. The mathematical models start from van der Waals (1893) and refer to equations known as Cahn-Hilliard and Allen-Cahn.

11.30-11.40 *Break*

11.40-12.30 **Dr Anna Trykozko, Dr Kerstin Kantiem** *Application of Finite Element Method in materials modelling in macroscale*

Finite Element Method (FEM) has become widely applied to numerical solving of models including partial differential equations. In this talk an application of FEM to problems in the materials modelling will be outlined. A short practical

introduction to FEM will be given, followed by elementary examples. Finally, numerical simulations of diffusion-driven structure formation phenomena governed by Cahn-Hilliard models will be presented.

12.30-12.40 *Break*

12.40-13.20 **M.Sc. Michal Lopuszynski, M.Sc. Robert Sot** *Ab-initio methods in Materials Science and their application to calculation of elastic properties of solids*

In this talk a short introduction to *ab-initio* methods for simulations in solids will be given. Particularly the framework of density functional theory (DFT) will be outlined. This theoretical introduction will be followed by a brief overview of existing DFT software packages and their functionality. Finally, as an example of practical engineering problem, application of the above techniques to calculating the elastic properties of materials will be discussed.

13.20-14.00 *Break*

14.00-16.00 **M.Sc. Michal Lopuszynski** *Introduction to MedeA modeling*

MedeA is an environment for computer-assisted design of materials. The name MedeA stands for 'Materials Exploration and Design Analysis' and these words aptly describe MedeA's function. MedeA focuses on the properties of solids, surfaces and interfaces of inorganic materials and properties, but can also be applied to organic matter.

MedeA software can be applied to bulk materials, layered materials, interfaces and to surfaces, including surface chemistry and chemical reactions. Amorphous materials can be treated within a supercell model, where amorphous domains are replicated with periodic boundary conditions. The validity of this approach depends of course on the size of the repeated cell and the type of system and property.

3 Secretariat of Workshop on Modelling Applications in Materials Science

Participation in the workshop is free of charge and the number of participants is limited by the size of the teaching laboratory.

Registration by e-mail: workshop-icm@icm.edu.pl

M.Sc. Robert Sot
Interdisciplinary Centre
for Mathematical and Computational Modelling
(Warsaw University)

4 Workshop Place

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Lecture room - 3089 (11.00-13.20), Computer Lab - 3083 (14.00-16.00)