

Preface

Most properties of contemporary materials in advanced technologies follow from structural transformations whose dynamics are governed by atomistic mechanisms that must be controlled. This general goal cannot be achieved on one hand without elucidating the nature of nano-structural (atomistic) phenomena both experimentally and by means of modelling or simulations covering the problems of structural defect thermodynamics and physics of atomic migration in condensed phases, and on the other hand, without elaborating links between nano- and meso-scale approaches to modelling the processes. As is apparent from many meetings and discussions, advanced methods and concepts of condensed-matter physics are now definitely entering the domain of contemporary materials science. This is to a great extent due to the current rapid development of hardware and software computational facilities.

The main idea of the Symposium: Multiscale Kinetic Modelling of Materials organized within the Fall Meeting of the European Materials Research Society, Warsaw 4-8 September 2006 was to gather physicists, materials scientists/engineers and other scientists carrying out interdisciplinary research dedicated to the multiscale modelling of time-evolving phenomena in materials. Although such problems have recently been taken up in contributions scattered over various conferences/sessions, it seemed appropriate to organize a special symposium with its programme clearly focused on materials dynamics aimed at stimulation of new insight into the subject matter that would give rise to the development of new material technologies that are well-grounded in materials physics.

The symposium focused on two basic aspects of investigations:

- (i) The current development of theoretical and model approaches to structural kinetics (links between quantum electron theories of solids and non-equilibrium thermodynamics);
- (ii) Computer simulations as an effective tool for studying atomistic mechanisms of structural kinetics (Monte Carlo and Molecular Dynamics: suitability, efficiency, limitations, results).

Almost 40 oral and poster contributions addressing the above basic aspects were presented during 7 sessions: Simulation Techniques for Bridging Length and Time Scales; Phase Transformations; Ordering Processes; Precipitate Formation; Simulation of Defect Processes; Microstructure, Layers and Thin Films; Simulation of Nanostructures.

This volume contains selected and refereed papers presented at the Symposium.

Rafał Kozubski

Graeme E. Murch

Paweł Zięba