

Preface

It would be difficult to find a process running in any material technology, which would not involve atomic migration. The phenomenon is a mechanism of not only the mass transfer (diffusion), but also of a great variety of structural transformations occurring and observed in all distance and time scales.

The general intention of the book is to give the readers a wide image of physical problems connected with the processes controlled by atomic migration and of the methods of their modelling. It is composed of seven extended articles showing the subject matter studied in particular scales.

The presentation starts with a chapter devoted to the “ab-initio” (DFT) modelling directly based on the ideas of Quantum Mechanics and thus linking the contemporary nano-scale Materials Science to the Physics of Condensed Matter. The power of Molecular Dynamics (MD) as an efficient technique for atomic-scale modelling is demonstrated in the following four articles which show not only a wide scope of the modelled phenomena, but also point at particular problems to be solved in order to make the MD simulation results valuable.

The last two chapters of the book lead a reader beyond the atomic scale modelling. The path goes through the Phase Field technique to the Finite Element method and shows the wide scope of time and distance scales covered by the contemporary modelling techniques. The development of the PF illustrates in addition the efforts for linking the particular methods and creating the new ones adequate for really multiscale modelling of materials.

The volume straightforwardly addresses researchers and graduate students working in the field of diffusion and diffusion-controlled processes in condensed matter.

Due to the wide scope of the presented topics it should, however, be interesting to all scientists active in the fields of condensed-matter physics and materials science. In view of the fast development of materials technologies, it is expected that representatives of industrial R & D centres will also be found among the volume readers.

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