Preface

Alongside theory and experiment, simulation is today considered equally as a fundamental means for scientific investigation. Materials science is a field where computational methods have found particularly widespread application.

There is a wealth of reports in the scientific literature presenting the results of computational material science studies, but the actual machinery used to perform these calculations is much less well documented. Against this backdrop, the *Software Development for Process and Materials Design* symposium was held in Moscow on September 15-16, 2002 as a satellite symposium to the *Nano and Giga Challenges in Microelectronics* meeting. The focus of the symposium was to introduce and discuss software tools used to explore questions related to materials science and technology development, with an emphasis on detailing the algorithms and software tools used to accomplish the calculations. We will continue these important exchanges with the *US-Russian Workshop on Software Development to Bridge Atomic and Macroscopic Scales for Materials, Process, and Device Design* to be held at Arizona State University, Tempe, AZ, November 13-15, 2003.

To capture the latest advances in software technology we present this special issue which have enabled the remarkable achievements of computational materials science in recent years. It is our hope that this special issue will simultaneously serve as an overview to the types of computer tools currently being developed and applied within the field of computational materials science, and to provide detailed information to readers on specific implementions across a wide range of problems. Papers in this volume cover important software categories: atomic scale simulation; materials structure, chemistry, and thermodynamics, electronic structure computation, nanotechnology, and graphical and informatics approaches in materials design.

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