Responsable :
Fabien BRUNEVAL
01 69 08 43 49

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Kinetics and thermodynamics of defects, impurities, nanostructures and interfaces

Matthias Posselt

Forschungszentrum Dresden-Rossendorf
Institute of Ion Beam Physics and Materials Research
Dresden, Germany

Computer simulations using classical interatomic potentials are an efficient and promising tool to investigate and understand atomic-level properties and processes in advanced materials. They allow the consideration of length and time scales which are often hardly accessible by experiments. However, the accuracy of the interatomic potentials employed in such type of simulations determines decisively the quality of the obtained results. Therefore, these potentials must be continuously improved and evaluated.
In the present contribution three applications of atomistic computer simulations are illustrated. The focus is on kinetics, energetics and thermodynamics of defects, impurities, nanostructures and interfaces in materials for micro- and nanoelectronics and in structural materials for fission reactors.

The first example deals with molecular dynamics simulations on basic migration mechanisms of mono- and di-(self-)interstitials in Si. Both the atomic mobility due to the presence of the defect and the defect mobility itself were determined. The mechanism of di-interstitial migration depends on temperature, in contrast to that of the mono-interstitial.

In the second example amorphous Si and Ge as well as their solid-phase epitaxial recrystallization (SPER) are considered. Results obtained by different interatomic potentials are compared. The molecular dynamics simulations yield amorphous material with realistic structural and thermodynamic properties, but the SPER rate is strongly overestimated. It is shown that a more realistic SPER rate can be obtained using a modified interatomic potential which yields a higher melting temperature of the amorphous phase. This is explained by the fact that both melting and SPER are essentially determined by the flexibility of atomic bonds.

The subject of the third example is the formation of coherent clusters containing vacancies, Cu and Ni in bcc-Fe. Using the most recent interatomic potential for Fe-Cu-Ni alloys, the structure, energetics and thermodynamics of the clusters were determined. Many clusters up to a size of 200 monomers (vacancies, Cu and Ni atoms) were studied. In the case of vacancy-Cu clusters a core-shell structure is found where Cu atoms coat the outer surface of vacancy clusters. In a vacancy-Cu-Ni cluster Ni atoms are never first nearest neighbors of vacancies, and the Ni atoms cover the Cu-surface of inner vacancy-Cu cluster. The total and monomer binding energy as well as the nucleation free energy of the clusters were calculated. The monomer binding energy is an important input parameter of rate theory and object kinetic Monte Carlo simulations. For further application in these calculations compact and physically-based fit formulae were derived from the atomistic data.

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