

MM 31 Hauptvortrag Walter Wolf

Zeit: Montag 14:00–14:30

Raum: TU H1058

Hauptvortrag

MM 31.1 Mo 14:00 TU H1058

Finite temperature ab initio modeling of formation and migration of impurities, point defects and planar faults — •WALTER WOLF — Materials Design, Le Mans, France and Taos, (NM) USA

Ab initio methods have proved to be powerful in exploring properties of defects such as vacancies, antisites, impurities, stacking faults or grain boundaries. Nowadays, even temperature effects can be routinely included by ab initio lattice dynamics. In this contribution, emphasis is put on effects from finite temperature, defect migration and interaction.

Impurities are of large impact on phenomena such as stress corrosion cracking and may cause serious materials fatigue. Since cracking typically occurs at grain boundaries, a large variety of impurities (H, O, S, P, B, alloying metals) and combinations thereof are investigated for their impact on grain boundary cohesion in metals. Their statistic distribution is estimated from grain boundary and surface segregation energies and site preference energies. Temperature dependent energy and entropy contributions are included. As a result, candidates responsible for grain boundary weakening or strengthening are identified.

Formation and migration of point defects are studied. Energy profiles of diffusion paths are explored and metastable and transition states are analyzed thermodynamically. As a result, solubility and diffusion processes can be quantitatively predicted. In particular for hydrogen impurities, zero point vibrations are critically important. Taking into account temperature dependence enables reliable predictions at working temperature for technological applications, and has pushed the ab initio approach into direct application within the industrial research process.