INTERDISCIPLINARY CENTRE FOR
ADVANCED MATERIALS SIMULATION

ICAMS Special Seminar

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Lattice instabilities in metallic elements

Most metallic elements have a crystal structure that is either body centered cubic, face centered close-packed or hexagonal close-packed. If the bcc lattice is the thermodynamically most stable structure, the close-packed structures usually are dynamically unstable, i.e., have elastic constants violating the Born stability conditions or, more generally, have phonons with imaginary frequencies. Conversely, the bcc lattice tends to be dynamically unstable if the equilibrium structure is close-packed. This striking regularity essentially went unnoticed until ab initio total energy calculations in the 1990s became accurate enough to model dynamical properties of solids in hypothetical lattice structures. After a review of stability criteria, I discuss thermodynamic functions and how instabilities may arise or disappear when pressure, temperature and/or chemical composition is varied. I also comment on the ideal strength of solids, amorphization and melting.