Multiscale Modelling of Interstitial and Vacancy Defects in bcc Metals

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We develop a comprehensive multiscale model for single self-interstitial atom and vacancy defects in body-centred cubic transition metals forming groups 5B (vanadium, niobium and tantalum) and 6B (chromium, molybdenum and tungsten) of the Periodic Table. The model spans the electronic, atomistic and mesoscopic scales, and describes the electronic structure, interatomic interactions, and thermally activated mobility of defects.

Density-functional calculations show that in all the non-magnetic bcc metals the axially-symmetric 111 self-interstitial atom configuration has the lowest formation energy. In chromium the difference between the energies of the 111 and the 110 self-interstitial configurations is very small, making the two structures almost degenerate. Local densities of states for the atoms forming the core of the 111 crowdion configurations exhibit systematic widening of the local d-band and an upward shift of the anti-bonding peak in empty states. Using the information provided by electronic structure calculations, we derive a family of the Finnis-Sinclair-type interatomic potentials for vanadium, niobium, tantalum, molybdenum and tungsten.

Using these potentials, we perform molecular dynamics simulations of thermally activated migration of self-interstitial atom defects in tungsten, and compare the results with the earlier studies of thermal migration of self-interstitial atom defects in vanadium. We rationalize the results of simulations using analytical solutions of the multi-string Frenkel-Kontorova model describing non-linear elastic interactions between a self-interstitial defect and phonon excitations. We find that the discreteness of the crystal lattice plays a dominant part in the picture of mobility of defects. We are also able to explain the origin of the non-Arrhenius diffusion of crowdions observed at elevated temperatures.

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