INTERDISCIPLINARY CENTRE FOR ADVANCED MATERIALS SIMULATION

MMM Seminar

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Room IC 02/718

Maarten de Jong
University of California, Berkeley

First principles-design of rhenium-based alloys for improved ductility and lower cost

Amongst refractory metals, hexagonal close packed (hcp) rhenium (Re) is uniquely distinguished by its absence of a measured brittle-ductile transition. This makes the material particularly attractive for applications involving exposure to extreme variations in temperature. However, the usage of Re-rich alloys is inhibited by its high cost and world-wide scarcity. In this work, first principles total energy-calculations are employed to identify potential substitutional solute elements that can be used to create Re-based alloys with lower cost, while maintaining important mechanical properties such as room-temperature ductility.

First principles-calculations are used to assess elastic properties and defect energies (twin boundaries, surfaces, stacking faults) as a function of solute content. From this, intrinsic ductility parameters can be extracted. Trends in two independent ductility parameters with solute species are found to be consistent and to correlate with d-band filling.

Further, it is shown that the high ductility of pure Re is likely related to its anomalously low {1121} twin boundary energy. A theoretical justification of the anomalously low twin boundary energy and its variation with alloying (band filling) is provided. The justification is based on the structural similarity between the {1121} twin boundary and topologically close-packed (tcp) phases, which are metastable but close in energy to hcp near the Re band filling.