Atomistic Studies of Deformation and Fracture in Materials with Mixed Metallic and Covalent Bonding

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Abstract
Materials with high melting temperatures (over 2000°C) tend to be brittle at ambient and even relatively high temperatures. High melting temperatures originate in strong interatomic bonding arising from formation of \(dd\) or \(dp\) bonds that also affect and/or control crystal structures and properties of extended defects, such as dislocations, grain boundaries. These, in turn, govern plastic deformation and fracture.
General goal: Establish relationship between electronic structure and mechanical behavior

Comments
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General goal: Establish relationship between electronic structure and mechanical behavior.

Materials studied

**BCC transition metals:** Mo, W, Nb, Ta, V  
**FCC transition metal:** Iridium  
**Intermetallic compounds:** MoSi$_2$, Mo$_5$Si$_3$, Ir$_3$Nb, Ir$_3$Zr

**MOTIVATION OF RESEARCH**

**CORE STRUCTURE OF THE 1/2[111] SCREW DISLOCATION IN MOLYBDENUM**

Bond-order potential and $ab$-initio DFT-based calculations of Woodward and Rao

**MOLYBDENUM**

Tension and compression compared with corresponding pure shear in the direction of the Burgers vector. If only the shear stress parallel to the Burgers vector controlled glide, the CRIS would be the same for pure shear, tension and compression.

**FUTURE RESEARCH**

**SHORT TERM**

Properties of special and general grain boundaries in iridium and comparison with other fcc metals to clarify the propensity for intergranular brittleness in polycrystalline iridium.

Studies of stacking faults and dislocations in molybdenum silicides: MoSi$_2$ (tetragonal C$11_b$, hexagonal C40, orthorhombic C54) and Mo$_5$Si$_3$ (D$8_m$).

**LONG TERM**

Transition bcc metals (Mo, W, Ta, Nb, V)

Establish general rules of the dependence of their plastic behavior on electronic structure, in particular filling of the d-band. Investigate effects of point defects, in particular interstitials produced by irradiation, impurities and alloying elements on dislocation glide and thus deformation and fracture of these materials.

**FERROMAGNETIC IRIDIUM**

Development and testing of BOP that includes ferromagnetism. Using this BOP to investigate dislocations, interstitials, grain boundaries, alloying elements and their interactions in bcc iron with emphasis on effects of ferromagnetism and comparison with non-magnetic bcc metals.