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Intrinsic solid-solution softening in BCC Mo from dislocation-solute interactions DALLAS TRINKLE, SATISH RAO, CHRISTOPHER WOODWARD, Air Force Research Laboratory, Wright Patterson AFB, OH — Solid solution softening observed in the group VA and group VIA transition metals has traditionally been attributed to either extrinsic effects—such as interstitial scavanging—or intrinsic effects—direct solute/dislocation interaction. We invesitgate intrinsic mechanisms using first principles methods. First, density functional theory calculates directly the interaction of Re, Hf, Os, W, Ir and Pt solutes with a straight $< 111 >$ screw dislocation in Mo. The local strain field associated with the dislocation core is self-consistently coupled to the long-range elastic field using the recently developed lattice-Green function boundary-condition method. The construction of simple interaction models from the *ab initio* data allows the extension of chemically accurate calculations to physically relevant length scales. We contrast the direct interaction energies with size- and modulus-misfits of solutes using the work of Fleischer. The misfits alone are unable to explain the presence of both softening and hardening, requiring the more complete treatment provided by *ab initio* methods.

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