Abstract Submitted
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Intrinsic mechanism of the solid solution softening and hardening in bcc transition metal alloys: combined first principles calculations with atomic row modeling[1] N. I. MEDVEDEVA, YU. N. GORNOSTYREV, A. J. FREEMAN, Northwestern U. — The solute–dislocation interaction is of great interest since it determines one of the important strengthening mechanisms in alloys. It is still unclear why some alloying elements lead to hardening but others give rise to softening at low temperature. To reveal the intrinsic mechanisms in solution softening/hardening, the interaction of d transition metal additions with dislocations in bcc metals was studied by using a combined approach including the atomic row model with *ab-initio* parametrization of interatomic interactions. We found opposite trends in solute-dislocation interaction for the Groups V and VI bcc metals. Additions with extra valence electrons, which enhance the double kink nucleation and result in softening in the Group VI metals, cannot lead to softening in the Group V metals and vice versa; additions with fewer electrons may give rise to softening in the Group V metals but lead to strong hardening in the Group VI metals. We demonstrate that the electronic structure, rather than atomic size or shear modulus misfits, plays an important role in the softening/hardening effects in bcc transition metal alloys.

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