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Chemistry effects on dislocation mobility in refractory bcc metals

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Using a novel concurrent multiscale approach we demonstrate that the *local environment* of transition-metal solutes in refractory bcc metals has a large effect on the mobility and slip paths of dislocation. The results reveal that solid solutes or nano-clusters of different geometries may lead to solid-solution hardening (SSH) or softening (SSS), in agreement with experiment, including spontaneous dislocation glide and activation of new slip planes. The underlying electronic mechanism is also studied by the multiscale approach. Solutes nano-cluster can affect Peierls potential surface (PPS) dramatically. The results indicate that it is the change of the anisotropy of the lattice resistance induced by solutes that result in the different behavior of the dislocation according to the different geometries of solutes nano-clusters.

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