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Effect of alloying on screw dislocation structure in Mo: atomistic modelling approach with ab-initio parametrization[1] YU.N. GORNOSTYREV, N.I. MEDVEDEVA, A.J. FREEMAN, Northwestern University — The plastic deformation in bcc metals is realized by the motion of screw dislocations with a complex star-like non-planar core. In this case, the direct investigation of the solute effect by first principles electronic structure calculations is a challenging problem for which we follow a combined approach that includes atomistic dislocation modelling with *ab-initio* parametrization of interatomic interactions. The screw dislocation core structure in Mo alloys is described within the model of atomic row displacements along a dislocation line with the interatomic row potential estimated from total energy full-potential linear muffin-tin orbital (FLMTO) calculations with the generalized gradient approximation (GGA) for the exchange-correlation potential. We demonstrate (1) that the solute effect on the dislocation structure is different for "hard" and "easy" cores and (2) that the softener addition in a "hard" core gives rise to a structural transformation into a configuration with a lower energy through an intermediate state. The softener solute is shown to disturb locally the three-fold symmetry of the dislocation core and the dislocation structure tends to the split planar core.

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