Evaluation of dislocation mobility and plastic properties of molybdenum using molecular dynamics.

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Being a widely spread construction material, alloyed and pure molybdenum is usually affected by continuous external stresses. Therefore it has to be studied in terms of plasticity and creep which is helpful for safety issues. Plastic properties of metals are considered to be governed by variety of processes including twining, martensite transitions and dislocation movement. In case of body-centered cubic metals, the contribution of twinning and martensite transitions to plastic properties can be neglected and plasticity can be studied in terms of motion of dislocations.

Since dislocations in real materials usually form a complex forest, it is challenging to study the behaviour of a single dislocation in an experiment. The use of molecular dynamics, which has already shown good results in simulation of atomic-level processes, allow one to consider the movement of a single dislocation. In this work the dislocation movement was studied using the method of molecular dynamics with ADP interatomic potential.

To perform dislocation mobility estimation, the calculation cell with a single dislocation was created. The results of calculations showed the screw dislocation to be less mobile than edge one which is in a agreement with the common conception. It means that plastic properties of molybdenum is controlled by the motion of screw dislocations. In addition, two regimes of dislocation motion are shown to exist: thermo-activated and viscous regimes. The main differences between these two regimes are the forms of velocity-stress and velocity-temperature dependencies. Moreover, the movement in the thermo-activated regime is characterised by kink-pair nucleation and migration. In contrast, the behaviour of kinks do not govern the motion in the viscous regime.

Using theoretical models of a dislocation movement, we estimated the enthalpy of a kink-pair nucleation and the friction coefficients of the dislocation motion in the viscous regime. In addition, making a comparison to experimental data we estimated the density of dislocations in the molybdenum single crystal. Finally, the obtained dislocation mobility functions allowed us to make the estimation of yield stress of molybdenum using the method of dislocation dynamics.