Macroscopic characteristics of plastic deformation in bcc metals described through dislocation mobility properties

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Plastic deformation of bcc metals is a complicated phenomenon that links behaviour of the crystal defects with a macroscopic change in a sample shape. It is known that one of the basic mechanisms of plasticity is motion of dislocations under applied stress. In this work, the plastic deformation in bcc metals (Mo and Nb) was studied with large-scale atomistic modelling. The temperature-dependent mobility functions of screw and edge dislocations were calculated from molecular dynamics simulation. The simulations of screw dislocation movement under applied shear stress revealed that the process can proceed in two different regimes: through thermally activated motion and athermal motion. Hence, the dislocation velocity depends on the shear stress in a non-trivial way. The calculated data provide a way to evaluate the basic macroscopic characteristics of plastic deformation (yield stress, activation volume and strain rate sensitivity) at various temperatures and strain rates. The obtained results agree well with the existing experimental data (see Fig.1) and give opportunity to predict a plastic behavior in case where the measured data are absent.

Keywords: dislocations, bcc metals, multiscale modeling

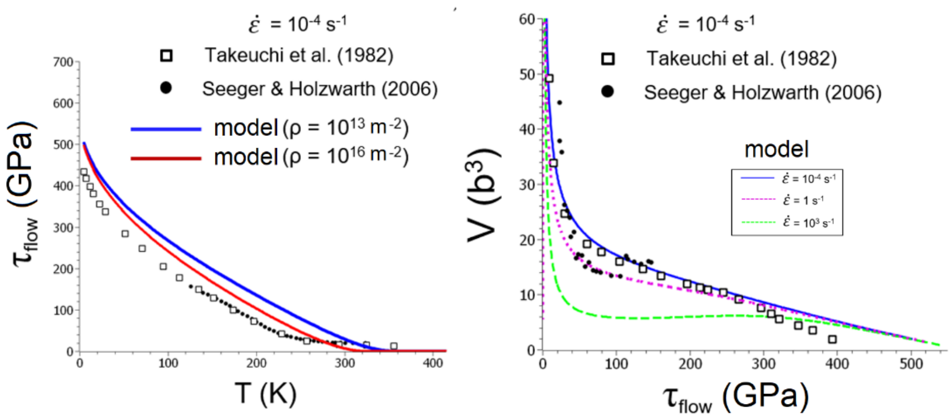

Fig.1 The comparison of the calculated characteristics of plastic deformation in Nb with the existing experimental data.

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