Ab-initio simulations of grain boundary sliding in aluminum and nickel

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The Hall-Petch relationship predicts an increase in material yield strength with decreasing grain size. However, a breakdown has been reported at smaller grain sizes, where plastic deformation gradually becomes grain boundary dominated. Studying grain boundary sliding process is therefore key to understanding the mechanical properties of polycrystalline materials. In the present work, we use density functional theory to examine the microscopic processes that accompany grain boundary sliding in aluminum and nickel for a $\Sigma = 11(113)$ tilt grain boundary. Sliding of tilt boundaries is also accompanied with grain boundary migration, where grain boundary movement normal to the boundary surface takes place. Heat of solution of tungsten in nickel was calculated and is also presented. Sliding in nickel was studied for both pure nickel and in cases where a few atoms of nickel at the grain boundary were substituted with tungsten atoms. The effect of adding tungsten on the sliding process is also reported.