

[PO-E1]Poster Session 1

Symposium E

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[P1-23]Study of solute effect on the yield strength of Fe-based dilute alloy using atomistically informed kinetic Monte Carlo method

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Solid solution hardening/softening is one of the ways to control mechanical properties of alloys. The trend of change in mechanical properties of solid solution alloys due to solute addition is generally non-linear against a solute element, concentration, strain rate, and temperature. In order to develop the advanced alloy, prediction of mechanical strength is important to reduce the cost and development time.

It is well known that the solute atoms in crystalline metals affect mechanical strength by interacting other lattice defects such as dislocation. Although many researchers have studied the interaction between dislocation and solute atoms to understand solid solution hardening/softening, detail of solute effect on dislocation motion is not fully clarified yet.

In this work, we investigate the solute effect on the yield strength of body-centered cubic (BCC) alloy by analyzing dislocation motion using kinetic Monte Carlo (kMC) model based on atomistic understanding. We focus on dilute BCC Fe-based alloy including substitutional solute Si atom.

First, we analyze the solute effect on screw dislocation motion, which mainly dominates plastic deformation of BCC metals, based on atomistic modeling. In order to estimate the solute effect on screw dislocation motion, we performed nudged elastic band calculation to obtain activation energy of dislocation motion via kink mechanism which includes a kink-pair nucleation and kink migration processes.

Then, obtained activation enthalpy of each process and solute effect on them is introduced to kMC model to calculate activation rate of dislocation motion. By performing kMC simulation, we estimate dislocation velocity in different concentration, temperature, and stress conditions, and evaluate the solute effect on dislocation velocity.

Finally, we predict yield strength from estimated dislocation velocity and discuss the effect of solute atoms.