

# DISLOCATION DYNAMICS SIMULATION OF PRECIPITATION HARDENING

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Investigation of the effect of solute-atom precipitates on the material strength is a very important issue in the materials science. Solute-atom precipitates work as obstacles to dislocation motion, resulting in the hardening of the material. Therefore, understanding the interaction between a dislocation and a solute atom precipitate is very important to determine the material strength of metals. The hardening of the material due to the solute-atom precipitation has been theoretically and experimentally investigated, but simulation technique to study the precipitation hardening mechanism has not been well established yet.

Recently, a dislocation dynamics (DD) computer simulation technique is becoming a very promising approach to study the strength of metals based on the fundamental behavior of dislocations in the metals<sup>[1]</sup>. The DD method handles short-range interactions of dislocations, such as dislocation annihilation and jog formation, by the use of appropriate local rules<sup>[2]</sup> that can be determined theoretically and/or numerically using lower length- and time-scale computer simulations such as molecular dynamics (MD). In our simulations, local rules for the interaction between a dislocation and a solute-atom precipitate are first determined based on the results of the MD simulations, and the rules are further used in the DD simulations to understand the effect of precipitates on stress-strain behavior of the material of interest. This approach enables us to simulate the dislocation motions interacting with the solute-atom precipitates with no empirical parameters.

In this paper, we demonstrate the DD simulation of the precipitation hardening. We focus on the bcc-Fe containing Cu precipitates. Local rules for the interaction between dislocation and Cu precipitate are, as described above, determined based on the results of MD simulations, and the local rules are further used in the DD simulations. The availability of the local rules in DD simulation is tested with a simple model, and it can be confirmed that the local rules can reproduce well the interactions that can be seen in the MD simulations. Then, we perform DD simulations of the materials with different number densities of the Cu precipitates to understand the effects of the number density and the spatial distribution of the Cu precipitates. The yield stresses obtained by the DD simulations are compared with available experimental data. The capability of our approach to predict the yield stress is also discussed.

## References

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