Molecular Dynamic Research of the Energy dissipation during Plastic Deformation

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Purpose

For the improvement of the accuracy of the prediction of the microstructure and properties which depend on the heat dissipation during the deformation, molecular dynamic simulation was performed to give a precise prediction of the friction of the dissipation of plastic deformation work into heat during plastic deformation, Taylor-Quinney coefficient (TQC: β).

Outline

We constructed single-crystal atomic models of pure metals (Fe, Al, Ni, Cu, Ag, Mg) with various crystal structures (BCC, FCC, HCP), on which simple shear strain was applied. β was calculated by a new method using the energy stored in crystal defects during the deformation. The correlation of β with stacking fault energy (SFE: Γ_{SF}) was also discussed.

Result

The curves and predicted values of β were obtained in agreement with existing numerical models and experimental data. β also showed a dependence on crystal orientation and Γ_{SF}.

Computing system	OCTUPUS & SQUID
Node-hour	938.92 CPU Node-hours
Application	LAMMPS
Memory usage	5 TB
Parallelize	Maximum 8×76 mpi

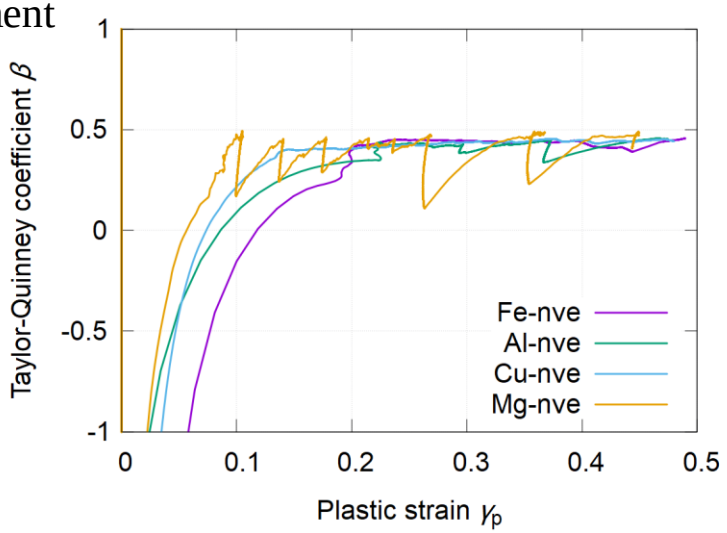

Fig. 1 TQC curves.