Molecular Dynamic Research of the Energy dissipation during Plastic Deformation

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Purpose

Molecular dynamic (MD) simulation of simple shear deformation were performed to verify the reliability of the new equation and investigate the dependence on stacking fault energy (SFE) and crystal orientations of Taylor-Quinney coefficient (TQC: β), which represents the fraction of the conversion of plastic deformation work into heat.

Outline

The new equation of TQC is derived from the energy conservation law considering thermodynamic boundary conditions. MD simulation of simple shear deformation was performed on single crystal atomic model of aluminum, copper and nickel. β was calculated using conventional equation β_0 and new equation β_1, the results were compared with experimental data reported in literatures. The dependence of β on stacking fault energy (SFE) and crystal orientations were also investigated.

Result

The results of β_0 and β_1 agreed well with each other and β reported in literatures.

The mechanism of the dependence on SFE and crystal orientations is the change in mobility and behavior of crystal defects.

$$\beta_0 = \frac{\Delta Q}{\Delta W^{\mathrm{p}}}$$

$$\beta_1 = 1 - \frac{\Delta E^{\mathrm{stored}}}{\Delta W^{\mathrm{p}}} = \begin{cases} 2\left(1 - \dfrac{\Delta E_{\mathrm{p}} - \Delta E^{\mathrm{e}}}{\Delta W^{\mathrm{p}}}\right) \\ 1 - \dfrac{\Delta U - \Delta E^{\mathrm{e}}}{\Delta W^{\mathrm{p}}} \end{cases}$$

Q: Heat generation during the deformation

W^{p}: Plastic deformation work

E_{p}: Interatomic potential

E^{e}: Elastic energy

U: Internal energy of the system (material)

Computing system	SQUID
Node-hour	6,000 CPU Node-hours
Application	LAMMPS
Memory usage	5 TB
Parallelize	Maximum 32×76 mpi