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# Extension, Compression and Bending Simulation of Nanowire with Nosé-Poincaré Molecular dynamics

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## ABSTRACT

With the recent advance of nanotechnology, nanostructure materials such as nanowire, nanofilm, nanocomposite and nanocrystalline have been received more attentions. As fabrication technique on nanosize has been developed, it is possible to make a nanowire which has a several nanometers for its width. Nanowire can be considered as a 3D solid beam which is a long and very small on nano level. In the order of nano-meter, surface effect appears strongly. It is not appropriate to apply the classical conventional continuum theory directly to analyze the nanowire. Therefore we should use the other method such as molecular dynamics (MD).

Molecular dynamics shows the atomistic deformation well. Nanowire can be simulated through Nosé-Hoover and Nosé-Poincaré method. Both method of Nosé-Hoover and Nosé-Poincaré maintain a temperature stably. Nosé-Hoover method doesn't guarantee the time reversibility and symplecticity. On the other hands Nosé-Poincaré guarantee the time reversibility and symplectic condition. [1]

In this study, we focus on mechanical behaviour of nanowire through Nosé-Poincaré molecular dynamics. Copper nanowire is arranged with an face-centered-cubic (FCC) and single crystal on (100). Total numbers of atoms are about 3500. MD simulations are carried out within Nosé-Poincaré NVT ensemble setting without periodic boundary conditions. With these setting, extension, compression and bending behaviours are studied.

In the simulation of extension and compression, MD simulations of nanowire are performed with constant strain rate and temperature. We provide the stress-strain curve constructed from the calculated Cauchy stresses and specified strain value [2]. We could observe dislocation slip and twinning. When dislocation takes place, Cauchy stress decrease. [3] After this instance, nanowire shows the nonlinear behaviour.

By the extension simulations, we characterize the mechanical properties of nanowire such as elastic modulus. Through this elastic modulus, we applied the displacement boundary condition at the tip which is equivalent to the externally applied end moment [4]. In bending simulation, bending moment curve which is calculated from molecular

dynamics and continuum theory shows similar behaviour before the dislocation occurs. As the rotated angle increase, dislocation occurs on nanowire. With this dislocation, bending moment curve deviated from the linear curve.

From the proposed MD simulation with the Nose-Poincare thermostate, the mechanical behaviours of single crystal nanowires are investigated.

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