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Ideal Strength of Nano-polycrystalline diamond under High Temperature and High Pressure using MD Simulation

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The aim of this work is to study the hardness of nano-polycrystalline diamond. Nano-polycrystalline diamond is a nanosized artificial diamond. It has diamond crystalline structure [1] and the same physical property as natural diamond, strong hardness, high thermal conductivity, and excellent electrical insulators. It is also harder than natural diamond, because it has various kinds of crystal planes. That is why it is applied for the Diamond Anvil Cell used in the high pressure experiment. It is important to synthesize nano-polycrystalline diamond and study its physical properties.

Ideal strength is the limit value of elasticity before the solid gets above the limit of elasticity and irreversible deformation occurs when the infinite, defect-free solid are gradually put more load on [2,3]. For the preparative simulation, we performed Molecular Dynamics (MD) simulations for studying ideal strength of crystalline diamond. The LAMMPS codes [4] with Tersoff potential [5] (SiC.tersoff) were used in all simulations. Temperature and time steps were set at 300 K and 0.001 ps, respectively. After constant pressure and constant temperature (NPT) simulation was performed for 1 ps, constant volume and constant temperature (NVT) simulation was performed for 210 ps. The share strength was evaluated at the {010} slip plane in the <100> slip direction, at the {110} in the <-110>, and at the {111} in the <1 1 -2> by performing NVT simulations with strain increasing at every 1000 steps. Our simulation data showed the ideal shear strength 202.0 (GPa) at critical strain of 0.39, 93.4 (GPa) at 0.33, and 87.9 (GPa) at 0.16 of the {010} slip plane in the <100> slip direction, of the {110} in the <-110>, and of the {111} in the <11-2>, respectively.

In the main simulation we study whether or not Hall-Petch behavior [6,7] are applied for nano-polycrystalline diamond. We will perform MD simulations for larger grain size of nano-polycrystalline diamond than 4.1 nm that was reported by Branicio et al. [8]. We study also hardness of nano-polycrystalline diamond with the ideal strength. We will perform MD simulations for nano-polycrystalline diamond with the same method as preparative simulation.

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