Shear strength of metals under uniaxial deformation and pure shear

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Abstract. In this paper, we investigate the dynamic shear strength of perfect monocrystalline metals using the molecular dynamics simulation. Three types of deformation (single shear, uniaxial compression and tension) are investigated for five metals of different crystallographic systems (fcc, bcc and hcp). A strong dependence of the calculated shear strength on the deformation type is observed. In the case of bcc (iron) and hcp (titanium) metals, the maximal shear strength is achieved at the uniaxial compression, while the minimal shear strength is observed at the uniaxial tension. In the case of fcc metals (aluminum, copper, nickel) the largest strength is achieved at the pure shear, the lowest strength is obtained at the uniaxial compression.

1. Introduction
Mechanical properties of materials considerably depend on the defects substructure. Dislocations consist one of the main types of defects determining the material plasticity and shear strength. A large number of dislocations usually exist in material in the initial state before deformation; motion and multiplication of these pre-existing dislocations provide the plastic relaxation in quasi-stationary conditions, as well as at dynamic deformation with moderate strain rates (up to about $10^8$ s$^{-1}$). At the same time, increasing of the strain rate or decreasing of volume of the deformed area leads to a dislocation starvation, which means that the density of pre-existing dislocation becomes insufficient for providing the plastic relaxation. The first situation takes place, for instance, at ultra-fast intensive laser irradiation of thin foils [1]; the second situation takes place at nanoindentation. A homogeneous nucleation of dislocations [2] determines the shear strength of material in these conditions; the crystal can be treated as a perfect one. Therefore, calculation of shear strength of perfect crystals has a sense.

Molecular dynamics (MD) simulations [3] for iron single crystal (bcc lattice) had shown that under uniaxial compression the lattice withstand the shear stress, at least up to 15 GPa, while under uniaxial tension the shear strength is much less. In order to verify this fact and identify the dependence of the critical shear stress on the lattice type and the type of deformation, in present paper we carry out the MD simulations of uniaxial compression and tension and pure shear for five metals with different crystal lattice; bcc (iron), hcp (titanium) and fcc metals (aluminum, copper, nickel) are considered.
Figure 1. Ti. Shear stresses versus degree of deformation in a titanium (hcp). Uniaxial compression, uniaxial tension and pure shear. The model contains 864 000 atoms.

Figure 2. Ni. Shear stresses versus degree of deformation in a nickel (fcc). Uniaxial compression, uniaxial tension and pure shear. The model contains 864 000 atoms.

2. Simulations

Investigations are performed using the MD simulator LAMMPS [4]. The following potentials of interatomic interaction are used: [5] for aluminum, copper and nickel, [6] for titanium and [7] for iron. We use models of perfect single crystals located in the thermostat at constant temperature with periodic boundary conditions. The model in thermostat is set in equilibrium state at a given temperature, at first, and then subjected to deformation. Temperatures of 300, 500 and 700 K are considered. In the course of dynamic loading, the shear stress in metal grows while achieving a critical point; thereafter, the stress drops sharply. This drop indicates the nucleation of dislocation in the model and subsequent plastic relaxation. In all cases the examined strain rate is $10^{10}$ s$^{-1}$. Therefore, the obtained values of shear strength meet the threshold for homogeneous nucleation [2]. Sizes of systems (number of atoms) are chosen from additional tests on the shear strength dependence on the system size.

3. Results

The calculated strain-stress dependences for different types of deformation and different temperatures are presented in figures 1–5. At first, the shear stress grows with the increasing of deformation; deformation is elastic at this stage and defects are absent. The beginning of the nucleation and motion of dislocations and, consequently, the plastic relaxation, leads to a sharp drop in the value of the shear stresses. The maximum determines the shear strength of the material (the threshold for homogeneous nucleation) at the certain type of deformation; the values of shear strength are shown in Table 1. A strong dependence of the calculated shear strength on the deformation type is observed, the difference can reach several times.

4. Conclusion

A strong dependence of the calculated shear strength on the deformation type is observed, the difference can reach several times. In the case of bcc (iron) and hcp (titanium) metals, the maximal shear strength is achieved at the uniaxial compression, while the minimal shear...
strength is observed at the uniaxial tension. In the case of fcc metals (aluminum, copper, nickel) the largest strength is achieved at the pure shear, the lowest strength is obtained at the uniaxial compression. The uniaxial compression or tension leads to action of a positive or negative pressure respectively in addition to shear stress. Therefore, the obtained results evidence an importance of pressure dependences of the shear strength and parameters of kinetics and motion of dislocations in metals. Tacking these pressure dependences into account can substantially influence the results of calculation of the shock wave dynamics. A detailed numerical investigation of the pressure dependences should be a continuation of the present work.
Table 1. Shear strength of metals at different types of deformation: the results of molecular dynamics calculations at a strain rate of $10^{10}$ s$^{-1}$.

| Temperature (K) | Compression (GPa) | Tension (GPa) | Shear strength (GPa) |
|-----------------|-------------------|--------------|---------------------|
|                 | hcp               |              |                     |
| Ti              | 300               | 15.4         | 1.8                 |
|                 | 500               | 13.9         | 1.5                 |
|                 | 700               | 12.2         | 1.3                 |
| fcc             | 300               | 3.2          | 4.2                 |
| Ni              | 500               | 3.0          | 3.6                 |
|                 | 700               | 2.7          | 3.0                 |
| Al              | 300               | 0.6          | 1.3                 |
|                 | 500               | 0.5          | 1.0                 |
|                 | 700               | 0.4          | 0.8                 |
| Cu              | 300               | 1.5          | 2.3                 |
|                 | 500               | 1.3          | 1.8                 |
|                 | 700               | 1.1          | 1.4                 |
| bcc             | 300               | 29.5         | 2.9                 |
| Fe              | 500               | 24.2         | 2.2                 |
|                 | 700               | 19.7         | 1.7                 |

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