HOMOGENEOUS NUCLEATION OF DISLOCATIONS IN METALS UNDER UNIAXIAL DEFORMATION AND PURE SHEAR

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Dislocations are linear defects in the crystal lattice, their movement is a major mechanism of plastic deformation. Usually dislocations already exist in material. Homogeneous nucleation can be observed under dynamic loading, when the strain rate is so high that shear stresses do not have time to relax at the expense of reproduction and movement of existing dislocations [1]. Homogeneous nucleation of dislocations restricts the shear strength of perfect crystals. The report presents the results of molecular dynamics study of ideal shear strength of single crystals of aluminum, titanium, iron and nickel in a pure shear strain, uniaxial tension and compression. The simulation was performed using the package LAMMPS [2]. We consider a system consisting of different number of atoms at different temperatures and strain rates. Were defined shear stress at which the system begins to form dislocations and plastic deformation began. As can be seen from the simulation results, depending on the type of crystal lattice of metal better resists deformation of a certain type.

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