Atomistic simulation of single crystal copper nanowires under tensile stress: Influence of silver impurities in the emission of dislocations

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The transition from elastic to plastic behaviour in single crystal copper nanowires under uniaxial tensile stress at different concentrations of silver (0.0-0.5 at.% Ag) and at different temperatures (0.1, 100, and 300 K) using the molecular dynamics method is investigated. The tensile stress is applied along â?©100â? crystallographic orientation and the silver atoms are placed randomly on the surface of the nanowire, as substitutional point defect. The simulations indicate that silver atoms lower slightly the unstable stacking fault energy, making them act as sources of partial dislocation nucleation, due to the local strain field they produce in the lattice structure. The defects generated in the material also act as sources for nucleation, giving rise to a competition of two mechanism. Also, it is observed that the yield point decreases with the temperature and the presence of impurities.