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

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ABSTRACT

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 ⟨100⟩ 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.

1. Introduction

Electronic devices are getting smaller from year to year in the last decade, reaching molecular levels. Thus, materials with good mechanical properties and electrical conductivity are required. The unusual electrical behaviour of metallic nanowires make them a material of interest in such area [1–6], increasing their importance. Studies on the mechanical properties are necessary to understand the behaviour of the nanowires in their different applications. In the recent years, different research regarding mechanical properties of materials using computational techniques have been carried out, such as dislocation nucleation [7,8], grain size effects [9,10], void growth and them serving as crack seed [11–14], surface defects [15], among many others. In most cases the crystal structure of materials are not defect free, so imperfections, such as vacancies, impurities, and grain boundaries are needed to be included in the studies. However, to our knowledge, there is limited information about the effects of impurities on the mechanical properties of metals using computational simulation [16–19], making necessary studies which describe the influence of this kind of defect on the mechanical properties of the material.

In the present work, we study the influence of silver impurities on the partial dislocations nucleation, analysing its effect on the unstable stacking fault energy of copper. Also, the yield point of copper nanowires with silver impurities at different concentration levels (from 0.0 to 0.5 at.% Ag) and at different temperatures (0.1, 100, and 300 K) is investigated. We use the molecular dynamics method, submitting the system to uniaxial tensile stress.

The paper is organized as follows: In Section 2 we explain the simulation procedure used and the tools for analysis employed, in Section 3 we present and discuss our results, and in Section 4 we draw the conclusions.

2. Methodology

The system under study consists of a face centred cubic (fcc) copper nanowire with square cross-section, like most nanowires studied in previous works [20–23], with a size corresponding to $40 \times 10 \times 10$ in terms of the lattice parameter, which is 3.61 Å for copper. The orientation is such that the axial axis is along [100] direction, with six {100} side surfaces, as is shown in Fig. 1. Free boundary conditions are imposed in all directions. Different silver impurity concentrations (0.0–0.5 at.% Ag) are added on the surface as substitutional defects, since it is well-known that silver segregates to Cu grain boundaries and surfaces [24–26] due to its limited solubility [27] (in Fig. 1 blue atoms represent copper and the red ones silver). The procedure to create the different impurity concentration systems is straightforward. First, a concentration of 0.1 at.% Ag is placed randomly on the surface of the impurity free nanowire, obtaining the Cu 0.1 at.% Ag system. Thus,

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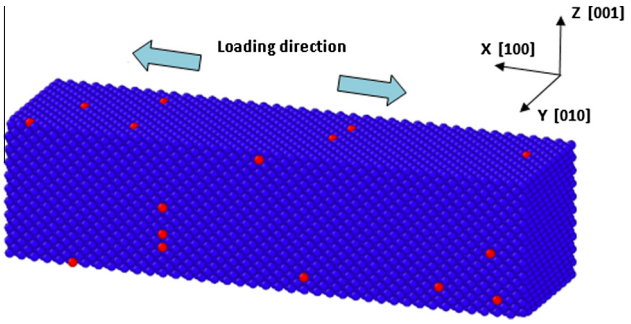

Fig. 1. Initial configuration of the copper nanowire. Copper and silver atoms are represented by blue and red color, respectively. The loading of the system is along the axial direction, which lies in the [100] direction. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

a particular realization of this system is created. Then, a concentration of 0.1 at.% Ag is added, again randomly, on the surface of this system, thus obtaining the Cu 0.2 at.% Ag system. This procedure is repeated three more times in order to obtain the Cu 0.3, 0.4 and 0.5 at.% Ag systems.

The simulation is carried out using the classical molecular dynamics code LAMMPS developed by Plimpton et al. at Sandia National Laboratories [28] and the visualization by means of OVITO [29]. The inter-atomic potential employed for copper-silver alloys is the well established embedded-atom method (EAM) potential developed by Williams et al. [30] which is based on the previous potential developed by Mishin et al. for Cu [31]. In general, the EAM gives the total energy of an atomic system in the form [32]

$$E = \frac{1}{2}\sum_{ij} V_{ij}(r_{ij}) + \sum_{i} F_i(\bar{\rho}_i), \tag{1}$$

where E is the total energy of the system, and V_{ij} is the pair potential between atoms i and j separated by a distance r_{ij}. F_i is the energy of atom i embedded in an electron density $\bar{\rho}_i$, given by

$$\bar{\rho}_i = \sum_{i \neq j} \rho_j(r_{ij}). \tag{2}$$

The quantity $\rho_j(r_{ij})$ represents the electron density at atom j as function of the distance r_{ij}.

The procedure of the simulation is the following. First, the energy of the system is minimized using conjugate gradient method. Then, a thermalization at 0.1 K, 100 K or at 300 K (depending on the temperature wanted to be studied), is performed using velocity rescaling for 10 ps, using 1 fs as the integration time step. After this procedure, the system is loaded along the axial direction at a strain rate of 10^8 s^{-1}. For this purpose, the positions of atoms are rescaled each time step. The temperature is kept constant during the tensile process in order to avoid thermal effects related to dislocation propagation.

The stress in the system is calculated from the stress tensor expression as implemented in LAMMPS [28]

$$\sigma_{ij} = -\frac{1}{V}\sum_{\alpha}\left(m^{\alpha} v_i^{\alpha} v_j^{\alpha} + \frac{1}{2}\sum_{\beta \neq \alpha} r_i^{\alpha\beta} F_j^{\alpha\beta}\right), \tag{3}$$

where V is the volume of the system, m^{α} is the mass of atom α, v_i^{α} and v_j^{α} are the i and j-component of velocity respectively, $F_i^{\alpha\beta}$ is the i-component of the force between atom α and β, and $r_j^{\alpha\beta}$ is the j-component of the distance between atom α and β. The first term is associated with the kinetic energy due to thermal vibration and the second term with the potential energy due to the deformation of the system. Note that since the loading is in the (100) axial direction, only the σ_{ii} stress component is required.

To study the partial dislocation nucleation and stacking faults in the system, the centrosymmetry parameter (CSP) [33] is used, which is defined for a particular atom i as

$$c_i = \sum_{j=1}^{N/2} \left| \vec{R}_j + \vec{R}_{j+\frac{N}{2}} \right|^2, \tag{4}$$

where N is the number of nearest neighbours of atom i, $\vec{R}_j$ and $\vec{R}_{j+\frac{N}{2}}$ are the vectors from the atom to a pair of opposite nearest neighbours. Note that for a face centred cubic structure $N = 12$. The CSP value is zero for atoms in a perfect lattice and it increases for any defects and atoms close to the free surface. In this study, $3.7 < c_i < 4.5$ represents a partial dislocation, $4.5 < c_i < 6.5$ corresponds to stacking fault and $c_i > 6.5$ for free surface.

3. Results and discussion

The stress–strain curves for the six copper nanowires (0.0, 0.1, 0.2, 0.3, 0.4, 0.5 at.% Ag) at 0.1 K are shown in Fig. 2 [34]. As it can be seen, three main features are clearly distinguishable. Firstly, the elastic regimen of the systems is essentially the same, thus the stiffness is almost unaffected by the impurities at the considered concentration levels. Secondly, both the yield stress and yield strain change with the concentration of impurities. Thirdly, after the yield point, a sawtooth behaviour of the curve is observed. This is indicative of a successive emission of dislocations.

3.1. Reduction of the yield point and emission of dislocations

Table 1 presents the calculated values of the yield strain and yield stress for each system. The change of the yield point according to the presence of impurities can be rationalizes in terms of the local strain field generated in the lattice due to the size mismatch

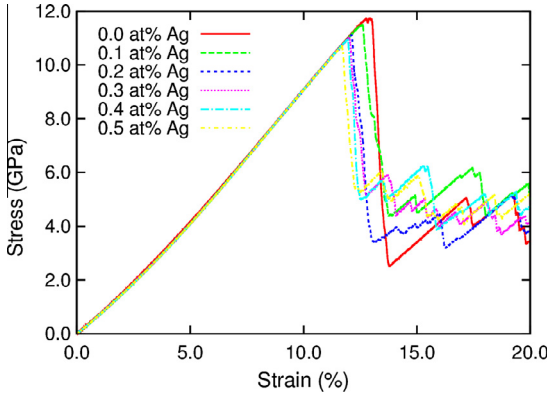

Fig. 2. Stress–strain relationships for single crystal Cu nanowire along [100] direction at different concentrations levels of Ag.

Table 1
Yield strain and yield stress for different concentrations of Ag.

Ag content (at.%)	Yield strain (%)	Yield stress (GPa)
0.0	12.9	11.7
0.1	12.6	11.5
0.2	12.0	11.1
0.3	11.9	11.0
0.4	11.8	10.9
0.5	11.6	10.7