Computational Materials Science 152 (2018) 381–392

Contents lists available at ScienceDirect

Computational Materials Science

journal homepage: www.elsevier.com/locate/commatsci

MD-based characterization of plastic deformation in Cu/Ag nanocomposites via dislocation extraction analysis: Effects of nanosized surface porosities and voids

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ARTICLE INFO

Keywords:
Cu/Ag nanocomposite
Porosity
MD simulation
Plastic deformation
Dislocation

ABSTRACT

Recently, copper-silver nanocomposites (NCs) have been utilized in medical instruments owing to their ability in destroying the bacterial cell wall, which prevents inflammation of the body tissue. It has been revealed that introducing nanosized porosities in their structure can lead to an increase in the interfacial surface area with the tissue promoting the quality of treatment. However, since yielding and occurrence of plastic deformation are not acceptable in medicine, analyzing the mechanical behavior of these NCs having nanopores is an important challenge. Therefore, the focus of this study is to assess the role of porosities on the deformation mechanism of Cu/Ag NCs under uniaxial tensile loading conditions. Accordingly, several perfect and defected samples are systematically studied through molecular dynamics simulation. It is observed that plastic deformation of perfect sample occurs through twinning. For samples with surface voids, this is happened as a result of perfect dislocations gliding. Meanwhile, for volumetric porosities, the deteriorating effect is stopped passing the critical void content. This is ascribed to the formation of many motionless dislocations such as stair-rod, Hirth and Frank as confirmed via the dislocation extraction analysis. Consequently, it is demonstrated that presence of surface voids can be more destructive.

1. Introduction

In recent years, the use of copper and silver as two antibacterial agents has been extensively interested in medical instruments. According to studies conducted by researchers in the field of microbiology, copper and silver prevent inflammation of the body tissue by destroying the bacterial cell wall [1,2]. On the other hand, metal matrix nanocomposites (MMNCs) have been extensively implemented due to their excellent mechanical properties and commercialization of their manufacturing processes [3]. Accordingly, Cu-Ag nanocomposites (NCs) can be widely utilized in medical implants leading to intensification of the antimicrobial activity. Meanwhile, owing to the increased interfacial area, the use of nanoporous implants can accelerate the process of ion exchange at the NC surface, which reduces time of the treatment period [4]. Since release and absorption of drugs are increased by reducing the dimensions of the voids to the nanoscale, creation of nanopores can also be considered in terms of the drug delivery issue [5]. However, the presence of voids is not always useful. Various defects can occur in the structure of a NC over its formation process. Surface voids with uncontrollable dimensions or the presence of them in the volume of materials can lead to substantial challenges in their mechanical properties. Whereas, the presence of defects in substances with medical applications, causes a high sensitivity. Any yield and plastic deformation in the implants are not acceptable [6]. Therefore, characterization and analysis of the mechanical behavior of implants are very important. Although failure of NCs is a macroscopic phenomenon, this is resulted by atomic-scale structural variations of the sample. Therefore, to understand the failure mechanism and to investigate the structural changes during deformation, it is necessary to use a tool that can detect the displacement of atoms in the crystalline structure of material.

A suitable option for simulating mechanical properties and investigating atomic structural changes of nanostructured materials is utilizing atomic-scale modeling techniques such as molecular dynamics (MD) simulation [7]. The plasticity of crystal materials is usually controlled by dislocation slipping. According to the Hall-Petch relation, grain boundary prevents the activity of dislocations, which in turn, results in the different mechanisms affecting the plastic deformation of nano-sized grains [8]. By reduction of the grain size to below 10 nm, plastic deformation occurs through grain boundary sliding, while increasing this parameter enhances nucleation of partial dislocations and, as a result, the concentration of stacking faults and twins are increased

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https://doi.org/10.1016/j.commatsci.2018.06.018
Received 11 April 2018; Received in revised form 6 June 2018; Accepted 8 June 2018

[9,10]. According to the previous studies, temperature, strain rate and sample geometry are the most important factors affecting the nucleation and slipping of dislocations [11–13]. It has been well established that by increasing the temperature, decreasing the strain rate and reducing the dimensions of the specimen under tension, the stress required for nucleation of dislocations is decreased. Subsequently, the yield strength and strain of the samples are reduced. According to the study of Zhang et al. [14] on the effect of sample geometry, nucleation of dislocations in a cubic sample of single crystal copper occurred easier and faster than that of its cylindrical specimen. This was attributed to the much greater stresses in the cube edges compared to the stress distributions in the cylinder wall. Study of stacking faults is another subject that has been considered by the researchers [15–20]. According to these investigations, stacking faults can change the deformation mechanism by creating twins. Also, these areas can change the slip direction of the dislocations. Consequently, formation of stacking faults can prevent dislocation movements by changing the crystal lattice structure from FCC to HCP [21].

In addition to the external variables such as temperature, strain rate and sample geometry, internal factors have also been studied by researchers. They include presence of crystalline defects and voids within the structure, which can influence the deformation mechanism. For example, Xu et al. [22] demonstrated that presence of voids within the single crystal copper can accelerate the propagation of dislocations from their surroundings. In addition, Traiviratana et al. [23] showed that most of the dislocations nucleated from the surrounding of a void are the partially dislocation type. Based on the previous studies, stacking faults can also be extended from the voids into the material [24–26]. Asari et al. [27] showed that by increasing the dimensions of the void, internal dislocations need more stress to pass through it. Therefore, these imperfections can also appear as an obstacle for slipping of dislocations. In general, position and amount of defects can be considered as the most important factors affecting the mechanical properties of the samples. So far, significant parts of studies have been focused on the developments of single phase nanostructures. However, the NCs deformation has some remarkable differences compared to other materials. Most of the researches in this field focus on the effect of the second phase on the matrix deformation. For example, in the research of Sun et al. [28], influence of the second phase geometry and its distribution was investigated. It was found that the presence of particles with spherical shape and random distribution can lead to formation and expansion of the stacking faults. According to the conducted studies, the interface of nanoparticles (NPs) with matrix has a significant contribution in determining the mechanical properties of NCs. In addition, difference between the atomic radius of the second phase and matrix, as well as the increase of temperature, can weaken the strength of the interface [23,29,30]. Mathiazhagan et al. [31] showed that dislocations can be emitted from the interface. The amount of reinforcement phase is also very effective in the nucleation and movement of dislocations [32]. In this study, to investigate the deformation mechanism of Cu-Ag NCs, first, the perfect nanocomposite sample is examined through uniaxial tensile test using MD simulations. Then, the tensile procedure is repeated under the same conditions in the presence of surface and volume voids at different amounts. This is followed by comparing the results with those of the perfect sample. Accordingly in the second part, details of MD simulation and sampling techniques are introduced. Then, in the third section, the results of the tensile test are presented for all samples. Also, the governing deformation mechanisms are systematically described in this part. Finally, results of the research are summarized and the conclusions are made.

2. Details of MD simulation

In this research, MD simulation method was used for analyzing the effect of surface and volumetric porosities on the deformation mechanism of Cu-Ag NCs. All simulations were conducted utilizing the

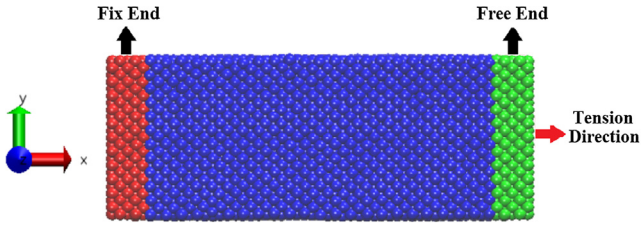

Fig. 1. Schematic illustration of the uniaxial tensile test in LAMMPS.

open-source LAMMPS code developed by Sandia National Laboratory [33]. In order to determine the interatomic interactions between copper–copper, silver-silver and copper-silver atoms in the force and energy fields, Embedded Atom Model (EAM) function was implemented. This potential function has been successfully used in many previous studies to simulate copper-silver systems [34–37]. Simulations were carried out using the canonical ensemble (NVT) at a constant temperature of 300 K. The Nose-Hoover thermostat was used to maintain the simulation temperature at 300 K. The use of this thermostat causes fewer fluctuations than other methods [38]. The initial velocities were determined based on the Maxwell-Boltzmann distribution at the desired temperature. In addition, velocity-Verlet integration algorithm [39] with a time-step of 2 fs was used for solving equations of motion through time. Since the initial configuration of the samples may not be in the equilibrium state, the system was relaxed to 100,000 steps (i.e., 200 ps) before loading. After relaxation, according to the quasi-statics method introduced by authors [40], the left side of the representative volume element (RVE) was kept fixed during imposing the uniaxial tensile loading. This was followed by applying the incremental displacement on the other side to obtain the desired strain. Fig. 1 presents schematic illustration of a typical RVE under uniaxial tension. At each loading step, a displacement of 0.1 Å was applied along the sample length. After each displacement, the system was relaxed for 30,000 steps. Free boundary conditions (BC's) were considered in direction of the axial stretch. Also, periodic BC's were imposed in the lateral directions.

As shown in Fig. 2a, rectangular RVE with the dimensions of $10 \times 4 \times 4$ nm in the x, y, and z directions, respectively, was constructed to resemble the copper-reinforced with Ag and the porous samples. The basic MD cells were created in two steps. First, the NC matrix consists of Cu atoms were created using the built-in tools in LAMMPS guided by the specific metal lattice parameters. At a later stage, a central hole with the diameter of 2 nm was included to accommodate the Ag atoms (Fig. 2b and c). In all of the simulations, there was no overlapping between silver inclusion and copper atoms as depicted in Fig. 3. It is noted that all graphical illustrations have been made using OVITO software [41]. The geometrical characteristics of silver nanoparticle and the RVE were chosen so that a sample containing 2.6% mass fraction of Ag was achieved in each case.

To model porous samples, some voids with the diameter of 1 nm were distributed at the surface or in the volume of the copper matrix (See Fig. 4). The volume fraction (VF) for a void with the mentioned diameter was about 0.32%. Therefore, the VF for a surface void was half of this amount for the volumetric pore. Accordingly, to produce different cases having various VF of these porosities, the corresponding amount of them could be introduced in the RVE as shown in Table 1.

The centro-symmetry (CS) parameter [42] was used to identify the partial dislocations, twinning and stacking faults. For the specified atom i, this parameter is defined as follows:

$$CS = \sum_{i=1}^{N/2} |\overrightarrow{R_i} + \overrightarrow{R_{i+N/2}}|^2 \tag{1}$$

where N is the number of nearest neighbors of atom i equal to 12 for the FCC metals. Also, $\overrightarrow{R_i}$ and $\overrightarrow{R_{i+N/2}}$ are vectors from the central atom to a