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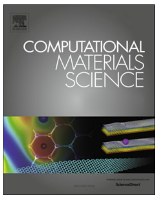

Molecular dynamics simulations of tensile tests of Ni-, Cu-, Mg- and Ti-alloyed aluminium nanopolycrystals

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ABSTRACT

Molecular dynamics simulations are used to investigate tensile strengths and failure mechanisms of aluminium nanopolycrystals with an average grain diameter of 8 nm containing dissolved Ni, Cu, Mg or Ti atoms. It is shown that tensile strengths are influenced by several factors such as stacking fault energies as well as types, concentrations and positions of the dissolved atoms. A strong strengthening was found in case of Cu whereas Ni or Ti lead to a moderate increase of strength, while Mg even lowers the tensile strength.

It was found that both dislocation processes as well as grain boundary dominated effects contribute to plastic failure mechanisms. Type and concentration of dissolved atoms possess a significant influence on these failure mechanisms. Whereas alloying with Ni, Cu or Mg supports grain boundary dominated failure processes, dissolved Ti atoms lead to a significant increase of stacking faults and dislocations.

1. Introduction

Polycrystalline materials with grain sizes in the nanometer region (nanopolycrystals) exhibit an enormous strength in tensile or compression tests and are therefore favourable for industrial applications which require strong components. Significant progress has been made in understanding the mechanisms of plastic failure and hardening in these nanopolycrystals [1–6]. The method of choice is molecular dynamics (MD) because in MD simulations direct observations of the underlying processes are possible. A main focus of the previous research is the dependence of the tensile strength on the grain size. The well known Hall–Petch relationship [7] where strength increases with decreasing grain size was found in MD simulations of nanocrystalline copper [1,2]. Additionally, a decreasing strength with decreasing grain sizes known as inverse Hall–Petch effect [8] was observed in these simulations for grain sizes below 11 nm. The inverse Hall–Petch effect was also confirmed in MD simulations of aluminium polycrystals with grain sizes below 10 nm [3]. Whereas plastic deformation is caused by the generation of dislocations and stacking faults at the grain boundaries for larger grain sizes, the number of these defects is significantly diminished in the inverse Hall–Petch region. Instead, grain boundary mediated processes such as grain boundary sliding or grain rotations contribute dominantly to plastic failure in these materials with very small grain sizes [4].

Detailed investigations of the dislocations and stacking faults generated at grain boundaries in fcc structures revealed that the generalised stacking fault energies have a significant influence on the mechanisms of plastic failure [5]. The generalised stacking fault energies contain the unstable stacking fault energy (γ_{USF}) which corresponds to the energy maximum which has to be surmounted by the Shockley partials and the stable stacking fault energy (γ_{SF}) which is the interface energy of the planar stacking fault generated by a displacement of $a_0/6^{1/2}$ along the $<112>$ type directions. It was shown in Ref. [5] that the ratio γ_{USF}/γ_{SF} determines the type of defects generated at the grain boundaries. In materials with a low γ_{USF}/γ_{SF} ratio (e.g. nickel) initial Shockley partials are generated and move through the grain leaving behind stacking faults which intersect the grain. But in case of a γ_{USF}/γ_{SF} ratio close to one (e.g. aluminium) trailing partials are also emitted from the grain boundaries and, therefore, the stacking faults exist between the travelling initial and trailing partials only.

It is well known that alloying elements can have a significant influence on tensile strengths and the mechanisms of ductile failure. Most investigations in this field concentrate on the interaction between a dislocation and solute atoms. It was found for several materials, e.g. Al–Mg [6], Fe-based alloys [9] and Ni-based alloys

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[10] that the dislocation mobility is impeded by the foreign atoms. However, in nanopolycrystals it has to be taken into account that the generation of defects at the grain boundaries is also influenced by foreign atoms. In case of polycrystalline Ni–Fe with grain sizes of 15 nm MD simulations showed that the tensile strength depends significantly on the chemical composition of the grain boundaries whereas the chemical composition inside the grains is negligible [11].

The objective of this work is a detailed investigation of the behaviour of Ni-, Cu-, Mg- and Ti-alloyed aluminium nanopolycrystals during tensile tests. Foreign atoms with concentrations up to 20% of all atoms are placed at different locations, namely at the grain boundaries, inside the grains or at both positions. Tensile strengths are determined in dependence of types, concentrations and positions of foreign atoms. Additionally, the generalised stacking fault energies are calculated for the foreign atom concentrations considered. In order to understand the changes in tensile strengths and the underlying failure mechanisms an analysis of the generated crystallographic effects is performed using the common neighbour analysis (CNA) [12]. Within this method the number of atoms located in stacking faults as well as the number of atoms belonging to other crystallographic defects are identified allowing to distinguish grain boundary mediated plasticity and dislocation based ductile failure.

2. Computational details

2.1. Basics

All molecular dynamics (MD) simulations of this work are carried out using the IMD package [13]. The reliability of results from MD simulations are determined by the quality of the interaction potentials used. Therefore, we use potentials which reproduce the material properties with high accurracy. A widely used approach for the simulation of metals is the embedded atom method (EAM) [14,15]. In this model each atom is embedded in an electron density consisting of contributions from neighbouring atoms. The potential energy is the sum of the pair interaction and the embedding term U_i. U_i describes the energy of embedding atom i in an electron density n_i, which is the sum of contributions ρ_j from neighbours j at distances r_{ij}:

$$V = \frac{1}{2}\sum_{i \neq j} \Phi_{ij}(r_{ij}) + \sum_i U_i(n_i), \quad n_i = \sum_{i \neq j} \rho_j(r_{ij}), \tag{1}$$

For the binary systems Al–Ni and Al–Ti we use potentials of this type [16,17]. Calculations of lattice constants, cohesive energies, elastic constants and phonon frequencies of Al, Ni, Ti and several structures of the Al–Ni and Al–Ti phase diagrams with these potentials agree well with literature data. Additionally, the energies of defects in these metals such as surface energies, vacancy formation energies and stacking fault energies are also obtained with reasonable agreement. The potential for aluminium is identical in the Al–Ni and Al–Ti potentials used in this work. Details about the Al–Ni and Al–Ti potentials can be found in Ref. [16] and Ref. [17].

Simulations of the Al–Mg system were carried out using potentials of the Finnis–Sinclair type [18]. This approach differs from the EAM in the functions $\rho(r_{ij})$. Whereas in the EAM there is one density function $\rho_j(r_{ij})$ for each atom type j, the Finnis–Sinclair potentials contain a function $\rho_{ij}(r_{ij})$ for each combination of atom types i and j. Due to their good reproducibility of physical properties of Al–Mg structures we chose the Al–Mg Finnis–Sinclair potentials of Ref. [19] for our simulations of this system. It must be stated that these Al–Mg potentials were optimised for the simulation of solid–liquid interfaces whereas the potentials used for Al–Ni, Al–Ti and Al–Cu were optimised to reproduce many more properties of the solid phases existing in these material systems. Nevertheless the Al–Mg potentials are capable to reproduce the lattice parameters of various solid Al–Mg phases and the elastic constants of aluminium obtained with these potentials are in agreement with literature data.

In case of the Al–Cu system strong deviations from cubic symmetry can occur, a well known example is the clustering of Cu atoms in disc shaped precipitates, the so-called Guinier–Preston zones. In order to improve the description of material properties in case of deviations from cubic symmetry angular dependent potentials (ADP) were developed by Mishin et al. [20]. ADP potentials are a generalisation of the EAM where angular dependent forces are taken into account. This is achieved by adding additional terms to Eq. (1). The extension consists of dipole vectors and quadrupole tensors which contain two additional functions for each pair combination of types i and j. The Al–Cu potential applied in this work [21] is suitable for several structures of the Al–Cu phase diagram and as stated in Ref. [21] it is applicable to simulations of hardening in Al–Cu alloys.

2.2. Structures

All structures used in the tensile test simulations are based on the same nanopolycrystal. It was constructed by a Voronoi tesselation of a $17.2 \times 17.2 \times 17.2\ \text{nm}^3$ cube with ten randomly placed grain centres. Each grain was filled with aluminium atoms in a randomly oriented fcc structure resulting in a nanopolycrystal with 292,000 atoms and an average grain diameter of 8 nm. With this initial structure a common neighbour analysis (CNA) [12] was performed. The CNA allows to determine the crystallographic structure of each atom. It distinguishes between fcc, hcp and other structure. Due to different orientations of the grains, the atoms at grain boundaries are identified by the CNA to be of the third structural type (other structure). It was found that 18% of all atoms are located at the grain boundaries. The knowledge which atoms are at grain boundaries and which ones are located inside the grains was used to generate structures with Ni, Cu, Mg or Ti foreign atoms. For each of these elements the following alloy structures were generated: (1) 2–20% of aluminium atoms at grain boundaries were replaced by foreign atoms. This percentage corresponds to 0.36–3.6% of all atoms. These structures are denoted as *gb rel* in Fig. 3. (2) 2–20% of aluminium atoms in grains were replaced by foreign atoms. This percentage corresponds to 1.64–16.4% of all atoms. These structures are denoted as *ig rel* in Fig. 3. (3) 2–20% of all aluminium atoms were replaced by foreign atoms. The foreign atoms of this structure are the same as in (1) and (2). (4) 11–100% of aluminium atoms at grain boundaries were replaced by foreign atoms. This percentage corresponds to 2–18% of all atoms. These structures are denoted as *gb* in Fig. 3. (5) 2.4–24% of aluminium atoms in grains were replaced by foreign atoms. This percentage corresponds to 2–20% of all atoms. These structures are denoted as *ig* in Fig. 3.

The structures used in the calculations of generalised stacking fault energies are single crystals with 76,000 atoms with foreign atom concentrations up to 20%. They are cuboid-shaped with edge lengths of 17.4, 17.2 and 4.2 nm and side plane orientations of the types {112}, {110} and {111}.

2.3. Simulation procedures

In order to allow reordering of the atoms in the nanopolycrystal at a given temperature, equilibration simulations of the polycrystalline structures were performed. The chosen temperature of these simulations is 300 K and a pressure control is applied in order to achieve zero values of the stress components $\sigma x, \sigma y$ and σz. A time step of 2 fs is used for 10,000 MD steps. A comparison