

Atomistic modeling of the effect of calcium on the yield surface of nanopolycrystalline magnesium-based alloys



Raghuram Reddy, Sébastien Groh*

Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg, 09599 Freiberg, Germany

ARTICLE INFO

Article history:

Received 5 June 2015

Received in revised form 6 October 2015

Accepted 11 October 2015

Available online 19 November 2015

Keywords:

Molecular dynamics

Modified embedded-atom method

Substitutional calcium binding energy

Intergranular fracture

ABSTRACT

The change of mechanical properties resulting from the addition of Ca alloying elements in nanopolycrystalline Mg-based alloys was investigated using molecular dynamics in the framework of the modified embedded-atom method. Using an energetic approach, it was demonstrated that grain boundaries and their vicinity are the favorable locations for substitutional Ca atoms in nanopolycrystalline Mg with average grain diameter in the order of 12 nm. Based on the McLean theory, a concentration around 8 at% of Mg can be substituted by Ca atoms at the grain boundaries. Thus, by increasing the concentration of substitutional Ca atoms from 1 at% to 5 at% in a nanopolycrystalline Mg sample, we demonstrated that the addition of Ca in Mg-based alloys leads to a systematic decrease of the yield surface. Moreover, a microstructural analysis was performed to identify the relation between the deformation mechanisms and the change in yield surface revealed by the addition of substitutional Ca atoms. It was found that the addition of substitutional Ca leads to (i) a decrease of the activity of $\langle \mathbf{a} \rangle$ dislocations, (ii) an increase of the activity of non-basal dislocations, and (iii) an enhancement of the intergranular fracture.

© 2015 Elsevier B.V. All rights reserved.

1. Introduction

Magnesium-based alloys became highly attractive due to their high strength, lightweight, good recyclability capability, biocompatibility and biodegradability properties, as well as the presence of large amounts of magnesium in natural resources at low cost. This new family of alloys is expected to replace more traditional materials such as stainless steel, aluminum alloys, and even titanium alloys in various application fields ranging from automotive and aerospace [32] to orthopedic [23,37] industries. However, to be fully integrated as new technological materials, certain limitations of magnesium and its alloys must be mitigated. Mg alloys have a high anisotropy in plastic deformation resulting in poor formability and limited ductility at room temperature, in addition to poor corrosion resistance. From the literature, two manufacturing routes were proposed to improve the formability. While the first route to improve the formability of Mg-based alloys is based on grain refinement by severe plastic deformation [50], the addition of alloying elements constitutes the second route to improve

the formability of Mg-based alloys. At the macroscopic scale, Agnew et al. [1] demonstrated using a visco-plastic-self-consistent method that alloying elements such as Al, Ca, Li, Zn, and Zr enhance the activity of $\langle \mathbf{c} + \mathbf{a} \rangle$ dislocations, and, therefore, improve the formability of Mg-based alloys. As a secondary effect, the addition of the above mentioned alloying elements improves the resistance to corrosion of this family of alloys.

The effect of grain size on the yield strength is explained by the Hall–Petch relationship [15]:

$$\sigma = \sigma_0 + k_{\text{hp}} d^{-1/2} \quad (1)$$

where σ is the yield stress, σ_0 is the frictional stress representing the overall resistance of the crystal lattice to the dislocation movement, k_{hp} is a constant (Hall–Petch slope, material dependent), and d is the average grain diameter. The Hall–Petch constant is a measure of the grain boundaries contribution to the relative hardening. From a macroscopic perspective, Eq. (1) reveals that the yield stress of a polycrystalline sample increases as the average grain size decreases. From a microscopic perspective, two microscopic mechanisms can be identified to recover the generic Hall–Petch behavior: (i) decrease of the dislocation mean free path [6], and (ii) diffusion at the grain boundary, also referred in the literature as Coble creep [21,49]. It has been shown experimentally [9], and numerically using molecular dynamics [38,21,49,5,43] that there is breakdown in the Hall–Petch relation when the grain size is decreased below

* Corresponding author at: Department of Biomedical Engineering of the University of Basel, Switzerland. Tel.: +41 612075426; fax: +41 612659668.

E-mail addresses: Sebastien.Groh@imfd.tu-freiberg.de, sebastien.groh@unibas.ch (S. Groh).

a material dependent critical size. Thus, developing nanocrystalline materials exhibiting an inverse Hall–Petch behavior is of high interest as their strength increases during deformation at high strain rate [40].

In view of identifying the structure–properties relation, Van Swygenhoven et al. [48] deformed under high strain rate polycrystalline Ni and Cu with grain size between 3 nm and 12 nm at 300 K using molecular dynamics method. Their data revealed that deformation is within the grain boundaries for the small grains, while for larger grains there is intra-grain deformation, which is revealed by the presence of stacking faults inside the grains. Furthermore, they observed that deformation starts at the triple points with grain boundary sliding followed by creation of an intra-grain Shockley partial which glides on the slip system. Within the same objective, Desai et al. [6] numerically deformed using molecular dynamics polycrystalline Mo and UO₂ with average grain size of approximately 12 nm at high temperature and constant strain rate. The two materials exhibited similar thermally activated creep rates, and their data suggested that Mo was deformed by Coble and Nabarro–Herring creep while UO₂ was deformed by Coble creep. It was concluded by the authors that the Hall–Petch effect was the consequence of diffusion creep accompanied by the Nabarro–Herring creep that shows decrease in yield stress, flow stress and creep rate with decreasing average grain size. Kim et al. [19,20] analyzed the plastic deformation of nanocrystalline Mg using molecular dynamics. These authors reported the signature of the different deformation modes in Mg. In addition, their calculations revealed a transition from basal slip to twinning deformation while decreasing the grain size below 30 nm. Finally, Sha et al. [39] investigated the effect of temperature on the deformation of nanocrystalline diamonds with average grain size between 2 nm and 5 nm at high strain rate using molecular dynamics simulation. Their data suggests a change in the failure mechanism when increasing the temperature in nanocrystalline diamonds. Grain boundary sliding resulting from the presence of large shear stress, and, thus, leading to crack initiation at an adjacent triple junction, may be the cause of failure in nanocrystalline diamonds at room temperature, while direct intergranular fracture was observed at high temperature. The change in failure mechanisms was explained by the temperature dependence of shear and tensile properties of the grain boundaries.

The objectives of this study are threefold: (i) identify the energetically more favorable location for substitutional Ca alloying elements in Mg nanopolycrystals when small concentrations of Ca are considered, (ii) reveal the macroscopic effect of Ca on the yield surface of nanopolycrystalline magnesium-based alloys, and (iii) shed light on the effect of substitutional Ca on the microscopic deformation mechanisms such as dislocation, twinning, grain boundary sliding, and intergranular fracture.

In this manuscript, the methodology used to (i) quantify the interaction between substitutional Ca atoms and grain boundaries, and (ii) calculate the yield surface of nanocrystalline magnesium using LAMMPS is given in Section 2, in addition to a review of the existing Mg–Ca semi-empirical potentials available in the literature. In Section 3, numerical data revealing the energetically more favorable location of substitutional Ca in nanocrystalline magnesium are presented together with the macroscopic effects of small concentrations of Ca on the deformation behavior of nanocrystalline magnesium. Apart from discussing the effect of Ca on the yield surface using molecular dynamics, a microstructural analysis was performed to reveal the effect of substitutional Ca on the relation between the microstructure and the yield surface. The corresponding numerical results are presented in Section 3 and discussed in Section 4. Concluding remarks are given in Section 5.

2. Methodology

2.1. MgCa potentials from the literature

Employed in a computational framework, empirical potentials are suitable to (i) reveal mechanisms to be later observed experimentally [13,10], (ii) validate continuum theories [4,2,12], (iii) model the mechanical properties of complex metallic alloys [36,35,24], or (iv) shed light on the nature of the interaction between defects of different dimensionalities [26].

The modified embedded-atom method (MEAM) proposed by Baskes [3] and extended to the second nearest neighbors by Lee and Baskes [22], allows the calculation of the thermodynamics forces and stress tensors for the atoms in the lattice based on the notion of mean field theory. The total energy, E , of an atomic system is approximated as the sum of the atomic energies, E_i , as follows:

$$E = \sum_i E_i. \quad (2)$$

The energy of atom i consists of the embedding energy F_i , i.e., the amount of energy required to embed an atom at an electronic site represented by an average background electronic density, ρ_i , and a perturbation given by the pair potential term, Φ , as follows:

$$E_i = F_i(\rho_i) + \frac{1}{2} \sum_{j \neq i} \Phi_{ij}(r_{ij}), \quad (3)$$

where j is any neighboring atom of i , and r_{ij} is the distance between atoms i and j .

From the literature, two MgCa potentials developed in the MEAM framework are available [11,18]. For simplification, G-MEAM and K-MEAM refer to the potentials proposed by Groh [11] and Kim et al. [18], respectively. Using the G-MEAM potential, it was demonstrated by Groh [11], in agreement with first-principle data, that substitutional Ca in Mg-based alloys increased the energy barrier for dislocation motion in the basal plane while decreasing the energy barrier for dislocation motion in the pyramidal second order slip system. As a consequence of such changes in the energy barriers for dislocation activity, the formability parameter proposed by [17] suggests that nanopolycrystalline Mg alloys can be alloyed with small concentrations of Ca to improve formability. As plotted in Fig. 1 using the so-called effective potential [16], it can be observed that the G-MEAM potential accurately reproduces the variations of the energy with respect to the volume for the B2 phase as predicted by Zhou and Gong [51] using density functional theory. Alternatively, the K-MEAM potential underesti-

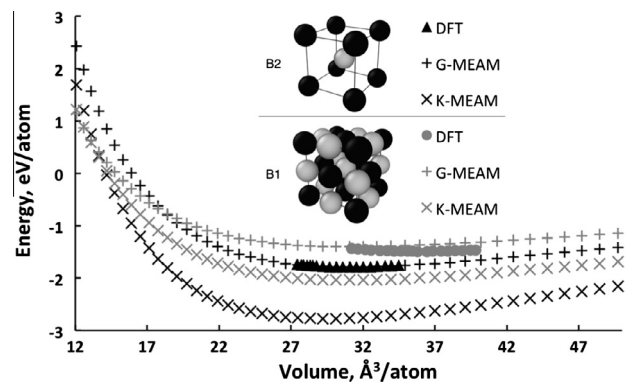


Fig. 1. Energy vs. volume of B1 and B2 MgCa compounds obtained using K-MEAM and G-MEAM, and compared with the first-principles predictions of Zhou and Gong [51].

Download English Version:

<https://daneshyari.com/en/article/1559959>

Download Persian Version:

<https://daneshyari.com/article/1559959>

[Daneshyari.com](https://daneshyari.com)