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Full Length Article

Molecular dynamics simulation of nanometer scale mechanical properties of hexagonal Mg—Li alloy

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Abstract

Nano mechanical behavior of Mg—Li nanowire is investigated under tension and compression to elicit property alteration due to Li alloying in Mg within hexagonal range. Embedded atom method (EAM) is employed to carry out present simulation work. Nanowire under consideration is supposed to be isotropic and mechanical behavior is uninfluenced by material texture. The elastic modulus, yield strength both in tension and compression is assessed with change in strain rate. Effects of temperature in tension and compression are studied. Results of present simulation work elicit serrated yielding under uniaxial tension, however, twin mediated deformation under compression is completely tuned with previously reported experimental works. This investigation bridges nanometer scale properties to microscale material response, which in turn can be applied for designing suitable robust processing routes of this material.

Keywords: Molecular dynamic simulation; Nanowire; Mechanical behavior

1. Introduction

Mg—Li based alloys are potential next generation structural material for automotive, aerospace and other transport industries for light weight, fuel efficient automotive components due to its high specific strength with stiffness [1–8]. This particular alloy design seems to be lightest ($\rho \sim 1.3$–1.7 g/ cm^3) among all commercial magnesium casting component as well as other metallic structural materials, hence draw attention as a competitive structural material. Depletion of Taylors five independent slip systems [9], below 225 °C deformation of polycrystalline hcp-Mg, is restricted to basal $(0001)<11\bar{2}0>$ slip and pyramidal $\{10\bar{1}2\}<1011>$ twins. Magnesium exhibits poor plasticity and strong deformation texture during conventional metal working like rolling, forging extrusion but addition of Li (bcc) to Mg (hcp) decreases c/a ratio from 1.624 (pure Mg) to 1.607 (Mg—17 at% Li, near solubility limit) [10]. Increasing activity of non basal prismatic slip plane improves room temperature ductility of Mg—Li α-solid solution [11]. Increase in critical resolved shear stress for basal slip with increase of Li concentration has been reported by previous researchers [12]. Moreover segregation of Li in Mg—Li or Mg—Li—Al alloy is also not very well understood [13,14]. Along with that assessment and understanding of deformation modes, thereafter correlation of microstructure and process parameters for optimum material performance for reliable and safe service condition is of great importance. Evaluation of mechanical behavior at molecular length scale bridges microscopic, in turn macroscopic continuum mechanical response of the material [15,16]. Therefore, molecular dynamics analysis is a potential method for understanding physical phenomena inexplicable and/or inaccessible in macroscopic length scale investigations. Pure magnesium has been well explored in molecular dynamics simulation, various attempts to simulate the large scale molecular dynamics of pure Mg for understanding its deformation behavior is well studied, special focus also given to twin formation as well in Mg [17,18]. Nanocrystalline modification of hcp-Co (similar c/a ratio ~1.63) exhibits superior mechanical properties than its micro-crystalline counterpart which is believed due to high density of stacking fault is noticeable on basal planes [19,20]. This idea can be extrapolated for pure Mg too. However, addition of alloying elements to Mg—Li alloy has been very less explored for its nanoscale properties [21], but many ab-initio studies have been done in

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recent time studying its mechanical and physical properties [22–24]. In previous MD simulation of Mg—Li a cubic box with 600 particles and periodic boundary conditions [25] structural properties was studied after an equilibration period of 10,000 time step, but it was based on LJ type potential. LJ pair potential does not imitate the structural properties of metallic system. That is why metallic bonds are described by embedded atom method (EAM) potential, which provides the best description of the metallic bonding in the work piece [26]. At present most of the simulation of metals are done using EAM or some kind of a modification of EAM potential like modified embedded atom method (MEAM) or 2NN (2nd nearest neighbor) MEAM to predict the molecular trajectories accurately [27–29]. Here we present our work which elicits a large scale molecular dynamics simulation of Mg—5Li alloys. Mg—Li is always interesting to study for its very light weight, computationally however it is very less explored. As the multiscale modeling is gaining popularity it is not necessary to study the deformation behavior of materials at nanoscale. Regarding Mg—Li there are ab-initio studies for shear modulus, bulk modulus [23], there are also a large set of studies on Mg—Li—X (X for various metals like Ni, Al etc.) [30]. Ab-initio DFT studies are derived from very fundamental assumptions by taking quantum mechanical properties into account, but as it is very fundamental in nature it is not computationally efficient to take a large number of electrons into the computation. That is where large scale molecular dynamics simulation is used to predict material properties to a very large number of atoms. Large scale molecular dynamics study of Mg—Li is not that frequent in literature. Especially our choice of 5.5% of Li in Mg—Li alloy which has a significant role in lightweight metal industry is yet to be studied with the help of molecular dynamics. Li addition to the alloy will result into two phase addition of Li between 5.5 and 11 wt % results in a two phase, α (hcp) and β (bcc), structure. Per the author's knowledge on Mg—Li alloy, there has not been a detailed nanoscale molecular dynamics study of this alloy. Apart from Mg—Li alloy, we can say particularly the hexagonal phase of it. Our work on the deformation mechanisms under tension and compression at a certain strain rate, effects of variable strain rates and evaluation of temperature dependence mechanical behavior may help to understand the atomic scale failure phenomena. This is the main aim and objective of the material.

2. Potential model and simulation methods

To obtain physically meaningful results from atomistic simulations, it is essential that reliable interatomic potentials are used, inter atomic potential track the atomic trajectories during any simulation. That is why only a reliable interatomic potential can reproduce various physical properties of relevant elements or alloys, including the elastic properties, structural properties, defect properties, surface properties, thermal properties etc. The potential use in this simulation is 2NN-modified embedded atom type potential (MEAM) developed by Kim et al. [31] Generally EAM potential accounts for the behavior of an atom placed in a defined electron density that is why this method can capture the physical reality of metallic bonding [26]. This approach represents the total energy of the system as a combination of two additive terms, a pairwise sum of interactions between atoms and a term representing the electron density of each atomic site. While calculating the forces on atoms EAM uses a linear superposition of spherically averaged electron densities. But MEAM, which was initially developed by Baskes26, allows background electron density to depend on local symmetry that is why it can consider the directionality of the bonding of the material. But the original MEAM considered interactions only among first nearest-neighbor atoms. So again MEAM was modified by Lee and Baskes [28] and Lee et al. [29] such that the interactions among second nearest-neighbor atoms (2NN MEAM) are partially considered overcoming some critical shortcomings of the original MEAM. In (2NN) MEAM the total energy has been given by,

$$E = \sum_i \left[F_i(\bar{\rho}_i) + \frac{1}{2} \sum_{j(\neq i)} S_{ij} \varphi_{ij}(R_{ij}) \right] \tag{1}$$

where *Fi* is the embedding function for an atom *i* embedded in a background electron density *ρi*. *Sij* and *φij*(*Rij*) are the screening function and the pair interaction between atoms *i* and *j* separated by a distance *Rij*. For energy calculations, the functional forms for *Fi* and *φij* should be given. As mentioned before the in 2NN MEAM potential background electron density at each atomic site is computed by considering the directionality of bonding, i.e. by combining several partial electron density terms for different angular contributions with weight factor. Each partial electron density is a function of atomic configuration and atomic electron density of each element. A perfectly ordered binary intermetallic compound, where one type of atom has only the same type of atoms as second nearest neighbors, is considered as a reference structure in the 2NN MEAM. For the Mg—Li system, a fictitious B2 ordered structure is chosen as a reference structure [31]. The total energy is given as follows,

$$\begin{aligned} E^{u}_{MgLi}(R) = \frac{1}{2}\Bigg[& F_{Mg}(\bar{\rho}_{Mg}) + F_{Li}(\bar{\rho}_{Li}) + Z_1 \varphi_{MgLi}(R) \\ & + \frac{Z_2}{2}\left[S_{Mg}\varphi_{MgMg}(aR) + S_{Li}\varphi_{LiLi}(aR) \right] \Bigg] \end{aligned} \tag{2}$$

where *Z1* and *Z2* are the numbers of first and second nearest-neighbors in the B2 MgLi structure respectively. In the present case, *Z1* and *Z2* are 8 and 6, respectively. *SMg* and *SLi* are the screening functions for the second nearest-neighbor interactions between Mg atoms and between Li atoms, respectively, and aids the ratio between the second and first nearest neighbor distances in the reference structure. The pair interaction between Mg and Li can now be obtained in the following form,

$$\begin{aligned} \varphi_{MgLi}(R) = \frac{1}{Z_1}\Bigg[& 2E^{u}_{MgLi}(R) - F_{Mg}(\bar{\rho}_{Mg}) - F_{Li}(\bar{\rho}_{Li}) \\ & - \frac{Z_2}{2}\left(S_{Mg}\varphi_{MgMg}(aR) + S_{Li}\varphi_{LiLi}(aR) \right) \Bigg] \end{aligned} \tag{3}$$