Molecular dynamics simulation of diffusion in Mg-Al system under pressure

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Abstract. The Mg-Al composite material possesses a large potential value in practical application due to its excellent properties. Molecular dynamics with the embedded atomic method potentials is applied to study aluminium-magnesium (Al-Mg) interface bonding during deformation. Study of fabrication techniques to obtain composites with improved mechanical properties, careful investigation of phase composition, dynamics and kinetics are of high importance. The loading scheme used in the present work is the simplification of the scenario, experimentally observed previously to obtain Al/Cu composites. It is shown that shear strain has a crucial role in the diffusion process. The results indicated that the symmetrical diffusion took place in the Mg-Al interface during deformation. Tensile tests showed that fracture took place in the Mg part of the final composite sample, which means that the interlayer region where the mixing of Mg and Al atoms observed is much stronger than the pure Mg part.

1. Introduction

High-pressure torsion (HPT) is an effective technique to manufacture nanostructured materials with improved mechanical properties [1-4]. Recently, this method was used to obtain metal-matrix composites based on strongly dissimilar materials consolidated during deformation treatment, like carbon-metal composite [5, 6], ceramic Al/Al2O3 composite [7, 8], metal-metal composites [9, 10].

Different initial elements can be used to obtain mixed composite structures like powders or discs. For example, previously, HPT followed by annealing was successfully used to obtain Al-Cu in-situ composites from stacked discs [9-11]. Magnesium and Mg alloys are increasingly used in various industrial applications, for example, for aerospace or automotive industry [12, 13]. A combination of Mg with the other metals can improve the properties of the final structure. Aluminium can prevent the corrosion process of Mg alloy and possess better properties for both Mg and Al [14-16]. Mg-Al alloys are promising for advanced engineering applications.

It was previously shown that temperature and pressure can affect the efficiency of diffusion on the Al and Mg interphase [17, 18]. Thus, studying the diffusion behavior in Al/Mg system is of high importance. To understand the atomic mixing between Al and Mg, the distribution of Al and Mg should be predicted in order to control the formation of intermetallic compounds. X-ray photoelectron spectroscopy or the electron probe micro-analyzer can be used to experimentally determine these distributions however, it is still very hard to get a close view locally in the zones of interests [19].
Molecular dynamics (MD) simulation is an effective tool for studying different processes on atomistic level [20-25]. Different binary systems were successfully studied by MD with the realistic interatomic potential. In the present work, MD simulation is applied in order to study atomic diffusion behavior at the bonding interface in the Al/Mg sample during compression combined with shear strain. Mechanical strength of the obtained composite is studied under uniaxial tension.

2. Simulation details

The atomic structure of a bimetallic AlMg interface is presented in figure 1. A bilayer model of Mg (HCP lattice, red atoms) and Al (FCC lattice, blue atoms) is assembled from two unrelaxed perfect crystals with lattice parameters of $a_{\text{Mg}} = 3.203$ Å and $a_{\text{Al}} = 4.05$ Å. Magnesium crystal has 31 periodicity-lengths along $x$ and $y$, $L_x = L_y = 100$ Å, and 15 periodicity-lengths along $z$, $L_z = 50$ Å; Al crystal has 24 periodicity-lengths along $x$ and $y$, $L_x = L_y = 100$ Å, and 12 periodicity-lengths along $z$, $L_z = 50$ Å. The interlayer distance between two crystals calculated as $(a_{\text{Mg}} + a_{\text{Al}})/2 = 3.6$ Å. The periodic boundary conditions are applied along $x$, $y$, and $z$ directions. The structure is initially relaxed at 300 K to find structural configuration with minimum potential energy.

![Figure 1. Simulation cell. Al atoms are shown by blue, Mg atoms are shown by red.](image)

The simulations are carried out by molecular dynamics using the LAMMPS free simulation package. Embedded atom method (EAM) interatomic potential for Mg and Al is used [26]. For temperature control, the Nose-Hoover thermostat is applied. Verlet algorithm to integrate the Newtonian equation of motion with an integration time-step of 2 fs is used.

To study the process of fabrication of Mg-Al composite and phase transformation in the system, pressure along $z$-axis $\varepsilon_{zz}$ combined with shear strain $\varepsilon_{xy}$. Strain rate is equal to $\varepsilon_{zz} = 0.00005$. Previously it was shown that this strain rate is small enough to obtain some phase transformations and not increase considerably the simulation time [27].

3. Results and discussion

3.1. Effect of loading

To visualize the evolution of diffusion over time, the representative atomic configurations are drowned out from the data obtained after the deformation of the material. Mg-Al interface is analysed at different strains and two types of loading conditions. The snapshots of interdiffusion processes of Mg and Al atoms at 300 K are displayed in figure 2, where Mg block in the model is shifted to the right by about 100 Å for a clearance. As can be seen, a small number of interdiffusion atoms are observed after pure compression along $z$-axis even after $\varepsilon_{zz} = 0.16$. Comparatively, when additional shear strain is
applied, the number of diffusing atoms considerably increases. It can be seen, that number of Mg atoms diffusing into Al matrix is almost equal to the number of Al atoms diffusing into Mg matrix, which can be connected with the equality of the atomic radius of Al and Mg atoms \( r_{\text{Mg}} = 1.45 \text{ Å} \) and \( r_{\text{Al}} = 1.43 \text{ Å} \). In addition, the lack of difference in the melting point for Mg (923 K) and Al (933.5 K) is worth considering, which means the bonds in both metals are similarly stronger to fraction.

It is found that key role in the process of atom mixing playing shear strain, because after pure compression (figure 2c,d) even after \( \varepsilon_{zz} = 0.16 \) only several atoms diffusing near the interlayer region. Thus, further only the case of combined loading would be considered.

![Figure 2](image)

**Figure 2.** Snapshots of the mutual diffusion of Mg and Al atoms at 300 K for two types of loading: (a,b) uniaxial pressure \( \varepsilon_{zz} \) combined with shear strain \( \varepsilon_{xy} \) and (c,d) uniaxial pressure \( \varepsilon_{zz} \). Snapshots after \( \varepsilon_{zz} = 0.04 \) (a,c) and after \( \varepsilon_{zz} = 0.16 \) (b,d). The red and blue balls represent Mg and Al atoms, respectively. The black dot line represents the initial position of Mg-Al interface.

Figure 3 shows the concentration distributions of Mg and Al atoms along \( z \) direction. The area on both sides of the interface where considered to calculate the atomic composition. The thickness of the layer where the diffusion of atoms during deformation took place is 42 Å. As it can be seen, after \( \varepsilon_{zz} = 0.04 \) thickness of the diffusion layer is equal to 29 Å, while after \( \varepsilon_{zz} = 0.16 \) equal to 38 Å. This figure also confirms that the number of Mg atoms diffusing into Al matrix is almost equal to the number of Al atoms diffusing into Mg matrix. However, the boundary of the mixing region in Mg part of the sample moves faster than in Al part: shift for 7 Å is observed for Mg part and only for 2 Å for Al part. It can be explained by a more porous HCP lattice of Mg.

### 3.2. Uniaxial tension

To study mechanical properties of the obtained composite structure, uniaxial tension along \( z \)-axis is applied after compression \( \varepsilon_{zz} = 0.16 \). In figure 4, the stress-strain curve is presented together with the snapshots of the structure close to the critical point. The process initiates with elastic deformation of structures (until about \( \varepsilon_{zz} = 0.02 \)). During plastic deformation, several drops in the stress-strain curve can be seen which is connected with defect structure transformation.

Fraction takes place at \( \varepsilon_{zz} = 0.22 \) and \( \sigma_{zz} = 11 \text{ GPa} \) in the Mg block of the composite. As it is known, Mg lattice is more prone to form defects than Al lattice. Analysis of the dislocation structure shows that most of the dislocations nucleated in Mg part of the sample.
Figure 3. The concentration of Mg and Al atoms along the z-direction after uniaxial pressure combined with shear at (a) $\varepsilon_{zz} = 0.04$ (blue line), (b) $\varepsilon_{zz} = 0.08$ (red line), (c) $\varepsilon_{zz} = 0.16$ (green line).

Figure 4. Stress-strain curve for Al-Mg with the snapshots of the structure close to the critical point. Snapshots are shown in accordance with the common neighbour analysis. The green colour is for FCC lattice, red - for HCP lattice, blue - for BCC lattice, and grey - for unknown.

4. Conclusions
In the present paper, the process of formation of Al/Mg composite from two initially separated crystals by severe plastic deformation is analysed on an atomistic level by molecular dynamics simulation. The proposed model is the simplification of scenario, experimentally observed previously in [10, 11, 9, 28]. In the HPT experiments, samples are polycrystals, while in the present model single crystal is considered. However, even such a simple model, allows understanding of mechanisms of diffusion bonding between Mg and Al.

It is found that uniaxial compression combined with shear deformation is an effective way to obtain the composite structure. Shear strain plays the most important role and considerably accelerates atoms mixing. As the strain increases, the number of diffusing atoms and the thickness of the interface region
grows rapidly. The symmetrical diffusion bonding took place during the deformation of the initial sample. Further analysis shows that Al atoms diffuse into Mg block easier than Mg atoms diffuse into Al block.

However, promising results are obtained, additional studies are required to underspend the effect of different factors on the diffusion process in Al/Mg binary system. For example, effect of mutual orientation near the interface, because their effect was previously shown for other binary systems.

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