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Research paper

Atomistic Simulations of Twist Grain Boundary Structures in Aluminum-Magnesium Alloys

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Abstract

The structures and energy of grain boundaries (GBs) have a significant influence on the mechanical properties of polycrystalline material. Most metal exists in the polycrystalline form but most of the metal applications are in term of their alloys. In this paper, twist GBs in magnesium (Mg)-aluminum (Al) were simulated using atomic simulation to understand the structure and properties of GBs in alloy. The energy of 45 twists GBs were calculated and plotted. The results indicate that the GB energy of a low-range misorientation angle agrees with the Read-Shockley equation for dislocation model. In high angle GB, special behaviour correspond to low ∑ values are observed.

Keywords: *Atomistic Simulation, LAMMPS, Read-Shockley Equation, Twist Grain Boundry Structures*

1. Introduction

Grain boundaries (GBs) are crystallographic defects that have a significant influence on the properties of polycrystalline materials. GBs refer to the region where two adjacent grains of different orientation are separated. GBs disturbed the dislocation in a material, which strongly affects the mechanical properties of the material. In metal alloys, the addition of the other substance further disturbed the lattice orientation. Most metal applications are in the form of their alloys. However, the effect of substance addition in alloys grain boundary properties is unknown. Over the past years, numerous studies have been done to study the basic properties of grain boundary in pure metals, such as the grain boundary energy, mobility and diffusivity via experiment and computer simulations. Atomic simulations are viewed as an effective way to understand the grain boundary structures and properties. At present, there are numerous studies on the GB crystallographic orientation and their properties; for example the study of GB energy as a function of GB disorientation in face-centered cubic (FCC) metals [1]–[3], GB mobility and grain growth [4]–[8] and deformation behavior of GBs under tensile force [9]–[11].

In this paper, the GB energy and structure of twist GBs was investigated using atomic simulations on Al-Mg alloys. Al-Mg alloys are binary alloys of 5xxx series aluminium alloys in non-heat treatable class. They possess moderate-to-high strength and toughness properties and high corrosion resistance, which are important properties in an automotive and marine application. Although high Mg content is desirable as it has higher tensile strength, the concentration of Mg more than 6% resulted in severe edge cracking[12]. In this study, only 0.05% of Mg concentration in Al alloy is used.

2. Computational models and methods

The atomic simulation was performed via LAMMPS [13]. The interatomic potential between atoms was obtained from Interatomic Potentials Repository Project [14]. The force field is calculated using embedded atom and Finnis-Sinclair (EAM/FS) method for diluted Al-Mg alloy and has been discussed elsewhere [15].

The method of creating and calculating the GB energy is similar to what is done by Tschopp et al. (2015). A schematic of a twist GB model is shown in Figure 1. The initial configuration of our model is a single crystal of Al-Mg alloy; which orientation are x<110>, y<001> and z <11$\bar{0}$>. Then both grains are rotated by θ/2 about z-axis clockwise and counterclockwise respectively. There are two GBs formed in this simulation, one periodic GB on both ends of the cell and the other GB is in the middle of the cell. In each grain, the concentration of Mg is set to be 0.05% randomly. The dimension of the simulation box is defined large enough to minimize the interaction between the two GBs. Each grain consist of ≈ 60000 atoms. The dimension of the simulation cell is set to be 10nm x 10nm x 20nm and is set to periodic in three directions (3D periodic box). Since atoms near the GB may overlap with each other, a critical distance [3] is defined as a deletion criterion for these atoms. The energy minimization is achieved by the non-linear cojugate gradient method.

The atomic simulation was done for misorientation angle $0 \leq \Theta \leq 180°$. Table 1 lists 32 examples of twist GB angles with their lattice orientation and ∑ value. The ∑ value denotes the reciprocal density of coincident site lattice (CSL). The grain boundary energy (GBE) can be calculated by$E_GB=\sum(E_o-E_c)/A_XZ$ whereE_0, E_c is the potential energy of the perfect crystal and twist GB respectively and A_xz is the area of GB plane $(L_x \times L_y)$.

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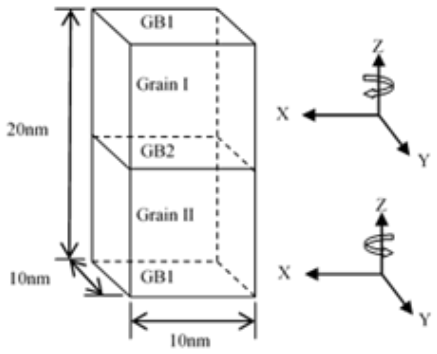


Fig 1: Schematic diagram of two grains with two GBs

Table 1: Misorientation parameter: twist angle, lattice orientation in the x-direction and the sigma value

Twist Angle (θ)	x-direction	∑	Twist Angle (θ)	x-direction	∑
1.00	<81 81 1>|<81 81 $\bar{1}$>	13123	80.63	<5 5 6>|< 5 5 $\bar{6}$>	43
2.03	<40 40 1>|<40 40$\bar{1}$>	3201	86.93	<3 3 4>|<3 3 $\bar{4}$>	17
4.05	<20 20 1>|<20 20$\bar{1}$>	801	89.42	<5 5 7>|<5 5 $\bar{7}$>	99
8.09	<10 10 1>|<10 10$\bar{1}$>	201	96.03	<7 7 11>|<7 7 $\bar{11}$>	219
11.54	<7 7 1>| <7 7$\bar{1}$>	99	105.42	<7 7 13>|<7 7 $\bar{13}$>	267
14.23	<17 17 3>|<17 17$\bar{3}$>	587	109.47	<1 1 2>|<1 1 $\bar{2}$>	3
17.23	<14 14 3>|<14 14 $\bar{3}$>	401	114.53	<5 5 11>|<5 5 $\bar{11}$>	171
20.05	<4 4 1>|<4 4 $\bar{1}$>	33	129.52	<1 1 3>|<1 1 $\bar{11}$>	11
26.53	<3 3 1>|<3 3 $\bar{1}$>	19	137.82	<3 3 11>|<3 3 $\bar{11}$>	139
31.59	<5 5 2>|<5 5$\bar{2}$>	27	141.06	<1 1 4>|<1 1 $\bar{4}$>	9
38.94	<2 2 1>|<2 2 $\bar{1}$>	9	148.41	<1 1 5>|<1 1 $\bar{5}$>	27
44.00	<7 7 4>|<7 7 $\bar{4}$>	57	153.47	<1 1 6>|<1 1 $\bar{6}$>	19
50.48	<3 3 2>|<3 3 $\bar{2}$>	11	159.95	<1 1 8>|<1 1 $\bar{8}$>	33
55.88	<4 4 3>|<4 4 $\bar{3}$>	41	162.14	<1 1 9>|<1 1 $\bar{9}$>	83
61.02	<6 6 5>|<6 6 $\bar{5}$>	97	165.35	<1 1 11>|<1 1 $\bar{11}$>	123
70.53	<1 1 1>|<1 1 $\bar{1}$>	3	175.91	<1 1 40>|<1 1 $\bar{40}$>	801

3. 3. Results and discussion

3.1 Grain boundary energy

Twist GBs is if the rotation axis is orthogonal to the grain boundary. If the adjacent crystals are mirror images of each other, then the GBs are symmetric. In this study, only symmetric twist GBs are studied. Figure 2 shows the dependence of GB energy on the misorientation angle. The GB curve for Al-Mg alloy has the similar pattern for low twist angle with iron [16] and tungsten [17]. The GBs are categorized into low angle GBs (LAGB) and high angle GBs (HAGB).

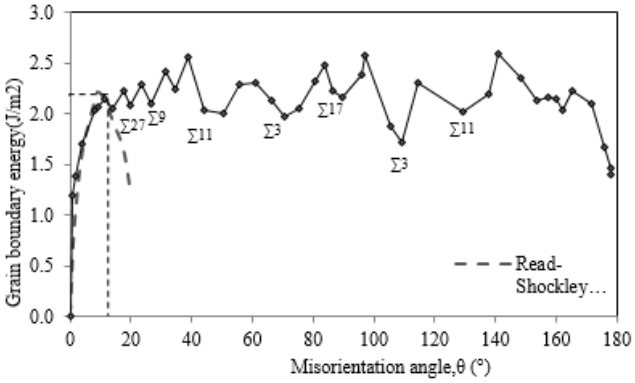


Fig 2: The dependence of GB energy with misorientation angle. The dotted line is the fitted curve based on Read-Shockley equation for low angle boundaries.

The GB energy, γ, dependence with low misorientation angle can be described using Read-Shockley equation [18] ,$\gamma = \gamma_0\theta(A - \ln\theta)$ where γ_0 and A are constants and θ is the misorientation in radians. The plot in Figure 2 are fitted into the Read-Shockley equation where $\gamma_0 = 11.189$ J/m^{2}and $A = -0.637$. The fitted curve agrees well with misorientation angle, $\theta \leq 11.54°$ and deviated at higher misorientation angles. The Read-Shockley does not work with higher angles since there is no regular dislocation network at those angles[16], [17].In the high angle, the properties of the GBs are independent of the misorientations. For two adjacent grains, the coincident site lattice (CSL) theory is used to describe the degree of fit, ∑ between two grains. ∑ is defined as the reciprocal of the density of coincident sites. In symmetric FCC crystal the ∑ value can be determined by, $\sum = \delta(h^2 + k^2 + l^2)$, where δ=1 if $(h^2 + k^2 + l^2)$ is odd and $\delta = 1/2$ if $(h^2 + k^2 + l^2)$ is even. As observed in the cusps in the high angle range in Figure 2, the GBs with low ∑ have lower GB energies. The GBs with low value of ∑ in high angle GBs are widely accepted as special GBs as they have the tendency to decrease the GB energy[16], [17].

3.2 Grain boundary structure

The structures of the twist GB are viewed using OVITO visualization software [19]. The centrosymmetry parameter is used to locate the dislocation in twist GBs. The centrosymmetry parameter is controlled in a threshold ($0.005 \sim 12$), the atoms outside this threshold are not displayed. Low angle GB structures are depicted in Figure 3 and high angle GB structure in Figure 4. In low angle GBs, an array of dislocation can be observed in the periodic tetragonal pattern. As the misorientation angle increases, the number of dislocation also increases and resulted in the space reduction between neighbouring dislocations. According to O-lattice theory, the upper and lower grains rotate around each O-point to improve lattice matching across the GB which resulted in a reduction of the GB energy in low angle. As the misorientation continues to increase, the dislocation will begin to overlap with each other and disrupt the array of dislocation at the boundary.

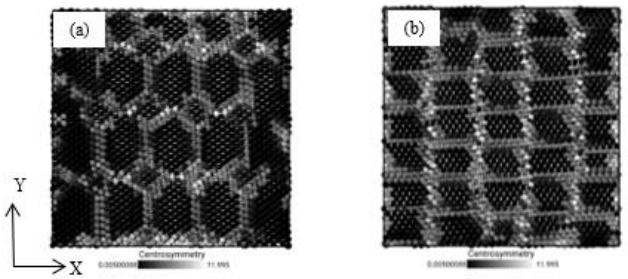


Fig 3: GB structure for low angle GBs: (a) 8.09° (b) ∑99- 11.54°

High angle GBs has poor lattice matching and the structures are disordered (Figure 4(a) and (b)) resulted in higher GB energy than at low angles. For special grain boundaries, due to their low ∑ values, they have good lattice matching thus, resulted in relatively lower GBs energy as in Figure 4(c). ∑3 GBs is known as coherent twin boundary with relatively low GB energies.

However in this work, as observed in Figure 2, the energies for ∑3 GBs are still quite high. This might be due to presence of Mg in Al. The Mg particles cause lattice distortion in Al that interferes with the motion of the dislocation, resulted in lattice mismatch, and thus increases the grain boundary energy.

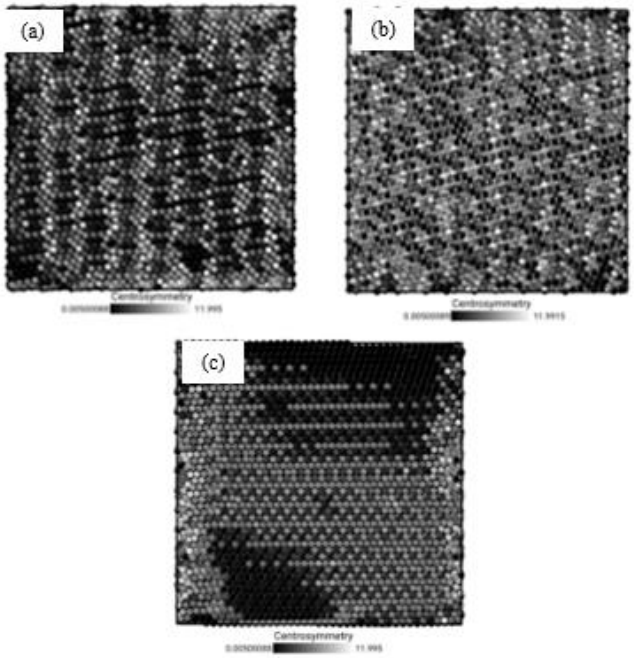


Fig 4: GB structure for high angle GBs (a) 20.05° (b) 44.00° (c) ∑3- 70.53°

4. Conclusion

In summary, the energy and structure of <110> twist GB in 0.5% Mg in Al alloy has been studied for misorientation angle 0 ≤θ≤180° via atomic simulation. The relationship between GB energy with misorientation angle is obtained and the analytic GB energy is calculated using Read-Shockley equation. The GB energy from prthe esent study is fitted into the Read-Shockley equation in low-angle range. In high angle range, there are no specific correlation between the grain boundary energy and misorientation angle. The GB energy with low ∑ values correspond to the cusps of the GB energy curve. The high angle GB with low ∑ value are special boundaries as they have good lattice matchinand relatively low boundary energy. However, in this study, the addition of Mg atoms cause lattice distortion in Al and interfere with the dislocation in the material and increases the GB energies in general.

Acknowledgements

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