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Effects of Zn atoms on the basal dislocation in magnesium solution from Peierls–Nabarro model

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ABSTRACT

Effects of Zn atoms on basal dislocation in Mg solution have been studied by means of the improved 2D Peierls–Nabarro model in combination with misfit approximation under the Fermi–Dirac distribution function of solute atoms. With increasing Zn concentration, the separation distance for edge dislocation is decreased, while the separation distance is increased for screw dislocation. From function of the total dislocation line energy surfaces as shift displacement of dislocation center and separation distance between the partials, it is found that with the increase of solute concentration of Zn atoms, the Peierls energies, Peierls stresses and yield stresses for edge dislocation increase more quickly than ones for screw dislocation, and the increase of edge dislocation is stronger.

1. Introduction

Magnesium and its alloys have attracted increasing interest in automobile and aerospace industry due to the light weight, high specific strength and environment-friendliness [1,2]. However, the strength and ductility of pure Mg are poor due to the anisotropic response of its hexagonal close-packed (hcp) structure. It has been shown that small addition of solute atoms causes a significant increase in both strength and ductility of Mg due to solid-solution strengthening [3–7]. Therefore, the study of solute strengthening in Mg solution is valuable.

Generally, the plastic deformation of Mg is accommodated by slip of $[11\bar{2}0]$ dislocations on basal and non-basal ($(10\bar{1}0)$-prismatic and $(10\bar{1}1)$-pyramidal) planes, $[11\bar{2}3]$ dislocations on pyramidal plane $(11\bar{2}2)$ and twinning on $(10\bar{1}2)$ and $(10\bar{1}1)$ planes [8–15]. Because the critical resolved shear stresses (CRSSs) of basal slip, twinning, prismatic slip and pyramidal slip are in ascending order [14,16–19], the basal slips are initially activated at finite temperatures during the deformation processing [14,19–21]. Therefore, the solute strengthening on basal plane would be essential to understand the improvement of strength of Mg solutions.

Recently, theoretical investigation of solute strengthening on basal plane in Mg solution has been performed using either direct *ab initio* calculation or atomistic simulation, in which random distribution (or average distribution) of solute atoms in alloys was assumed [22,23]. However, the solute atoms in materials are under a certain concentration distribution around the dislocation at finite temperatures due to interaction between solute atom and dislocation [24–26]. Therefore, their model can be further improved for the study of solute strengthening at finite temperatures, and further study of solute strengthening in Mg solution is necessary.

Zinc is widely used as a strengthening element in Mg solution owing to its excellent effect and non-toxicity [27–30]. In this work, the effects of Zn on basal dislocation of magnesium solution up to concentration limitation [31] at 300 K have been investigated using the combination of the improved 2D Peierls–Nabarro model with misfit approximation under the solute distribution of the Fermi–Dirac function.

2. Theoretical model and computational method

2.1. The improved 2D Peierls–Nabarro model

In the generalized 2D Peierls–Nabarro model [32–34], the total line energy of dislocation E_T consists of the elastic energy E_{el} in the two half-spaces and the atomic misfit energy E_A in the glide plane, that is, $E_T=E_{el}+E_A$. This total line energy E_T is a functional of disregistry $\boldsymbol{u}(\eta)$, which satisfies the boundary condition $\boldsymbol{u}(-\infty)=0$ *and* $\boldsymbol{u}(\infty)=\boldsymbol{b}$, where η is the coordinate in the glide plane normal to the dislocation line ξ.

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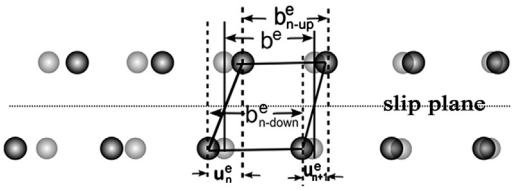

Fig. 1. Illustration of local volumetric strain for the edge component from the straight dislocation model. The faded spheres represent the perfect lattices.

The elastic energy E_{el} in the two half-spaces is expressed with Stroh tensor $\hat{H}=[H_{ij}]$ [35,36], which depends on the orientation of the dislocation line. For the (0001) plane of Mg, isotropy $\hat{H}$ is diagonal and has components $[H_{11},H_{22},H_{33}]=1/4\pi[K_{edge},K_{screw},K_{edge}]$. K_{screw} and K_{edge} of hexagonal crystals can be calculated by the following formula [37]:

$$K_{screw}=\left[\frac{1}{2}c_{44}(c_{11}-c_{12})\right]^{1/2} \tag{1}$$

$$K_{edge}=(\bar{c}_{11}+c_{13})\left[\frac{c_{44}(\bar{c}_{11}-c_{13})}{c_{33}(\bar{c}_{11}+c_{13}+2c_{44})}\right]^{1/2} \tag{2}$$

where $\bar{c}_{11}=(c_{11}c_{33})^{1/2}$ and c_{11}, c_{12}, c_{13}, c_{33}, and c_{44} are elastic constants. For the sake of convenience of following minimizing of the total line energy of dislocation E_T, the elastic energy E_{el} is then given by [32]

$$E_{el}(\boldsymbol{u})=\sum_q H_{qq}\sum_{i,j}u_i^q u_j^q \ln\left[\frac{R}{\omega_i^q+\omega_j^q}\right]-\frac{1}{2}\sum_{i,j}u_i^q u_j^q \ln\left[1+\frac{(r_i^q-r_j^q)^2}{(\omega_i^q+\omega_j^q)^2}\right]-\frac{1}{2}u_i^e u_j^s \ln\left[1+\frac{(r_i^e-r_j^s)^2}{(\omega_i^e+\omega_j^s)^2}\right] \tag{3}$$

with i, j being integers and $q=[e,s]$. $u_{i,j}^q$, $\omega_{i,j}^q$, $r_{i,j}^q$ are respectively disregistries, half widths and positions of the partials and R represents the normal outer cutoff radius of the elastic solution [38,39].

For a continuous displacement distribution, the atomic misfit energy E_A can be calculated by integrating the misfit energy density along the displacement path:

$$E_A(\boldsymbol{u})=\int_{-\infty}^{+\infty}\gamma(\boldsymbol{u}(\eta))d\eta \tag{4}$$

The misfit energy density along the specific path can be obtained by the generalized stacking fault (GSF) surface $\gamma(\boldsymbol{u}(\eta))=\gamma(u_x(\eta),u_y(\eta))$. For the following minimization of the total line energy of dislocation, the γ surface is expanded in 2D Fourier series in reciprocal lattice vectors [33]:

$$\begin{aligned}\gamma[u_x,u_y]=c_1+c_2[&\cos(2pu_x)+\cos(pu_x+qu_y)\\&+\cos(pu_x-qu_y)]+c_3[\cos(2qu_y)\\&+\cos(3pu_x+qu_y)+\cos(3pu_x-qu_y)]\\&+c_4[\sin(2pu_x)-\sin(pu_x+qu_y)-\sin(pu_x-qu_y)]\end{aligned} \tag{5}$$

where the reciprocal lattice vector along **x** direction is $p=2\pi/(\sqrt{3}a)$ and $q=2\pi/a$ is along **y** direction, $a=3.2$ Å is the lattice constant of Mg and c_1, c_2, c_3 and c_4 are coefficients.

In solution, the configurations and properties of dislocations are very complicated due to the interaction between solute atoms and dislocations, so the calculation of total dislocation energies thus is very difficult and time-consuming. Currently, misfit approximation of the solute strengthening model is proposed and applied to the study of dislocation in Mg solution [22]. In this approximate model, the misfit energy can be expressed as

$$E'_A(\boldsymbol{u})=E_A(\boldsymbol{u})+\sum_n c_0 E_{n-binding}(\boldsymbol{u}) \tag{6}$$

The first term is the misfit energy E_A of pure solid and the second term is the total interaction energy between solute atoms and dislocation, in which n represents the n-th atomic row parallel to the dislocation line, c_0 is the average concentration of solute atoms, and $E_{n\text{-}binding}(\boldsymbol{u})$ is the interaction energy of solute atoms with dislocations at n-th atomic row, which can be calculated in terms of the following chemical interaction and size interaction [22]:

$$\begin{aligned}E_{n-binding}(\boldsymbol{u})&=E_{n-chemical}(\boldsymbol{u})+E_{n-size}(\boldsymbol{u})\\&=E_{n-chemical}(\boldsymbol{u})-3BV_0\cdot e_{Vn}(\boldsymbol{u})\cdot\varepsilon_b\end{aligned} \tag{7}$$

The first term is the chemical interaction energy of single solute Zn atom with GSF, which is defined as follows:

$$E_{chemical}(\boldsymbol{u})=A[\gamma_{solution}(\boldsymbol{u})-\gamma_{pure\ Mg}(\boldsymbol{u})] \tag{8}$$

where A is the area of the fault plane. In Eq. (7) above, the second term is the size interaction energy, where B is the bulk modulus of Mg, V_0 is the equilibrium volume of a cell, e_{Vn} is the local volumetric strain at n-th atomic row and ε_b is the size misfit, which can be calculated as $\varepsilon_b=-(E'/3BV_0)$, where E' is the slope of the fitted quadratic strain energy of Mg solution. The local volumetric strain is defined as $e_{Vn}=V_n/V_0-1$, which can be represented by the disregistry $\boldsymbol{u}$. No local volumetric strain exists in the screw components of the partial, for the edge components, from the configuration as shown Fig. 1, the following expressions can be easily obtained based on the theory of straight dislocation [25,40]:

$$b_{n-up}^e-b_{n-down}^e=u_{n+1}^e-u_n^e \tag{9a}$$

$$b_{n-up}^e+b_{n-down}^e=2b^e \tag{9b}$$

Then the local volumetric strain at n-th atomic row in the final relaxed dislocation geometry can be obtained as

$$e_{Vn-up}=\frac{b_{n-up}^e+b_{(n-1)-up}^e-2b^e}{2b^e}=\frac{u_{n+1}^e-u_{n-1}^e}{4b^e} \tag{10a}$$

$$e_{Vn-down}=-\frac{b_{n-down}^e+b_{(n-1)-down}^e-2b^e}{2b^e}=-\frac{u_{n+1}^e-u_{n-1}^e}{4b^e} \tag{10b}$$

In the above approximate model of Eq. (6), the concentration c_0 in the misfit energy is assumed to be uniform. In fact, due to the interaction between solutes and dislocation, the solute should have certain distribution. The distribution of solute atoms at the n-th atomic row parallel to the dislocation line on the glide plane can be expressed using the Fermi–Dirac function [25]:

$$c_n=\frac{1}{1+exp\{[-E_{n-binding(\boldsymbol{u})}-kT\ln(c_0/(1-c_0))]/kT\}} \tag{11}$$

where c_0 is the average concentration of solute atoms Zn in the Mg solid solution, and $T=300$ K has been used at present. Then the total line energy of dislocation at finite temperatures can be expressed as

$$E_T(\boldsymbol{u})=E_{el}(\boldsymbol{u})+E_A(\boldsymbol{u})+\sum_n c_n E_{n-binding}(\boldsymbol{u}) \tag{12}$$

By minimizing dislocation line energy of the above 2D PN model, the effects of Zn on basal dislocations of Mg solution can be studied. The full details of minimizing procedure are described elsewhere [32,38,41].

2.2. Calculation method

The density functional theory (DFT) calculations were performed using VASP [42] with Perdew Wang (PW91) version of generalized gradient approximation (GGA) [43] and projector-augmented wave (PAW) [44] potentials. All calculations were performed at 0 K and the cutoff energy of plane wave basis was 350 eV. Brillouin zone sampling was performed using Gamma centered Monkhorst–Pack