

Molecular dynamics study of Al solute-dislocation interactions in Mg alloys

Luming Shen*

School of Civil Engineering, The University of Sydney, NSW 2006, Australia

(Received March 22, 2013, Revised April 7, 2013, Accepted May 7, 2013)

Abstract. In this study, atomistic simulations are performed to study the effect of Al solute on the behaviour of edge dislocation in Mg alloys. After the dissociation of an Mg basal edge dislocation into two Shockley partials using molecular mechanics, the interaction between the dislocation and Al solute at different temperatures is studied using molecular dynamics. It appears from the simulations that the critical shear stress increases with the Al solute concentration. Comparing with the solute effect at $T = 0$ K, however, the critical shear stress at a finite temperature is lower since the kinetic energy of the atoms can help the dislocation conquer the energy barriers created by the Al atoms. The velocity of the edge dislocation decreases as the Al concentration increases when the external shear stress is relatively small regardless of temperature. The Al concentration effect on the dislocation velocity is not significant at very high shear stress level when the solute concentration is below 4.0 at%. Drag coefficient B increases with the Al concentration when the stress to temperature ratio is below 0.3 MPa/K, although the effect is more significant at low temperatures.

Keywords: Mg alloys; molecular dynamics; solute effect; edge dislocation; drag coefficient; critical shear stress

1. Introduction

Magnesium (Mg) alloys have been constantly developed for various structural applications because of their light weight and high specific strength (Kainer 2000). However, due to the hexagonal close packed (HCP) structure their limited formability and mechanical anisotropy are the main obstacles for their wider applications. Since the mechanical properties of metals including strength and ductility can be influenced by alloy solute, a thorough understanding of the role of the solid solute in the microstructure-property relations is essential to the improvement of these mechanical properties of Mg alloys. In particular, studies at the atomistic level can help elucidate important aspects of solute-dislocation interaction and dislocation motion under different temperatures.

Dislocations in the alloys are pinned through interactions with the solute atoms. Compared with dislocation motion in pure crystal, higher shear stresses are therefore required for dislocation moving through a solute field. Solute strengthening is typically divided into two categories: strong

*Corresponding author, Professor, E-mail: Luming.Shen@sydney.edu.au

pinning, in which individual solutes are sufficient to pin the dislocation at the solute position; and weak pinning, in which the dislocation is pinned by a favourable collective configuration of solutes in a region of the material (Olmsted *et al.* 2006). In many cases, solute strengthening is the combination of both effects. As the dislocation attempts to move, or bow out in regions where it is not pinned, the remaining pinned dislocation segments experience increased forces, resulting from the dislocation curvature, which drive the unpinning. Thus, the amount of strengthening achieved by solutes is a function of the solute concentration, the fundamental strength and spatial range of the dislocation-solute interaction, the dislocation line tension, and the spatial configuration of solutes (Olmsted *et al.* 2006). The overall picture, however, is not clear and many unanswered questions remain with regards to the dislocation-solid solute interactions and the basic strengthening mechanisms in the alloys (Kong and Shen 2011).

Atomistic simulations can explicitly describe the dislocation core structure, including its splitting into partials, and solute-dislocation interactions in a physical and realistic manner, as compared with ad hoc continuum models. They also permit interatomic interactions, as relevant, among solutes, and the explicit consideration of solute configurations. Molecular mechanics (MM) simulations can be performed at zero temperature, where system energy is minimized, to analyse the unpinning of dislocation, or molecular dynamics (MD) can be carried out at finite temperatures to understand the thermal escape of dislocation from the energy barriers due to the solutes.

There have been quite a few atomistic studies of dislocation in various HCP materials (Bacon and Martin 1981, Bacon and Liang 1986, Ando *et al.* 2002). However, these works do not relate specifically to Mg. Only until recently there are a few atomistic simulations focused on the dislocation behaviour in pure Mg crystal (Yasi *et al.* 2009, Groh *et al.* 2009, Nogaret *et al.* 2010). Yasi *et al.* (2009) studied the core structures of screw and edge dislocations on the basal and prism planes in Mg, and the associated gamma surfaces, using an *ab initio* method and the embedded-atom-method interatomic potentials developed by Sun *et al.* (2006) and Liu *et al.* (1996). Their results showed that the dislocation core structures from *ab initio* were well represented by the Sun potential in all cases while the Liu potential showed some notable differences (Yasi *et al.* 2009). Groh *et al.* (2009) investigated the motion of dislocations with $\frac{1}{3}[1\ 1\ -2\ 0]$ Burgers' vector lying on the basal, prismatic and pyramidal slip planes in pure Mg under static and dynamic loading conditions using molecular mechanics (MM) and molecular dynamics (MD). Nogaret *et al.* (2010) examined screw and edge $\langle c + a \rangle$ dislocation core structures and Peierls stresses at 0 K and finite temperature using the embedded-atom-method potentials. It appears that there are even fewer atomistic simulations of the dislocation-solid solute interactions in Mg alloys in the open literature. Leyson *et al.* (2012) studied the finite-temperature yield stress of Mg-Al alloys undergoing basal slip using a recently developed parameter-free solute strengthening model, which took input from first-principles calculations of the dislocation/solute interaction energy and evaluated the solute strengthening due to fluctuations in solute concentration, taking into account the correlation of these fluctuations as a function of dislocation roughening. Tsuru *et al.* (2013) calculated the generalized stacking fault (GSF) energies for basal and prismatic planes in magnesium using density functional theory, and examined the effect of the GSF energy on the dislocation core structures using a semidiscrete variational Peierls-Nabarro model.

In HCP crystals, dislocations lying on different slip and twin systems can accommodate the plastic deformation (Hirth and Lothe 1992). Basal, prismatic and $\langle c + a \rangle$ -pyramidal are the most active slip systems in HCP and are commonly used to model the plastic behaviour at the mesoscale (Groh *et al.* 2009). Research has shown that the Peierls/critical shear stress of basal plane

dislocation is much lower than those in the other two planes (Yasi *et al.* 2009, Groh *et al.* 2009, Conrad and Robertson 1957, Reed-Hill and Robertson 1957). This study is thus focused mainly on the role that the basal plane dislocations plays on the deformation and strength of Mg alloys. We present extensive atomistic simulation results aimed at elucidating the effect of random Al solute additions on dislocation motion in a binary Mg-Al alloy and the associated solute strengthening as a function of concentration. In particular, edge dislocation structures in the basal plane of Mg/Al alloy will be investigated using molecular mechanics at zero temperature and molecular dynamics at finite temperature. Quantitative comparisons among available theoretical and numerical results will be presented. The work here on the solute–dislocation interactions could also provide a starting point for future physically-based crystal plasticity model for Mg alloys.

The remaining sections of the paper are arranged as follows. The computation procedures for the MM and MD simulations of dislocation-solute interaction are described in Section 2, which is followed by the demonstration of simulation results and discussions in Section 3. The concluding remarks are given in the last section.

2. Simulation procedure

In this study, MD simulations are performed to investigate the interaction between basal plane dislocation and Al solid solute and to study the effect of Al solute on the motion of dislocation and the critical shear stress of Mg alloys at different temperatures. In the atomistic simulations, software LAMMPS (Plimpton 1995) is adopted and the embedded atom method (Daw and Baskes 1984) is used to describe Mg-Mg, Al-Al and Mg-Al interactions with the potential model parameters being obtained from Mendelev *et al.* (2009). The computational configuration of the proposed MD simulations was initially developed in Shen *et al.* (2010) with the intention to allow the analysis of both edge and screw dislocations in an infinite periodic glide plane. The material is an Mg crystal with randomly inserted Al atoms deforming only through dislocation slip. The paper aims to investigate the effect of Al concentration on (1) the critical shear stress of the basal slip plane and (2) the motion of the edge dislocation in the basal slip plane, at a finite temperature.

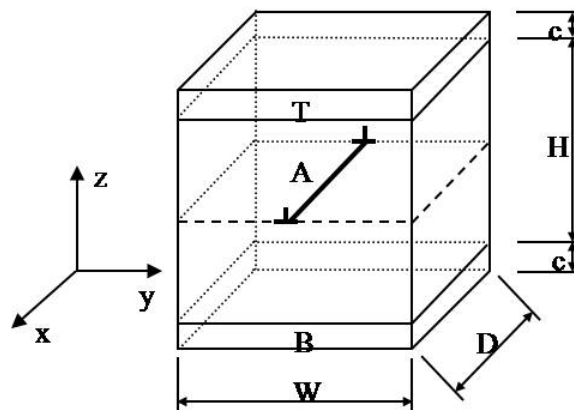


Fig. 1 Schematic diagram of the computational super-cell for simulating the behaviour of a dislocation in the HCP crystal

As shown in Fig. 1, the computational super-cell is a three-dimensional box where x , y and z are the global coordinates. The simulation cell consists of two parts. One part is referred to as the active zone (labeled as “A”) in which the atoms move according to the interactions among the neighboring atoms; the other part, labeled with a letter “T” or “B”, is referred to as the boundary zone, where the atoms are either fixed or assigned with a prescribed displacement to simulate a shear loading. The dimensions of the active zone are indicated by D , W and H , while the thickness of each boundary zone (T or B) in the z -direction is $c=\sqrt{3}a$ with a being the lattice parameter of Mg. The simulation cell uses a z coordinate normal to the glide plane. In standard HCP crystallographic notation, the crystal orientation has $x = [1 \ -1 \ 0 \ 0]$, $y = [1 \ 1 \ -2 \ 0]$ and $z = [0 \ 0 \ 0 \ 1]$ for the basal edge dislocation. Free surfaces are used along the z direction and periodic boundary conditions are applied along the x - and y -directions. In this case, the system can be represented as an array of dislocations periodically repeating in space.

The following procedure is used to form a basal plane edge dislocation: (1) The ideal crystal (super-cell) is evenly divided into the upper and lower half regions in the z -direction; (2) In the lower half region, two adjacent atomic half-planes (1 1 -2 0) are removed from the ideal crystal structure; (3) The y -coordinators of the remaining atoms in the lower half region are readjusted so that the distance between any two adjacent half-planes is the same while their x - and z -coordinates are kept the same and (4) The atoms in the “T” and “B” regions are then frozen while the atoms in region “A” are relaxed to minimize the potential energy of the entire system. It is necessary to emphasize the importance of the final stage in the above procedure because, at this stage, the pure dislocation, which is energetically less favourable for the HCP lattice, splits into two partial edge dislocations

$$\frac{1}{3} [1 \ 1 \ -2 \ 0] \rightarrow \frac{1}{3} [1 \ 0 \ -1 \ 0] + \frac{1}{3} [0 \ 1 \ -1 \ 0].$$

The dissociation of an Mg basal edge dislocation into two Shockley partials can be simulated using MM (Shen *et al.* 2010). Fig. 2 demonstrates the dissociation of a basal edge dislocation into two Shockley partials with 0.5 at% Al atoms randomly introduced into Mg matrix. In this study, the centro-symmetry deviation (CSD) method (Kelchner *et al.* 1998) is used to differentiate

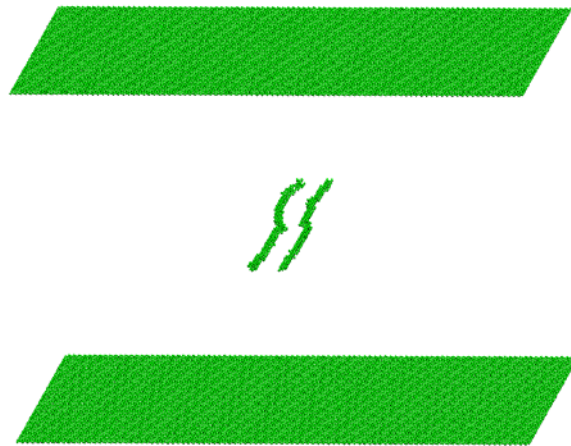


Fig. 2 Dissociation of an Mg basal edge dislocation into two Shockley partials with 0.5 at % Al

the surface and dislocation atoms from the bulk atoms, and only the atoms near the free surfaces and partial dislocations are shown in Fig. 2. The atoms with CSD parameter falling in the range of $0.5\text{\AA}^2 < P < 4\text{\AA}^2$ correspond to the cores of the partial dislocations, while the range of $P > 20\text{\AA}^2$ to the free surfaces. Due to the interactions between the dislocations and Al solutes, the two Shockley partials are not straight lines as those observed in pure Mg system in Shen *et al.* (2010).

After the basal edge dislocation is dissociated into two Shockley partials at zero temperature using MM, MD simulation are performed at a finite temperature. Those atoms in the boundary zone are fixed and the system is equilibrated in NVT ensemble for 50 ps. The Nose/Hoover temperature thermostat (Osetsky and Bacon 2003) is used to maintain the constant temperature. As shown in Fig. 2, with the atoms in region “B” being fixed, a constant velocity in the y-direction is then applied on the atoms in region “T” to simulate a displacement-controlled shear loading or a constant shear stress is applied on these atoms in region “T” to simulate a force-controlled shear loading. During the loading period, the temperature of the system is kept at constant using Nose/Hoover thermostat after excluding the y-component of the atom velocity. The time step is 1 fs in the MD simulation.

3. Simulation results and discussions

To study the effect of Al concentration on the critical shear stress of basal plane edge dislocation at a finite temperature, the Mg system with 0, 0.25, 0.5 and 1.0 at% Al is subjected to shear loading in the MD simulation. Following the convergence study in terms of simulation box size and loading rate in Shen *et al.* (2010), MD simulations are performed with active zone dimension of $100d \times 50d \times 40d$, where the magnitude of d is a , $\sqrt{3}a$ and $\sqrt{8/3}a$ in the x -, y - and z -directions, respectively, and the strain rate of 10^8 s^{-1} . Fig.3 demonstrates the shear stress-strain curve of Mg crystal containing different at% Al and a basal plane edge dislocation at temperature $T = 300\text{ K}$. It can be found from the figure that the critical shear stress increases with the increase of the Al concentration, although the slope of the shear stress-strain curve is almost a constant. The simulated edge dislocation is somehow pinned through interactions with the Al solute atoms. Compared with dislocation motion in pure Mg, higher stresses are therefore required for dislocation movement through a solute field and the magnitude of the required stress increases with the solute concentration.

Fig. 4 demonstrates the effect of Al solute concentration on the critical shear stress of edge basal dislocation at temperatures $T = 1\text{ K}$, 100 K , 200 K , 300 K and 400 K . It can be found from Fig. 4 that the critical shear stress of edge basal dislocation increases with the Al concentration regardless of temperature. In particular, the increase of critical shear stress is very significant when the Al concentration increases from 0 at% to 0.25 at%, where the critical shear stress increases by 6-8 times. The shear stress increase $\Delta\tau_c$ due to solid solution strengthening is proportional to the concentration of solutes C through the relation of $\Delta\tau_c \propto \sqrt{C}$. Based on the curves in Fig. 4, it is proposed that the critical shear stress-concentration relation of Mg-Al system can be described by

$$\tau_c = \tau_{c0} + 110\sqrt{C} \quad (1)$$

where τ_c is the critical shear stress of Mg with Al solutes, τ_{c0} is the Peierls stress of pure Mg with $\tau_{c0} = 1.0\text{ MPa}$ (Shen *et al.* 2010) and C is the atomic percentage of Al concentration. As can be

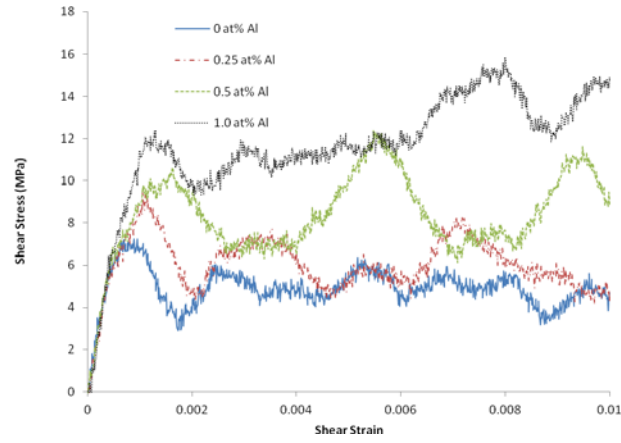


Fig. 3 Stress-strain curve of Mg/Al alloy with basal plane edge dislocation at $T=300$ K

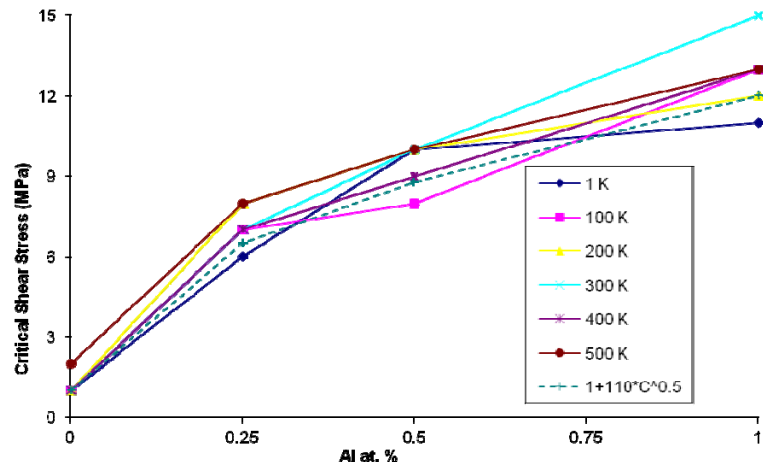


Fig. 4 Stress-strain curve of Mg/Al alloy with basal plane edge dislocation at $T=300$ K

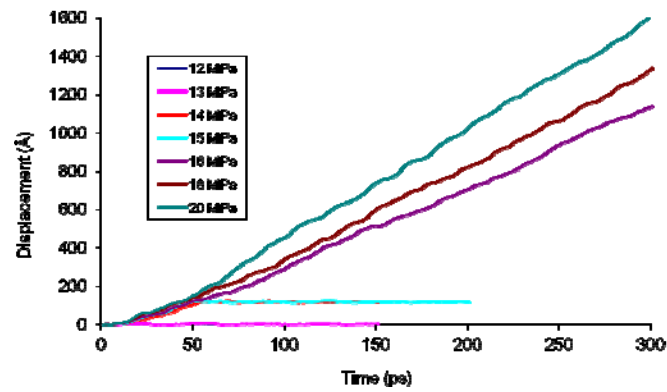


Fig. 5 The displacement history of a basal plane edge dislocation in Mg system with 2.0 at% Al under a given shear stress at temperature $T=100$ K

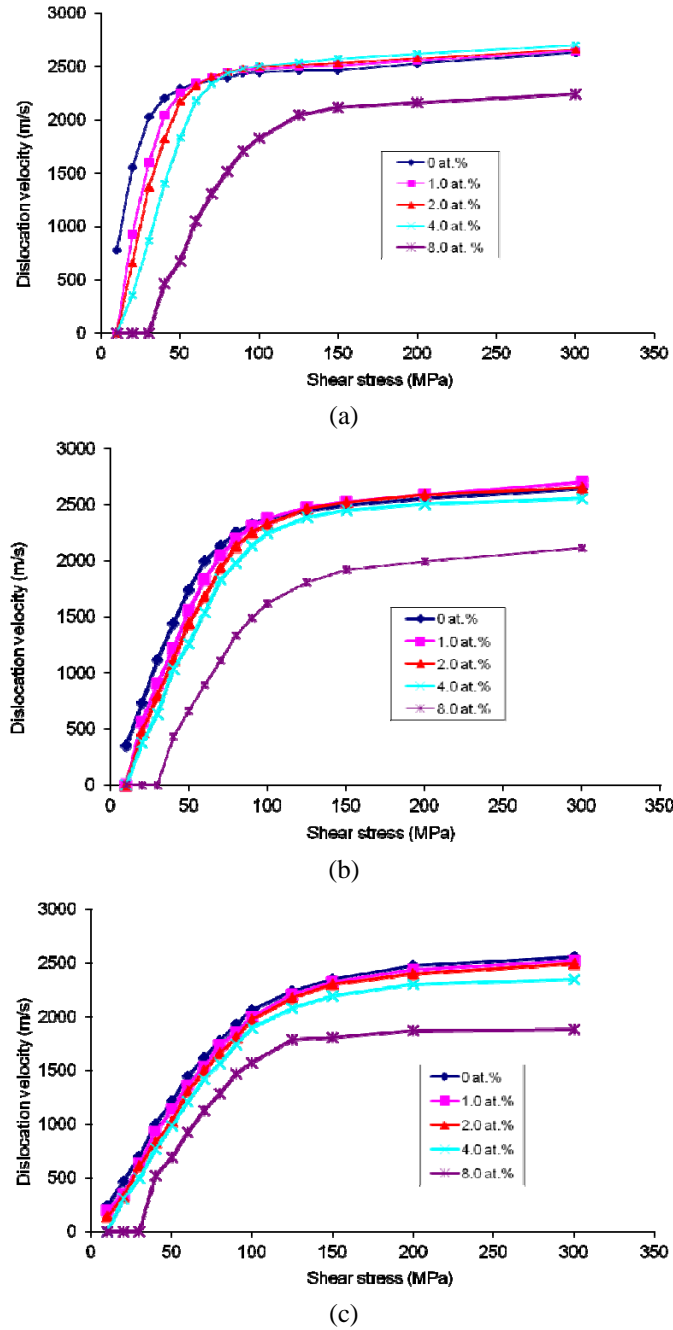


Fig. 6 The effect of Al concentration on the dislocation velocity at temperature of (a) $T = 100$ K, (b) $T = 300$ K and (c) $T = 500$ K

seen from Fig. 3, the proposed critical shear stress-Al solute concentration relation can approximately match the calculated data.

To study the effect of Al solute concentration on the motion of edge dislocation in Mg alloy, MD simulation of the behaviour of a basal plane edge dislocation embedded in different Al concentration under shear stress is performed. Fig. 5 demonstrates the displacement-time curve of a basal plane edge dislocation in Mg system with 2.0 at% Al under a given shear stress at temperature $T=100$ K. As can be seen from the figure, the edge dislocation does not move when the applied shear stress is smaller than 13 MPa, suggesting that the applied shear stress is too low to push the dislocation out of the barrier induced by the Al solutes. The edge dislocation starts to move for about 50 ps and then stops under shear stress of 14 or 15 MPa, indicating the applied shear stress is high enough to take the dislocation out of the initial barrier of the Al solutes. However, the motion of the edge dislocation is not sustained and can be stopped when there is slight increase of the obstacle due to the uneven distribution of Al solutes. A continuous nonstop motion of the edge dislocation is recorded when the applied shear stress is larger than 16 MPa, which is the critical shear stress of the Mg system under the given Al concentration and temperature. A dislocation velocity can be obtained using the slope of the displacement-time curve. It is obvious that the dislocation velocity increases with the applied shear stress.

To further study the effects of Al concentration on the Mg edge dislocation velocity at different temperature, MD simulation of the motion of edge dislocation at Al concentration of 0 to 8.0 at% under the temperatures of $T = 100$ K, 300 K and 500 K are performed. Fig. 6 demonstrates the velocity of edge dislocation in the Mg system with different Al concentrations under different shear stresses and temperatures. As can be seen from these figures, under a given temperature and external shear stress, the dislocation velocity generally decreases with the increase of the Al concentration. In particular, there is a significant drop of dislocation velocity when the Al concentration increases from 4.0 at% to 8.0 at%. Since the dislocation in the alloy is pinned through interactions with the solute atoms, the strength of the barriers increases with the increase of Al concentration as a result the dislocation velocity decreases regardless of the temperature.

However, it is found from the further detailed examination of Figs. 6(a) and 6(b) that at temperature $T = 100$ K and 300 K the dislocation velocity increases linearly with shear stress and decreases with Al concentration when the shear stress is smaller than 50 MPa. When the Al concentration is less than 4.0 at%, the solute effect is not significant when the shear stress is larger than 100 MPa. On the other hand, it can be found from Fig. 6(c) that the dislocation velocity increases linearly with the shear stress when the shear stress is smaller than 100 MPa and the dislocation velocity clearly decreases with the Al concentration.

The evolution of the dislocation velocity as a function of stress to temperature ratio, τ/T , can be further plotted at the three temperatures: 100 K, 300K and 500 K (figures not shown here). The velocity is nearly linear for $\tau/T < 0.3$ MPa/K. This result agrees with the scaling predicted by phonon damping theory (Hirth and Lothe 1992). The dislocation drag coefficient B can be calculated using the following equation

$$B = \tau b / v \quad (2)$$

where τ is the applied shear stress, b is the burger's vector and v is the dislocation velocity. The calculated drag coefficient B for $0 < \tau/T < 0.3$ MPa/K is shown in Fig. 7. When there is no Al concentration (0 at% Al), the calculated B is around $5.12 \sim 13.9 \times 10^{-6}$ Pa-s, which is close to $4.7 \sim 18.0 \times 10^{-6}$ Pa-s in Groh *et al.* (2009). Moreover, dislocation drag coefficient B increases with temperature T and Al concentration and the Al concentration effect is more significant at lower temperature.

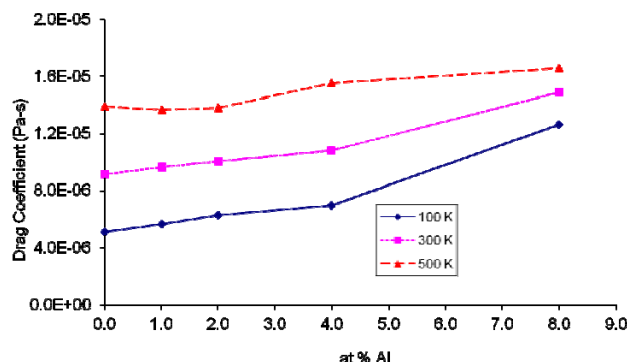


Fig. 7 The effects of Al concentration and temperature on the drag coefficient B

4. Conclusions

In this study, atomistic simulations have been performed to simulate the interaction between basal plane edge dislocation and Al solute in Mg system. In the atomistic simulations, the Mg-Mg, Al-Al and Mg-Al interatomic interactions are described by the embedded atom method with the potential model parameters being obtained from Mendelev *et al.* (2009). It appears from the simulations that generally the critical shear stress increases with the Al solute concentration at both zero and finite temperature. Comparing with the solute effect at $T = 0$ K, however, the critical shear stress at $T = 300$ K is lower due to the kinetic energy of the atoms at the finite temperature. The dislocation velocity decreases as the Al concentration increases under low to medium shear stresses. The Al concentration effect on the dislocation velocity is not significant at very high shear stress level if the concentration is below 4.0 at. %. Drag coefficient B increases with the Al concentration for $0 < \tau/T < 0.3$ MPa/K, although the effect is more significant at low temperatures.

Acknowledgements

This research was supported in part by the Australian Research Council Centre of Excellence for Design in Light Metals (CE0561574). The simulations were undertaken on the NCI National Facility in Canberra, Australia, which was supported by the Australian Commonwealth Government. Fig. 2 was produced by utilizing software VMD developed by Humphrey *et al.* (1996).

References

- Ando, S., Gotoh, T. and Tonda, H. (2002), "Molecular dynamics simulation of $\langle c+a \rangle$ dislocation core structure in hexagonal-close-packed metals", *Metall. Mater. Trans. A*, **33**(3), 823-829.
- Bacon, D. and Liang, M. (1986), "Computer simulation of dislocation cores in h.c.p. metals I. Interatomic potentials and stacking-fault stability", *Phil. Mag. A*, **53**(2), 163-179.
- Bacon, D. and Martin, J. (1981), "The atomic structure of dislocations in h.c.p. metals I. Potentials and

- unstressed crystals", *Phil. Mag. A*, **43**(4), 883-900.
- Bulatov, V.V. and Cai, W. (2006), *Computer simulations in dislocations*, Oxford University Press, New York.
- Conrad, H. and Robertson, W.D. (1957), AIME 209 503.
- Daw, M.S. and Baskes, M.I. (1984), "Embedded-atom method: derivation and application to impurities, surfaces, and other defects in metals", *Phys. Rev. B*, **29**(12), 6443-6453.
- Groh, S., Marin, E.B., Horstemeyer, M.F. and Bammann, D.J. (2009), "Dislocation motion in magnesium: a study by molecular statics and molecular dynamics", *Model. Simul. Mater. Sc. Eng.*, **17**(7), 075009.
- Hirth, J.P. and Lothe, J. (1992), *Theory of dislocations*, Krieger, Malabar, FL.
- Hoover, W.G. (1985), "Canonical dynamics: Equilibrium phase-space distributions", *Phys. Rev. A*, **31**(3), 1695-1697.
- Humphrey, W., Dalke, A. and Schulten, K. (1996), "VMD: visual molecular dynamics", *J. Mol. Graph.*, **14**(1), 33-38.
- Kainer, K.U. (2000), *Magnesium alloys and their applications*, Wiley-VCH, Weinheim.
- Kelchner, C.L., Plimpton, S.J. and Hamilton, J.C. (1998), "Dislocation nucleation and defect structure during surface indentation", *Phys. Rev. B*, **58**(17), 11085.
- Kong, Y. and Shen, L. (2011), "Strengthening mechanism of metallic nanoscale multilayer with negative enthalpy of mixing", *J. Appl. Phys.*, **110**(7), 073522.
- Leyson, G.P.M., Hector, L.G. and Jr., Curtin, W.A. (2012), "First-principles prediction of yield stress for basal slip in Mg-Al alloys", *Acta Mater.*, **60**(13-14), 5197-5203.
- Liu, X.Y., Adams, J.B., Ercolessi, F. and Moriarty, J.A. (1996), "EAM potential for magnesium from quantum mechanical forces", *Model. Simul. Mater. Sc. Eng.*, **4**, 293.
- Mendelev, M.I., Asta, M., Rahman, M.J. and Hoyt, J.J. (2009), "Development of interatomic potentials appropriate for simulation of solid-liquid interface properties in Al-Mg alloys", *Phil. Mag.*, **89**(34-36), 3269-3285.
- Nogaret, T., Curtin, W.A. and Yasi, J.A. (2010), "Atomistic study of edge and screw $\langle c \text{ plus } a \rangle$ dislocations in magnesium", *Acta Mater.*, **58**(13), 4332-4343.
- Olmsted, D.L., Hector, L.G. and Curtin, W.A. (2006), "Molecular dynamics study of solute strengthening in Al/Mg alloys", *J. Mech. Phys. Solids*, **54**(8), 1763-1788.
- Osetsky, Y.N. and Bacon, D.J. (2003), "An atomic-level model for studying the dynamics of edge dislocations in metals", *Model. Simul. Mater. Sc. Eng.*, **11**, 427.
- Plimpton, S.J. (1995), "Fast parallel algorithms for short-range molecular dynamics", *J. Comput. Phys.*, **117**, 1-19.
- Reed-Hill, R.E. and Robertson, W.D. (1957), "Additional modes of deformation twinning in magnesium", *Acta. Metal.*, **5**(12), 717-727.
- Staroselsky, A. and Anand, L. (2003), "A constitutive model for HCP materials deforming by slip and twinning: application to magnesium alloy AZ31B", *Int. J. Plast.*, **19**(10), 1843-1864.
- Sun, D.Y., Mendelev, M.I., Becker, C.A., Kudin, K., Haxhimali, T., Asta, M., Hoyt, J.J., Karma, A. and Srolovitz, D.J. (2006), "Crystal-melt interfacial free energies in hcp metals: a molecular dynamics study of Mg", *Phys. Rev. B*, **73**(2), 024116.
- Tsuru, T., Udagawa, Y. and Yamaguchi, M. (2013), "Solution softening in magnesium alloys: the effect of solid solutions on the dislocation core structure and nonbasal slip", *J. Phys. Cond. Mater.*, **25**(2), 022202.
- Yasi, J.A., Nogaret, T., Trinkle, D.R., Qi, Y., Hector, L.G. and Curtin, W.A. (2009), "Basal and prism dislocation cores in magnesium: comparison of first-principles and embedded-atom-potential methods predictions", *Model. Simul. Mater. Sc. Eng.*, 17055012.