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K. Y. Chen
M. Li
S. J. Zhou

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ATOMISTIC STUDIES OF JOGGED SCREW DISLOCATIONS IN γ-TIAL ALLOYS

K. Y. Chen*, M. Li*, S. J. Zhou**

*Theoretical Division and Center for Nonlinear Studies, Los Alamos National Laboratory, Los Alamos, NM 87545, USA
**Applied Theoretical and Computational Physics Division, Los Alamos National Laboratory, Los Alamos, NM 87545, USA

ABSTRACT

The behavior of jogged screw dislocations in γ-TiAl alloys has been investigated with large-scale molecular dynamics (MD) simulations. We find a new mechanism for formation of pinning points in jogged screw dislocations. We also find that the critical height for the jogs in the ±[110] directions on the (001) plane to move nonconservatively is between 3\(r_0\) and 4\(r_0\), where \(r_0\) is the nearest neighbor distance of aluminum atoms. Interstitials and vacancies are created during the nonconservative motions of the jogs. In addition, the formation of dislocation dipole and loops around the jogs is also observed.

INTRODUCTION

Experimental results indicate that the anomalous yield stress of γ-TiAl alloys at ambient temperatures is closely associated with simple unit screw dislocations [1-4]. Recent work by Sriram et al. [1] showed that the deformation substructures at ambient temperatures are dominated by unit screw dislocations pinned by a number of jogs along screw character segments. Due to the compact core structures of screw dislocations in γ-TiAl alloys, the cross-slip and the double cross-slip, which play a major role in generating jogs, are profuse. Viguier et al. [2] suggested that a simple screw dislocation gliding on the primary as well as cross-slip planes is the intrinsic source for the formation of pinning points, and the pinning points can be erased by the lateral motion of superkinks. As one of the potential pinnings, a jog has a significant role in dislocation mobility. Investigating dynamic behaviors of jogs with different heights will be very important to understand the anomalous yield stress in γ-TiAl alloys. There have been some theoretical studies of nonconservative motion of jogs [5], but the detailed mechanism is poorly understood. With the current powerful computers, this problem can now be coped with [6,7]. In this paper, we are motivated to investigate jogged screw dislocations in γ-TiAl alloys by performing large-scale MD simulations.

SIMULATION PROCEDURE

The methodology of our large-scale MD simulations is briefly summarized here. We chose the embedded atom method (EAM) potentials for γ-TiAl alloys developed by Farkas [8]. These potentials were obtained by empirically fitting equilibrium lattice parameters, c/a ratio, heat of formation, elastic constants, etc.. Throughout the paper, we use as units the atomic mass \(m\) of aluminum, the distance \(r_0\) between nearest neighbors of aluminum atoms (or titanium atoms), the energy unit \(\varepsilon\). So the unit of time \(t_0\) is determined by \(t_0 = r_0\sqrt{m/\varepsilon}\). The time step is chosen to be 0.01\(t_0\). For the EAM potential used, the energy unit is \(\varepsilon = 0.73\ eV\), \(t_0 = 1.7 \times 10^{-13}\ s\), \(a = 3.95\ \AA\), \(c = 4.14\ \AA\), and \(r_0 = 2.7\ \AA\). In our simulations, each MD system is first allowed to relax for 10\(t_0\)
without any loading. Then a constant shear strain rate, \( \dot{\varepsilon}_{yz} = 5.4 \times 10^9 \text{s}^{-1} \), is exerted on the system for another 100\( t_0 \). At \( t=110t_0 \), the shear stress \( \sigma_{yz} \) is 5.7\( \times 10^3 \) MPa. We have performed similar simulations with lower strain rate, and have found the basic physical processes unchanged. In this paper, we study the behavior of the jogged screw dislocations without the complications of thermal fluctuations, thus the initial temperature is set to be nearly zero (30 K). The constant-temperature MD integration scheme is implemented to maintain the system temperature at 30 K.

The \( \gamma \)-TiAl alloy presents an \( L1_0 \) configuration. The system size throughout this paper is chosen to be \( L_x \times L_y \times L_z = 609 \times 211 \times 338 \AA^3 \), containing about 1.1 million atoms. Initially, we set the screw dislocation lines parallel to the [110] (z-axis) with a pair of jog segments in the \( \pm [110] \) directions (see FIG01(a)). These two jogs attract each other. The Burgers vector is chosen as \( b = -b \hat{z} \) and the sense vector \( \xi \) of the screw dislocation is along the direction [110] (z-axis), so the screw dislocation lines can move along the [112] direction (negative x-axis) on the (111) primary slip plane under the external shear strain rate \( \dot{\varepsilon}_{yz} \) (see FIG01(b)). That the jog segments in the \( \pm [110] \) directions on the (001) plane climb in the [112] direction (negative x-axis) is defined as the forward nonconservative motion. Periodic boundary conditions are maintained in the [110] direction. The external shear strain rate \( \dot{\varepsilon}_{yz} \) is exerted on \( \pm y \) surfaces and the two \( \pm x \) surfaces are set free. We chose the jogs lying on the (001) plane mainly for the computational simplicity. The conservative motion of a jog segment is much faster on the (111) slip plane than that on the (001) plane. That would cause the jog pair to annihilate in our MD computational cell in such a short time that the forward nonconservative jog motions do not have sufficient time to proceed. We found that the <110> jog on the (001) plane has dynamic behavior similar to that found on the (111) slip plane in larger MD systems (to be reported in future).

RESULTS AND DISCUSSIONS

We have investigated jogged screw dislocations of several different heights. Here the jogged screw dislocations of heights 4\( \sigma_0 \) and 15\( \sigma_0 \) will be discussed in detail to show
the typical observations. We have found that under the shear strain rate \( \dot{\varepsilon}_{yz} = 5.4 \times 10^9 \, s^{-1} \), the critical height for the jog to move forward in a nonconservative way is between \( 3r_0 \) and \( 4r_0 \). So it is reasonable to choose the critical height as \( 3.5r_0 \). FIG02 shows the evolution process of a jogged screw dislocation with the height \( 4r_0 \). In the first \( 10t_0 \), the two jogs as well as the screw dislocation segments relax on the (001) plane without any loading (FIG02(a)). As shown in FIG02(b), both of the jogs decompose gradually into small jogs with the jog heights \( \sim 2r_0 \) less than the critical length \( \sim 3.5r_0 \). In addition, due to the attractive interaction between a pair of jogs with the opposite sign, these small, newly generated jogs move toward each other. Under the external shear stress \( \sigma_{yz} \) (after \( 10t_0 \)), the newly generated jogs move nonconservatively on the primary slip plane \((1 \bar{1} 1)\). Similar to our previous observations for the jog with the height \( 2r_0 \) [9], interstitials and vacancies are created during the forward nonconservative motion in the \([1 \bar{1} 2]\) direction. A jog that can generate vacancies is defined as a vacancy jog. Similarly, a jog that can create interstitials is defined as an interstitial jog. In addition to the forward nonconservative motion, we find that the jog also moves conservatively along the \([1 \bar{1} 0]\) direction on the (001) plane. It can be clearly seen in FIG02(c) that the vacancy tube \( V_1 \) formed during the jog nonconservative motion is aligned in the \([01 \bar{1}]\) direction. FIG02(c) also shows that the screw dislocation segments bow out around the jogs on the primary slip plane \((1 \bar{1} 1)\). Based on the Peach-Koehler formula \( F = (b \cdot \sigma) \times \xi \) [5], we can identify that the external force \( F \) exerted on the jog segments due to \( \sigma_{yz} \) is along z-axis \([110]\) for the vacancy jogs and is along negative z-axis \([\bar{1} \bar{1} 0]\) for the interstitial jogs. Thus the Peach-Koehler forces would make the vacancy jogs deviate from the \([01 \bar{1}]\) direction and the interstitial jogs deviate from the \([1 \bar{1} 2]\) direction. However, FIG02(c) shows that under the shear strain rate \( \dot{\varepsilon}_{yz} = 5.4 \times 10^9 \, s^{-1} \) the Peach-Koehler forces have no strong effect on the conservative motions of interstitial jog \( J_{II} \) and vacancy jog \( J_{VI} \). It is known that the formation energy of an interstitial is higher than that of a vacancy [10]. The current applied shear strain rate \( \dot{\varepsilon}_{yz} \) is not large enough to move the interstitial jog \( J_{II} \) along the \([\bar{1} \bar{1} 0]\) direction. FIG02(c) also shows that the newly generated interstitial jog \( J_{I2} \) and vacancy jog \( J_{V2} \) are closer to each other. So their attractive interaction is stronger. Due to the attractive interaction of these jogs, the lateral conservative motion of interstitial jog \( J_{I2} \) along the \([\bar{1} \bar{1} 0]\) direction occurs on the (001) plane. This causes the interstitial jog \( J_{I2} \) to move along approximately along the \([01 \bar{1}]\) direction. Similarly, the vacancy jog \( J_{V2} \) bends to some extent towards the interstitial jog \( J_{I2} \). At \( t=50t_0 \), the interstitial cluster \( I_2 \) and the vacancy tube \( V_2 \) disappear gradually (FIG02(d)). From the shape of the dislocation segments, we can see that the dislocation line in the vicinity of two interstitial jogs moves slower than those around vacancy jogs. FIG02(c) and FIG02(d) also suggest that the directions of interstitial clusters and vacancy tubes are determined by the nonconservative and conservative motions of jogs.

The motion of a large jog with a height of \( 15r_0 \) (FIG03(a)) has also been investigated. Within the first \( 10t_0 \), the dislocation segments as well as the jog pairs relax on the (001) plane, and disintegrate into small jogs (FIG03(b)). This decomposition is more obvious for large jogs than for small jogs (see FIG02(b) and FIG03(b)). It is also found in FIG03(b) that the dislocation segments around the negative z-axis decompose into small jogs more prominently than those around the positive z-axis. Under the external shear strain rate \( \dot{\varepsilon}_{yz} \), similar to the above analysis, the nonconservative motion of the jogs occurs, producing a vacancy tube lying on a different \((1 \bar{1} 1)\) slip plane. Both FIG02 and FIG03 suggest that large jogs along the \( \pm[\bar{1} 10] \) directions on the (001) plane are not stable, decomposing into small ones. As indicated by the experiments of
Sriram et al. [1], cross-slip or double cross-slip is the major source of pinning points. Our simulations suggest a new mechanism responsible for creating jogs. In fact, the simulated configuration of the jogged screw dislocation line shown in FIG03(b) is very similar to the experimentally observed one (FIG02(b) in [1]). Based on the elasticity theory of dislocations [10], the dislocation elastic energies $E_{el}$ satisfy $E_{el}$(screw)<$E_{el}$(mixed)<$E_{el}$(edge). Thus the jogs (edge dislocations) are not stable. They are first transformed into mixed ones (see FIG03(b)) and then are decomposed into small screw and edge segments. The edge segments will be the candidates for the pinning points.

At $t=38t_0$, we see the formation of a dipole around the small newly generated jog $J_S$ with the jog height $2r_0$ (FIG03(c)). Due to the strong interaction between the segments $L_{II}$ and $L_{IV}$, they can not pass by each other, indicating the shear strain $\varepsilon_{yz} = 3.49 \times 10^{-2}$ at $t=38t_0$ is not high enough to move these two segments. It is interesting to note that the simulated configuration of the dislocation dipole around the small, newly created jog $J_S$ is very similar to the

FIG02 (a) The initial configuration of a jogged screw dislocation with the height $4r_0$. (b) The decomposition configuration of the jogged screw dislocation at $t=8t_0$. (c) The jogged screw dislocation configuration at $t=38t_0$. The vacancy tube $V_1$ is aligned along the [0 1 1] direction, and the interstitial cluster $I_1$ is approximately along the [1 1 2] direction (negative x-axis). The interstitial cluster $I_2$ is approximately along the [0 1 1] direction and the vacancy tube $V_2$ around the jog $J_{V2}$ bends towards the interstitials cluster $I_2$. (d) At $t=40t_0$, the interstitial cluster $I_2$ and vacancy tube $V_2$ annihilate each other almost completely.
FIG03 (a) The initial configuration of a jogged screw dislocation with a height of 15\(r_0\). (b) The decomposed configuration of the jogged screw dislocation at \(t=8t_0\). (c) At \(t=38t_0\), the segments \(L_I, L_{II}, L_{III}\) and \(L_{IV}\) bow out on the (1 1 1) slip plane. A dipole has formed around the small, newly generated jog \(J_S\). (d) At \(t=40t_0\), the segments \(L_I\) and \(L_{II}\) glide on the (1 1 1) slip plane and almost contact each other. (e) At \(t=46t_0\), the jogs \(J_{IV}\) and \(J_{IO}\) annihilate, and the segment \(L_{III}\) closes and creates a dislocation loop \(L_{C1}\) on the (1 1 1) slip plane. (f) At \(t=50t_0\), the segments \(L_I\) and \(L_{II}\) pass each other and form a dislocation loop \(L_{C2}\) on the adjacent (1 1 1) slip planes. The rest of segments of \(L_I\) and \(L_{II}\) move out of the -yz free surface.

experimentally observed one shown in FIG09 in [1]. As shown in FIG03(c), the dislocation segments \(L_I, L_{II}, L_{III}\) and \(L_{IV}\) bow out significantly on different (1 1 1) slip planes. They exert additional forces on the original jogs \(J_{IO}, J_{IV}\) and on the newly generated smaller jog \(J_S\). At \(t=40t_0\), we see the segments \(L_I\) and \(L_{II}\) pass across each other on the adjacent (1 1 1) slip planes.
The dipole around the small, newly generated jog $J_5$, however, can not glide along the [110] direction. It can only grow along the $[\overline{1} \overline{1} 2]$ direction on the $(\overline{1} \overline{1} 1)$ slip plane. At $t=46t_0$, the segment $L_{II}$ detaches the dipole, gliding further along the [110] direction on the $(\overline{1} \overline{1} 1)$ slip plane (FIG03(d)). Moreover, the attractive interaction between jogs $J_{I0}$ and $J_{II}$ have caused jogs $J_{II}$ and $J_{I0}$ to move on the (001) plane conservatively along the $\pm[110]$ directions. Then these two jogs leave dislocation loop $L_{CI}$ on the $(\overline{1} \overline{1} 1)$ slip plane (FIG03(e)). It is worth emphasizing the motion of the dislocation segments $L_I$ and $L_{II}$ shown in FIG03(c). These two segments bow out and glide towards each other on the primary $(\overline{1} \overline{1} 1)$ slip plane. At $t=50t_0$, these two segments form another dislocation loop $L_{C2}$ on the $(\overline{1} \overline{1} 1)$ slip plane, above the dislocation loop $L_{CI}$ (FIG03(f)). The rest of the segments of $L_{I}$ and $L_{II}$ move out of the -yz free surface. As shown in FIG03(f), the whole dislocation loop $L_{C2}$ is not totally on the same $(\overline{1} \overline{1} 1)$ slip plane. The portion of the loop formed by the segment $L_{II}$ is on the $(\overline{1} \overline{1} 1)$ plane while the rest of the loop formed by the segment $L_{I}$ is on the adjacent $(\overline{1} \overline{1} 1)$ plane. The processes shown in FIG03 reveal a new atomic-level mechanism for a jogged dislocation to depin from a pair of jogs.

CONCLUSIONS

Based on our MD simulations, we obtain the following results on the jogged screw dislocations in $\gamma$-TiAl alloys. Jogs can be generated through the decomposition of large jogs into smaller jogs. Under the shear strain rate $\dot{\varepsilon}_{yz} = 5.4 \times 10^9 \text{s}^{-1}$, the critical height for a jog in the $[\overline{1} \overline{1} 0]$ direction on the (001) plane to move nonconservatively is between $3r_0$ and $4r_0$. Interstitials and vacancies are created during the nonconservative motion of jogs. The dipole around a jog with a height $2r_0$ can exist stably. A jogged screw dislocation can depin from a pair of jogs by looping.

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