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Kinetic Monte Carlo approach to modeling dislocation mobility

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Abstract

We describe a kinetic Monte Carlo (kMC) approach to modeling dislocation motion, directly linking the energetics of dislocation kink nucleation and migration on the atomistic scale with the experimental data on the microscale. A study of planar glide of screw dislocation in Si, an ideal test-bed for our method is first discussed, followed by preliminary results for a more complicated problem, three-dimensional motion of screw dislocation in BCC metals. We find that accuracy of the model predictions, even in the favorable case of Si, cannot claim to be quantitative because of uncertainties in the atomistic results for kink energetics. On the other hand, the kMC method is useful for qualitatively probing the mechanisms controlling dislocation motion, and it is capable of providing plausible explanation of some puzzling features of the experimental data.

Keywords: Dislocation; Kinetic Monte Carlo; Silicon; BCC Metals

1. Introduction

Kinetic Monte Carlo (kMC) method is generally used to simulate the evolution of a physical system through numerical sampling of (Markovian) stochastic processes. While the traditional Monte Carlo (MC) method is applied to sample systems in or close to the thermal equilibrium, kMC has a "kinetic" character, in that it also evolves the system in real physical time making it possible to study non-equilibrium processes [1]. A connection between MC time-steps and the real physical time has been discussed within the theory of Poisson processes [2]. The appeal of the kMC method is that it can treat large length and long time-scale kinetic response while incorporating atomistic information, through appropriately determined transition rates. For example, it is widely used to simulate surface diffusion and growth processes [3], in which the energy barriers for the atomic mechanisms are obtained from atomistic calculations.

Plastic deformation in crystalline materials is another physical process in which kMC methods

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is naturally applicable. The deforming lattice is a system far from thermal equilibrium, evolving through a complex sequence of kinetic processes taking place on several length and time-scales. In this brief report we are concerned with two applications of the kMC method to the motion of a single dislocation through a perfect lattice. We examine two types of lattices in which the dislocation motion mechanisms are quite different: a diamond cubic lattice of Si, where dislocations are confined to glide in a single plane, and a BCC lattice of Mo, where screw dislocations move in three dimensions due to their ability to cross-slip.

2. KMC study of silicon

Understanding the mechanisms of dislocation motion can be very helpful for designing and processing materials with special properties, such as high strength alloys for high temperature applications. In the case of silicon, dislocation mobility is important due to the notorious ability of dislocations, residing initially in the relatively insensitive areas of the silicon substrate, to bring themselves in contact with active circuits, either during manufacturing or the working period of the electronic devices. Yet another aspect that makes silicon an important test-bed for experimental and theoretical work, is its unmatched purity and the possibility to grow single crystals of silicon that are essentially free of dislocations. Thus, it is possible to study mobility of individual dislocations that is intrinsic to silicon and not affected by dislocation interactions with other dislocations or with extrinsic defects.

Although there have been considerable progress both in theoretical modeling [4–11] and the experimental measurements [12–16] of dislocation motion in Si during the last three decades, a disconnect still exists between theoretical predictions and the experimental measurements of dislocation mobilities. While dislocation motion is usually observed on the length scale of multiple microns and during time intervals of several seconds, the theoretical work has been mostly focused on the atomic mechanisms and energetics of kink nucleation and migration on the scale of angstroms and picoseconds. To bring together the atomistic theory and the experimental measurements, we developed a mesoscopic model of dislocation motion that considers the overall dislocation motion as the cumulative effect of a large number of kink events, sampled by a kMC algorithm.

Fig. 1 shows a schematic representation of a screw dislocation in Si that we study in our kMC model. The dislocation line is lying mostly along the $\langle 1\bar{1}0\rangle$ direction (defined as z axis), dissociated into two 30° partials, with Burgers vectors b_1 and b_2, respectively, enclosing an area of stacking fault. Under the action of external stress and temperature, the dislocation moves along x direction through kink pair nucleation and subsequent migration of the kinks along the line, in both partials. A kink pair nucleation event and a kink migration event are shown in Fig. 1 in dashed lines. Periodic boundary conditions are applied so that the kinks leaving at one end re-enter the dislocation from the other end. The elementary kink width is b, and the kink height is $h = b\sqrt{3}/2$.

A simulation proceeds by sampling all the elementary events that are competing with one another. At each time-step, a list is generated that containing all possible kink pair nucleation event on each and every horizontal segment of the partials, and all possible lateral displacements (migration to the left or the right) of the existing

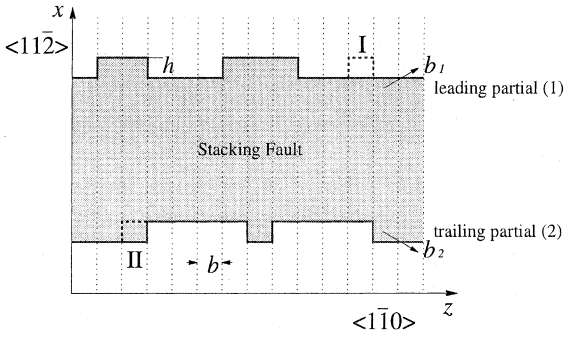

Fig. 1. Schematic representation of a screw dislocation in Si in the kMC simulation. The dislocation is dissociated into two 30° partials with Burgers vector b_1 and b_2, respectively, enclosing an area of stacking fault. Elementary kink width is b, while the kink height is $h = b\sqrt{3}/2$. A double-kink nucleation event is shown at position I, and a kink migration event is shown at position II, both in dashed lines.

kinks. A kMC algorithm [17] is then applied to select a particular event from the list, with the probability of selecting each event proportional to its occurrence rate. The selected event is executed, resulting in either nucleation of a kink pair or migration of an existing kink. The physical time increment is then evaluated as the inverse of the total (sum) rate of all the events in the current list and the simulation continues to the next time-step.

The rate of each event is calculated within the transition state theory [18]. Similar to the surface growth studies [3], the activation energy barriers for each transformation contain terms that are imported from atomistic calculations. However, since the dislocation segments can interact both with external stress and with each other, there is an additional energy term in the activation energy, defined by the local stress at the transformation site. This local stress is evaluated as a sum of the external stress and the internal stress due to all other dislocation segments. For example, the rate for kink migration on partial p ($p = 1$, 2 for leading and trailing partials, respectively) is calculated as,

$$j_{\mathrm{m}} = \omega_0 \times \exp\left(-\frac{W_{\mathrm{m}} - TS - (\pm\gamma_{\mathrm{SF}} - \sigma_{yz}b_{p,z} - \sigma_{yx}b_{p,x})A/2}{k_{\mathrm{B}}T}\right), \tag{1}$$

where ω_0 is the pre-exponential "frequency" factor that we set equal to the *Debye frequency*, W_{m} is the kink migration energy barrier which can be calculated using either empirical potential or first principles methods, S is the vibrational entropy, which is set to $3k_{\mathrm{B}}$, according to earlier theoretical and experimental estimates [19,20], γ_{SF} is the stacking fault energy, with "+" or "−" signs for the leading and trailing partial, respectively, σ is the stress tensor, $A = \pm bh$ is the area swept out by the dislocation during kink migration, with "+" or "−" sign corresponding to the dislocation moving upward (e.g., left kink move left) or downward (e.g., left kink move right), respectively, k_{B} is the Boltzmann's constant and T is the temperature.

Our experience is that the major bottle-neck of kMC simulations in general, including kMC simulations of dislocation motion, is an efficient treatment of very fast events that consume most of the computing time but do not contribute appreciably to the overall evolution. It is a general feature of *all* kMC simulations that they lack any natural dynamic or kinetic constraint. Unlike molecular dynamics (MD) in which dynamics is naturally defined by the interatomic potentials, kMC method will sample all and every process from its current event catalog. As is often the case, the catalog may contain a number of very fast events that are repetitive or otherwise uninteresting. It is up to the modeler to help such an ill-behaved simulation by integrating out, one way or another, such uninteresting events from the event catalog.

In the case of Si, a vast majority of fresh kink pairs (with kink pair separation b) recombine almost immediately after their formation. Unless specially treated, almost all of the kMC cycles are wasted on sampling these fast but unimportant processes, resulting in a very inefficient simulation unable to advance the dislocation over an appreciable distance within a reasonable amount of simulation time. To remedy such an unwanted behavior we considered kink pair nucleation and propagation as an isolated (Markov) stochastic process. Specifically, we examined a one-dimensional random walk with one absorbing end and derived a recursive formula that allows to compute the effective rate of formation of *sustainable* kink pairs of width ω_{s}, i.e., kink pairs that have considerable probability to expand further without recombination [21]. Based on this result, it became possible to speed up our kMC simulations by allowing only kink pairs of width w_{s} to nucleate. Parameter w_{s} was chosen as a compromise between efficiency and accuracy: a larger w_{s} means a more detailed and realistic sampling of the kink pair propagation processes. In our simulations we observed that any value of w_{s} between 10 and 20 was sufficient to generate reasonably large statistics of kink pair nucleation events and that the specific choice of w from this interval had no detectable effect on the final result for dislocation velocity. For more details on the kMC algorithm implementation in Si, refer to [21–23].

During each kMC simulation, the instantaneous average position of the moving dislocation

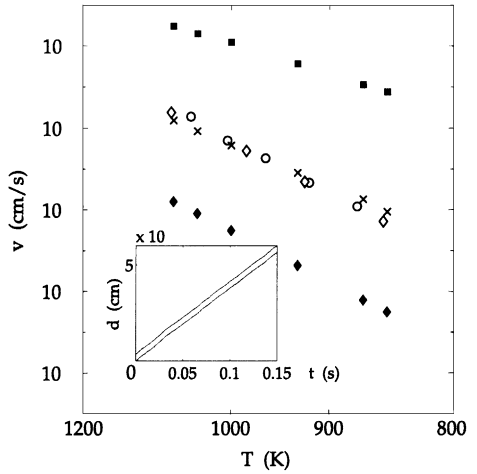

Fig. 2. Temperature-dependent velocities of screw dislocations at stress $\tau = 10$ MPa. Experiments are denoted by (◇) [12] and (○) [13], respectively. (■) and (◆) are kMC predictions using EDIP and TB kink energetics. kMC predictions for the optimized kink parameters, $E_k = 0.7$ eV and $W_m = 1.2$ eV, are also shown in (×).

is recorded as a function of time (the inset in Fig. 2 shows a typical result). Dislocation velocity is then computed as the slope of this curve. Fig. 2 shows a kMC prediction for the dislocation velocity as a function of temperature at 10 MPa shear stress, along with two sets of relevant experimental data [12,13]. Two sets of atomistic calculations were used in kMC simulations, one from empirical potential (EDIP) calculations [6], the other from tight-binding (TB) calculations [8]. Although atomistic calculations identified multiple species of kinks on partial dislocations in Si, our kMC simulation is based on a simplified model that includes ony one species of kinks. Using the procedure described in [21], we selected the nucleation energy E_k and migration energy W_m for this "generic" kink on 30° partial as $E_k = 0.52$ eV (EDIP) and 0.80 eV (TB), $W_m = 0.89$ eV (EDIP) and 1.52 eV (TB), as shown in the first two columns of Table 1. The predicted velocities based on these two sets of atomistic inputs are seen to differ by some four-orders of magnitude, bracketing the experiments. An Arrhenius fit of the simulated and the experimental velocity data produces an overall activation energy $Q = 1.31$ eV (EDIP), 2.23 eV (TB), and 2.20 (exp't).

Table 1
Kink's formation energy E_k and migration barrier W_m (in eV) on 30° and 90° partials in silicon obtained from atomistic calculations using EDIP potential, TB and DFT, and experimental measurements using TEM and high resolution electron microscopy (HREM)

	30°		90°	
	E_k	W_m	E_k	W_m
EDIP [6]	0.52	0.89	0.70	0.62
TB [8]	0.82	1.52	0.12	1.62
DFT [9]		2.1		
DFT [10]			0.1	1.8
DFT [11]			0.04	1.09
TEM [14]			$\geqslant 0.4$	$\leqslant 1.2$
TEM [15]		1–1.2		1–1.2
HREM [16]	0.8	1.55	0.74	1.55

A difference so large indicates that kMC predictions for dislocation velocity depend sensitively on the atomistic input. Simple analysis shows that to achieve reasonable agreement in the absolute values of dislocation velocity, the kink energy calculations have to reach the accuracy of 0.1 eV, which is only attainable for the first principles methods. However, as shown in Table 1, even density functional theory (DFT) calculations available for the partial dislocations in Si [9–11] have neither converged nor agreed with the experimental estimates which themselves show considerable scatter [14–16].

Based on various calculated and experimental values available at present, our best estimates for the energetics of the generic kink on 30° partial are $E_k = 0.7$ eV and $W_m = 1.2$ eV. Dislocation velocities calculated based on this effective parameters are also shown in Fig. 2. Although the result looks reasonably good, we would like to emphasize that quantitative agreement between the predicted velocities and the experimental data is not significant at this stage. This is because some other parameters, such as the sampling frequency ω_0 or the vibrational entropy S in Eq. (1), can easily shift the entire velocity curve by one- to two-orders of magnitude. Despite these uncertainties, the fact that the simulated dislocation velocities bracket the experimental data, and that they have similar temperature dependence with experiments are

significant, indicating that our kMC model is adequate but the accuracy is limited by the quality of its atomistic input. If and when a more reliable set of atomistic parameters becomes available, the model will be ready to incorporate the new data for more accurate prediction of the intrinsic dislocation mobility in Si.

Using the "optimal" set of kink energies, we examined the stress dependence of dislocation velocities. We observed that dislocation mobility is affected by the coupling between the two partial dislocations [23]. Depending on whether or not the average separation between the two partials is commensurate with the periodicity of Peierls potential, the dislocation velocity can differ by one-order of magnitude at low stresses. This suggests a possible explanation of the starting stress behavior alternative to the mysterious "weak obstacles" postulate traditionally invoked to explain such low stress anomalies of dislocation mobility [12,24,25].

3. KMC study of BCC metals

The mechanisms of dislocation motion in other materials can be very different from those in Si. For example, the picture of dislocation motion in BCC transition metals such as molybdenum can be quite complex. At low temperatures, screw dislocations are found to be much less mobile than edge and mixed dislocations [26]. These screws are believed to control the overall rate of plastic deformation. Due to the high Peierls barrier, the motion of screw dislocations in BCC molybdenum is believed to be controlled by nucleation and migration of kinks [27], just like in silicon. However, screw dislocations in BCC metals do not dissociate into a planar structure [28], as they do in Si, and their glide is not confined to a single glide plane. Instead, cross-slip should readily occur by which screw dislocations change their glide planes. In fact, each screw dislocation segment (aligned along $\langle 1\,1\,1\rangle$) can nucleate kink pairs on either of the three (1 1 0) planes of the $\langle 1\,1\,1\rangle$ zone, as shown in Fig. 3. Thus, motion of screw dislocations becomes three-dimensional and can involve a number of unusual mechanisms affecting dislocation mobility.

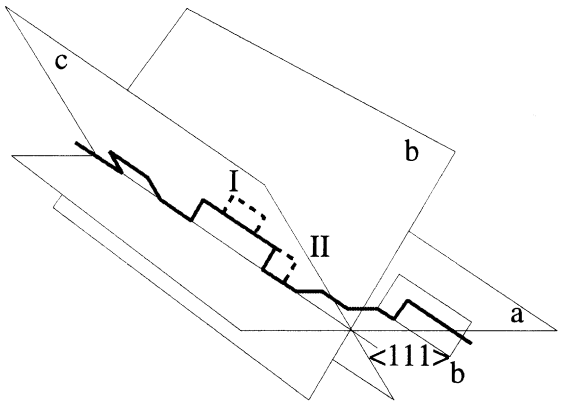

Fig. 3. A schematic of dislocation motion in BCC metals examined in the kMC simulations. The dislocation line is mostly aligned along the $1/2\langle 1\,1\,1\rangle$ Burgers vector. Kink pairs can nucleate on either of the three (1 1 0) planes a, b and c after which kink migration is constrained to the glide plane selected by kink pair nucleation. A kink pair nucleation event is shown at position I, and a kink migration event is shown at position II, both in dashed lines.

Similar to the case of Si, theory and simulations of dislocations in Mo have focused on the structure and energies of dislocations and kinks [28,29], whereas experimental observations [26,30,31] of dislocation motion dealt with the length scales of multiple microns. Recent MD simulations of dislocation motion at finite temperatures examined mobility of short dislocation segments and kinks [32–34]. At the same time, large scale dislocation dynamics (DD) [35] simulations have been applied to BCC metals, in an attempt to develop predictive material strength models (i.e., stress–strain relationships) based on the physics of dislocation behavior. In principle, atomistic simulations can provide mobility rules for the large scale DD simulations. In practice, however, the length and timescales of the atomistic simulations and those of the DD models remain disconnected. To close the gap between theory of the atomic core and dislocation mobility measurements and to eventually connect the atomistic mobility data to predictive large scale DD simulations of materials strength, an intermediate model for microscale behavior of individual dislocations is required. For this purpose, we develop here a kMC approach to modeling dislocation motion in BCC metals on the microscale, adapted from our study of dislocation glide in Si.

Fig. 3 shows a schematic representation of a screw dislocation in the kMC model. The dislocation is represented by a piecewise straight line mostly parallel the dislocation Burgers vector in a $1/2\langle 1\,1\,1\rangle$ direction. It consists of horizontal (H) and vertical (V) segments, with H-segments being pure screw and V-segments being pure edge. All V-segments have the same length h, the unit kink height, while the H-segments can be of any length. To model cross-slip, kink pair nucleation is allowed on any part of the H-segments and in any of the three $(1\,1\,0)$ glide planes a, b and c intersecting the $\langle 1\,1\,1\rangle$ direction. Once nucleated, a kink (V-segment) can move in its glide plane along the dislocation line until it recombines with another kink of opposite sign. Because a kink migrates in BCC metals against very small energy barrier (secondary Peierls barrier) [36], it requires a different treatment from that developed for Si. Specifically, kink motion is now modeled by a viscous drag mechanism with kink velocity proportional to the elastic force exerted on the kink. The kink mobility parameter associated with this kink drag mechanism has been obtained by direct MD simulations [34] at finite temperatures.

Our kMC simulations give a rather interesting picture of screw dislocation motion. At low temperature and low stress, the dislocation motion is controlled by the rate of kink pair nucleation. Due to a high energy barrier for kink pair nucleation and the relative ease of kink migration, there is no more than one kink pair at any given time on the entire dislocation line. Once formed, the kink pairs sweep quickly through the whole dislocation line and recombine after one of the kinks exits and re-enters the line (due to the periodic boundary conditions). Each of such kink pair nucleation and propagation sequences results in the dislocation moving by one repeat distance (the kink height h). Since the net rate of kink pair production is proportional to dislocation length, dislocation velocity under such conditions is proportional to the length, in agreement with earlier theories [27].

At a higher temperature and/or higher stress, kink pair nucleation rates increase dramatically. As a result, a large number of kinks may be simultaneously present on the dislocation line in which case dislocation velocity becomes length-independent. Furthermore, rather complicated mechanisms may result as a consequence of easy cross-slip. One scenario involves simultaneous presence of kink pairs nucleated on two intersecting slip planes. Such cross-kinks can now collide with each other and, being unable to recombine, form pinning points on the dislocation line. These events create conditions for pile-up of the kinks arriving at the pinning point from two opposite directions. Similar to the fast processes of kink pair nucleation and recombination in the case of Si, the kinks in these pile-ups tend to oscillate frequently between neighboring positions on the dislocation line, making no contribution to the overall dislocation displacement. Unless some sort of special treatment of such uninteresting events is applied, the simulation will become progressively less efficient as the kink pile-ups grow larger.

The physical effect of the pinning points and kink pile-ups is significant, in that they impede dislocation motion and may develop into cusps on the moving screw dislocations. These intrinsic obstacles can be overcome either by slow migration of the cusps along the line leading to possible partial recombination with other cusps, or by formation of closed (prismatic) loops left in the wake of a moving dislocation. While these processes are natural occurrences in our kMC simulation, previously they were postulated to explain the stress anomaly of dislocations in γ-TiAl alloy [37]. Recent transmission electron microscopy (TEM) experiments [38] in Mo and Ta also confirm such mechanisms, and further indicate that cusp migration is observed more frequently in Mo while formation of the debris loops is more prominent in Ta. Another predicted behavior which is in accord with TEM observations is that debris formation occurs more readily under higher temperature and/or higher stress conditions [38]. For more details of kMC simulation in BCC metals, refer to [39].

4. Concluding remarks

We have developed a kMC method to model dislocation mobility in diamond-cubic lattice of Si and BCC lattices of Mo. We will use this model to

study other observed behaviors of dislocation mobility which are not yet fully understood, such as mobility asymmetry [40,41]. We are also improving our kMC model of Mo to treat kink oscillation in superjogs more efficiently. The main objective of this work is to predict dislocation velocity at a wide range of temperature and stress conditions, which will serve as input to larger DD simulations [35] to model single crystal strength of BCC metals.

Acknowledgements

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