BROWNIAN MODEL OF DISSOCIATED DISLOCATIONS*

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Starting from the Volterra model of dissociated dislocations, a dislocation dissociated into two Shockley partials under the action of the periodic Peierls potential and a general external stress is modeled as a pair of coupled Brownian particles in a washboard potential. It is found that mobility shows a sensitive dependence on the parameters of the interaction between partials. In particular, a resonant-like behavior of the average velocity, for equilibrium separation distances close to half-integer multiples of the period of the Peierls potential, is observed.

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1. Introduction

The addition of noise to deterministic motion can give rise to interesting effects, such as stochastic resonance [1], resonant activation [2], and the mechanisms underlying the behavior of Brownian motors [3,4]. In particular, transport phenomena in periodic potentials is of relevance in numerous contexts. Several applications have been studied in condensed matter physics, nanotechnology, chemical physics, and molecular biology [3, 5–7].

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As for the study of two coupled Brownian particles in a periodic potential, attention has been focused on the overdamped limit [8–11], in which most biologically oriented applications are made [12, 13], and, in a general regime, on dimer diffusion on surfaces [14–16].

In this paper a model, consisting of two coupled Brownian motors moving in a periodic substrate potential, is applied to the dynamics of dissociated dislocations. In Sec. 2 the Volterra model of dissociated dislocations is recalled and it is shown that when the environment is taken into account through a Langevin dynamics it naturally leads to the model of two coupled Brownian particles in a washboard potential, illustrated in Sec. 3. This model presents a sensitive dependence on the main parameters of the interaction between the two particles, as pointed out in Refs. [14–16]. Also, detailed molecular dynamics simulations of dissociated dislocation dynamics with different equilibrium distances [17,18] have confirmed the prediction that a lower effective Peierls stress, corresponding to a lower critical tilt, results from a distance between the partials close to a half-integer multiple of the potential period, due to the destructive interference of the Peierls potentials felt by the partials [19, 20]. Here the same phenomenon is studied in Sec. 4 by numerical simulation of the mesoscopic model of two coupled Brownian particles, focusing on the effect of different equilibrium distances and coupling strengths on the mobility of the whole system. A resonant-like behavior in the average velocity as a function of the equilibrium distance is found and its origin is summarized. Results are discussed in Sec. 5.

2. The Volterra model of dissociated dislocation

In order to consider a concrete example, in the following we refer to a simple straight screw dislocation in a fcc crystal, but similar considerations apply to edge dislocations. For dislocations of this type it is energetically convenient to dissociate into partials dislocations, in the present case two Schockley partials, in the geometry represented in Fig. 1 [21, 22]. The two partials are in equilibrium at a separation distance determined by the competition between a long range repulsive force $\propto 1/r$ and a constant attractive force γ_0, due to the fact that a stacking-fault ribbon is formed between the partials. Novel phenomena take place, respect to the case of a single perfect dislocation, due to the interaction between partials, since under the action of an external stress partials can both move and change their separation distance. At low temperatures, a dissociated dislocation can be approximately described by the Volterra model, which provides its potential energy in the form [19, 20]

$$V(x_1, x_2) = E_0 \log\left(\frac{x_2 - x_1}{2w}\right) + \gamma_0(x_2 - x_1) + \sigma_\perp b_\perp (x_2 - x_1) - \sigma_\parallel b_\parallel (x_1 + x_2) + A_0\left[\cos\left(\frac{2\pi x_1}{a}\right) + \cos\left(\frac{2\pi x_2}{a}\right)\right]. \quad (1)$$

The first term on the right hand side represents the repulsion between partials and corresponds to a long range E_0/r force, where E_0 is an energy factor and $r = x_2 - x_1$ ($x_2 > x_1$), x_1 and x_2 representing the coordinates of the dislocation lines of the partials and w the dislocation core width. The second term, proportional to the stacking fault energy γ_0, represents the attractive interaction due to the energy required to form the stacking-fault ribbon between the partials. The third and fourth terms represent the contributions of an external stress applied to the system on the plane defined by the dislocation lines, with components σ parallel and perpendicular to the dislocation lines, b being the corresponding Burgers vector components. It is to be noted that a perpendicular stress $\sigma_\perp$ only affects the distance between partials, while a parallel stress $\sigma_\parallel$ acts on the whole dislocation complex. Finally, the periodic Peierls potential felt by the dislocations, represented by the last two terms, takes into account the discrete nature of the underlying lattice structure, with a representing the distance between lattice planes in the x-direction.

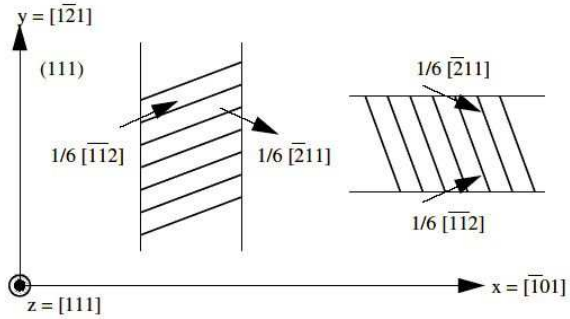

Fig. 1. Projections on the (111) plane of a generic fcc crystal of the system geometry for an edge (left) and screw (right) dislocation. Arrows denote Burgers vectors of partials. The area enclosed by the dislocation lines of the partials represents the stacking-fault ribbon.

The description of a dissociated dislocation through the Volterra model applies well to pure edge or screw dislocations near equilibrium and not too small separation distances but it represents a simplification in real situations. In this preliminary investigation the two-dimensional character of

dissociated dislocations in fcc crystals, due to their mixed edge-screw nature or revealed by kink–anti-kink pair formation is neglected. Also, the influence of the external stress on the crystal structure itself — *i.e.* on the periodic substrate potential — is not considered. Finally, since the Volterra model describes a dislocation at zero temperature, in the following Langevin dynamics is used to model the interaction with the rest of the crystal, assumed to be at constant temperature T. Despite its limited range of validity, the Volterra model can be fruitfully used for analyzing some general features of dissociated dislocations and their response to an applied field.

An important quantity in dislocation dynamics is the Peierls stress, defined as the minimum stress required to move a straight dislocation in the Peierls potential at $T = 0$. The Peierls stress corresponds to the critical tilt $f_{\rm cr}$ of a one-dimensional particle in a periodic potential. For one-dimensional motion in the potential $V(x) = A_0 \cos(kx)$, the critical tilt is given by $f_{\rm cr} = A_0 k = 2\pi A_0/a$ ($= 2\pi$ in rescaled units). However, for a system with two degrees of freedom moving in a periodic potential with the same amplitude A_0, the critical tilt $f_{\rm cr}$ can be much smaller, depending on the interaction parameters, as discussed in Sec. 4.

For the following considerations it is convenient to introduce the coordinates

$$\begin{aligned} x &= x_2 - x_1\,, \\ X &= \frac{x_1 + x_2}{2}\,, \end{aligned} \tag{2}$$

which describe the relative and translational motion of the dislocation complex, respectively. Then energy (1) can be rewritten as

$$V(X,x) = -E_0 \ln\left(\frac{x}{2w}\right) + \gamma x - fX + A_0 \cos\left(\frac{kx}{2}\right)\cos(kX)\,, \tag{3}$$

where we have introduced the effective stacking fault energy $\gamma = \gamma_0 + \sigma_\perp b_\perp$, the external tilt $f = 2\sigma_\parallel b_\parallel$, and the wave vector $k = 2\pi/a$. The first two terms on the right-hand side only depend on x and describe the interaction between the partials. The third term represents the external driving force acting on the dislocation complex and only depends on the center of mass coordinate X. Finally, the last term is the periodic Peierls potential, which couples the x and X degrees of freedom, and is shown in Fig. 2.

An estimate of the separation distance Δx can be obtained by replacing the Peierls potential $A_0 \cos(kx/2)\cos(kX)$ by its average (zero) value and then minimizing $V(X,x)$ respect to x, which gives

$$\Delta x = \frac{E_0}{\gamma}\,. \tag{4}$$

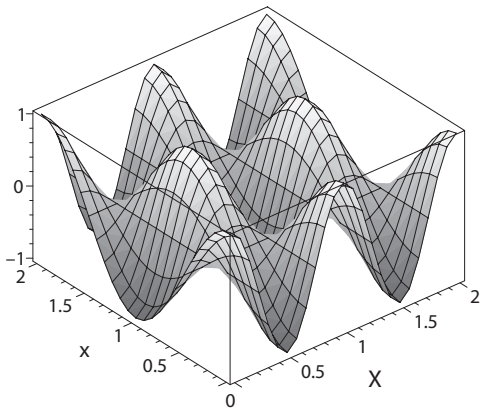

Fig. 2. Peierls potential $V(X,x) = A_0 \cos(kx/2)\cos(kX)$ in the X-x plane. The total potential (for zero tilt) is obtained by adding the x-dependent interaction potential, which is of the form $K(x-\Delta x)^2/2$ in the harmonic approximation, see text for details. Notice that the system can move along the X direction going round the potential barriers, rather than overcoming them across the steepest paths as in the one-dimensional case.

The variable x is expected to be equal to its equilibrium value Δx only on average, undergoing oscillations due to the x–X coupling. On the other hand, the center of mass coordinate will either oscillate within a potential valley or, if the tilt assumes large enough values, to vary over the X-axis range as the whole system moves with a nonzero average drift velocity.

3. Model system

In the following we employ a simplified version of the model illustrated above, in which the interaction potential between the partials is assumed to be harmonic. Its form can be obtained by considering the small oscillations around the equilibrium distance $\Delta x = E_0/\gamma$ through an expansion of the first two term in the potential (3) in powers of difference $(x - \Delta x)$. Then, apart from a constant, one obtains

$$V(X,x) = \frac{1}{2}K(x-\Delta x)^2 - fX + A_0 \cos\left(\frac{kx}{2}\right)\cos(kX)\,, \tag{5}$$

where $K = E_0/\Delta x^2 = \gamma^2/E_0$.

We begin by formulating the equations of motion for the particles coordinates x_1 and x_2, starting from the potential energy function (1), in which the first two terms are replaced by $K(x_2 - x_1 - \Delta x)^2/2$, according to the harmonic approximation introduced above. By adding a dissipative and a

random force to model the interaction with the crystal at constant temperature T and assuming a mass per unit length m, one obtains the two coupled Langevin equations

$$\begin{aligned} m\ddot{x}_1 &= kA_0 \sin(kx_1) - K(x_1 - x_2 + \Delta x) - \eta\dot{x}_1 + R_1(t) + f\,, \\ m\ddot{x}_2 &= kA_0 \sin(kx_2) - K(x_2 - x_1 - \Delta x) - \eta\dot{x}_2 + R_2(t) + f\,, \end{aligned} \tag{6}$$

where η is the damping constant and $R_1(t)$ and $R_2(t)$ are two independent stochastic Gaussian processes defined by

$$\begin{aligned} \langle R_i(t)\rangle &= 0\,, & & i = 1,2\,, \\ \big\langle R_i(t)R_j(t')\big\rangle &= 2\eta k_{\mathrm{B}} T\delta_{ij}\delta(t-t')\,, & & i,j = 1,2\,. \end{aligned} \tag{7}$$

Moving to the relative and center of mass coordinates the equations become

$$\begin{aligned} M\ddot{X} &= kA_0 \cos\left(\frac{kx}{2}\right)\sin(kX) + f - \eta\dot{X} + R(t)\,, \\ \mu\ddot{x} &= -K(x - \Delta x) + kA_0\,\sin\left(\frac{kx}{2}\right)\cos(kX) - \frac{\eta\dot{x}}{2} + r(t)\,, \end{aligned} \tag{8}$$

where $M = 2m$, $\mu = m/2$, and the Gaussian random forces $R(t) = [R_1(t) + R_2(t)]/2$ and $r(t) = [R_2(t) - R_1(t)]/2$ are defined by

$$\begin{aligned} \langle R(t)\rangle &= \langle r(t)\rangle = 0\,, \\ \langle R(t)r(s)\rangle &= 0\,, \\ \big\langle r(t)r(t')\big\rangle &= \big\langle R(t)R(t')\big\rangle = \eta k_B T\delta(t-t')\,. \end{aligned} \tag{9}$$

The Langevin equations (6) have been integrated numerically, through a standard Verlet algorithm with space unit a and energy unit A_0. The system evolution along one trajectory was simulated for a time period $t = 2000$, with a time step $\Delta t = 0.05$. Time averages have been obtained from that part of 2000 trajectories, after the transient depending on the initial conditions.

4. Results

In numerical simulations a value of (rescaled) temperature $T = 0.1$, a friction coefficient $\eta = 1$ and a tilt $f = 1.9$ were used. The value $f = 1.9$ was found to be critical for some distance value $x \approx 1.7a$, which is suitable to the following considerations, since it is between an integer and a half-integer multiple of the separation distance.

The asymptotic average velocity v of the system, in units of the free asymptotic velocity $v_0 = f/\eta$, is shown in Fig. 3 in the interval of separation

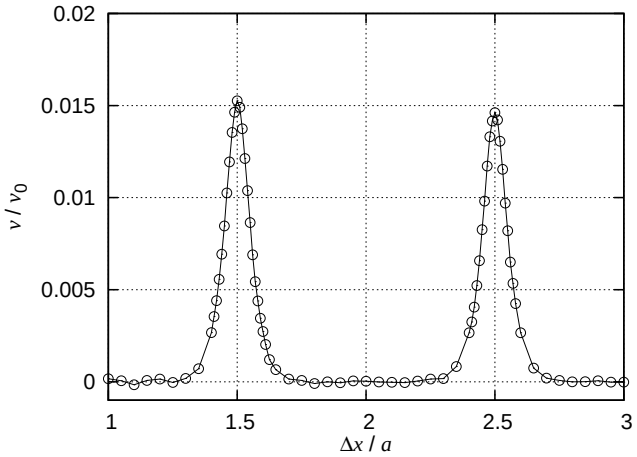

Fig. 3. Asymptotic rescaled average velocity v/v_0, with $v_0 = f/\eta$, obtained from 2000 trajectories, for an external tilt $f = 1.9$ and a coupling constant $K = 10$, for different values of the rescaled equilibrium distance $\Delta x/a$ between the particles. Peaks are located at distances equal to half-integer multiples of the period a.

distances $\Delta x \in (a, 3a)$. Its dependence on Δx is in fact periodic, with the same period a of Eqs. (6). While being practically equal to zero for separation distances $\Delta x < 1.3a$, $1.7a < \Delta x < 2.3a$, and $\Delta x > 1.7a$, close to integer multiples of a, it is appreciably larger than zero in the intervals $\Delta x = (1.3a, 1.7a)$ and $\Delta x = (2.3a, 2.7a)$, with sharp peaks in correspondence of half-integer multiples of a, namely $\Delta x = 3a/2$ and $\Delta x = 5a/2$.

The origin of the peaks is to be found in the fact that for half-integer multiples of the ratio $\Delta x/a$ the optimal situation takes place, in which the two particles can help each other's motion. The underlying mechanism can be illustrated from two different points of view.

In the picture of two coupled particles in a one-dimensional washboard potential, for distances $x = (n + 1/2)a$, with n an integer number, one partial going toward a potential well pushes the other partial climbing up a potential barrier or vice versa. Were it possible to maintain the distance exactly at a half integer multiple of the lattice period, the effective substrate potential felt by the center of mass degree of freedom would be identically zero according to Eqs. (6), since the substrate forces acting on the single particles would cancel each other, leading to a zero critical tilt.

Alternatively, one can reinterpret Eqs. (8) in terms of a two-dimensional analogy, as describing Brownian motion of a point-like particle in the X–x plane in the presence of potential (5). The periodic part of the potential is plotted in Fig. 2. One can see that the particle can cross the poten-

tial landscape moving around the potential peaks under the action of an external force, rather than through the steepest paths. The force necessary to ensure a running solution will be in general much smaller than in the one-dimensional case. One can also notice that the optimal trajectories correspond to a constant distance $x = (n + 1/2)a$, with n integer.

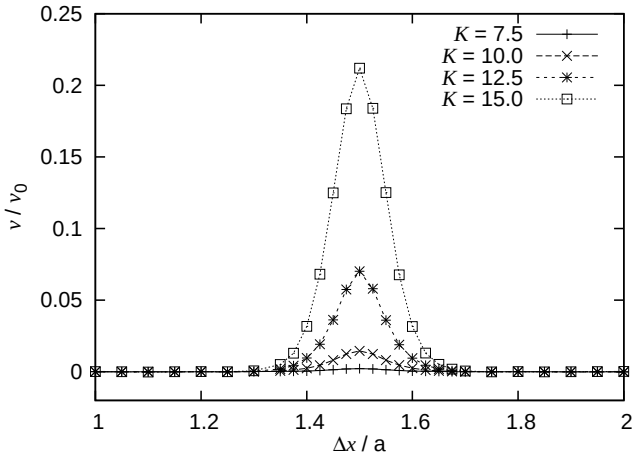

Fig. 4. As in Fig. 3, for different values of the coupling strength between the partials.

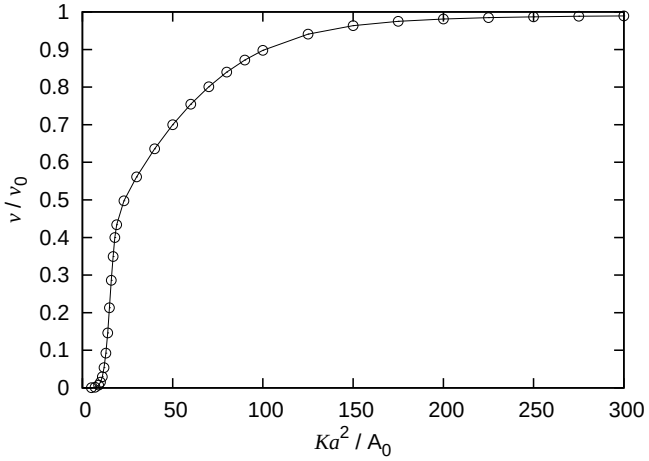

Fig. 5. Maximum value of the asymptotic rescaled average velocity v/v_0, with $v_0 = f/\eta$, corresponding to the peak at $\Delta x = 1.5a$ in Fig. 4, but for different values of the rescaled coupling strength.

In Fig. 4 the average velocity is plotted *versus* distance for different values of the coupling constant K. One can notice that the peak height increases monotonically with K. The ideal situation in which the particles are constrained at a fixed separation distance equal to a half-integer multiple of the period and the critical tilt is zero can in practice be realized by setting $\Delta x = (n + 1/2)a$ and a large enough value for K in Eq. (5), which reduces the oscillations of x. This is shown in Fig. 5, where the maximum values of the average velocity, taken from the curves in Fig. 4, are plotted as a function of the coupling constant K. For large enough values of K, the asymptotic value corresponding to the free case, that is $v/v_0 = 1$, is recovered.

Finally, in Fig. 6 the asymptotic average velocity is plotted *versus* the equilibrium distance Δx for different values of the applied tilt f. As in Fig. 4, the region in which the average velocity is different from zero determined the critical tilt, in turn depending on the equilibrium distance between the particles.

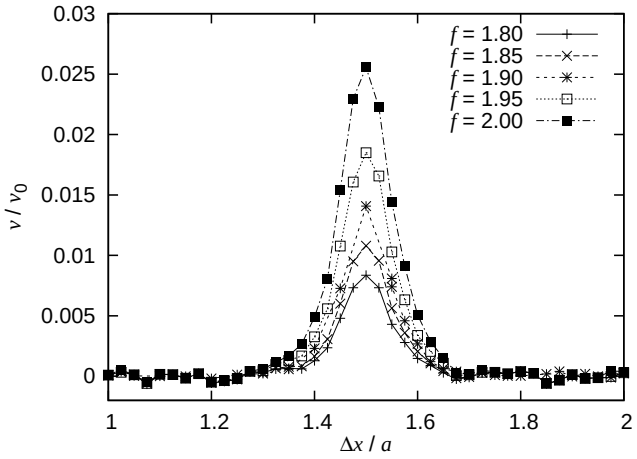

Fig. 6. As in Fig. 3, for different values of the applied tilt.

5. Conclusions

It has been shown that a system made up of two coupled Brownian particles in a washboard potential presents a resonant-like behavior in the mobility as a function of the separation distance, corresponding to half-integer multiples of the period of the underlying potential. Depending on the values of the other system parameters, the increase of the average velocity can be drastic and the system can also switch from a steady to a running solution. A physical interpretation of this effect has been illustrated and

a two-dimensional analogy of the model suggested. The model has been applied to dissociated dislocations in fcc materials in the low temperature regime, where they are described by the Volterra model, but the effect considered here should take place in any other physical system which can be modeled similarly.

A remark should be added concerning an apparent paradox, which especially arises in the case of a wide dislocations ($\Delta x \gg a$). The considerations done above suggest that in principle one can set the Peierls stress equal to a very small value if one makes the separation distance Δx equal to a half-multiple of the lattice constant a. This can be achieved by a suitable value of external stress $\sigma_\perp$ in Eq. (1), inducing a change Δx of an amount, which in general does not have to be larger than $a/2$. Such a change of the distance of a small percentage however would induce drastic changes in the plastic properties of the material.

The solution of the paradox is in the fact that the interaction coupling constant K and the equilibrium distance Δx are not independent quantities in the model, since $K = \gamma^2/2E_0 \equiv E_0/2\Delta x^2$, as explained in Sec. 2. Thus small coupling constants correspond to large separation distances while strongly interacting partials are at a small distance from each other. The ratio $\Delta x/a$ will correspondingly have a relevant role only when the distance Δx is not much larger than a and partials strongly interact. In this case a change of half a period requires a large stress and can represent a significant fraction of the equilibrium distance Δx. On the other hand, the effect of changing the separation distance becomes negligible for wide dislocations, where $\Delta x \gg a$, since partials are weakly coupled to each other and in practice behave independently, so that each partial sees the same effective Peierls stress.

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