Kink nucleation in the two-dimensional Frenkel-Kontorova model

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(Received 30 May 2000; revised manuscript received 25 April 2002; published 23 August 2002)

A computer simulation of thermofluctuation nucleation of kinks on dislocations and their dynamics is carried out in the framework of the two-dimensional Frenkel-Kontorova model. It is shown that at relatively low temperatures and applied stresses the kinks can appear as a result of developing instability of phonon modes localized in the vicinity of the dislocation. The transition from this mechanism to the ordinary thermofluctuation kink nucleation with temperature increase can reveal itself in the peculiarities of yield stress temperature dependence.

DOI: 10.1103/PhysRevE.66.027201 PACS number(s): 05.45.−a, 05.40.−a, 61.72.Lk

I. INTRODUCTION

Due to the translational symmetry of crystals the energy of a dislocation depends periodically on its position in the lattice (Peierls relief) [1,2]. This concept, having been formulated more than 50 years ago [3], proved to be very fruitful for dislocation theory, in particular, for elucidations of factors determining the dislocation mobility (see, e.g., Refs. [4,5]). At present it is commonly accepted that at finite temperatures the dislocations in crystals glide in the Peierls relief due to nucleation of kinks and their propagation along the dislocation lines. This mechanism determines the dislocation mobility in covalent crystals (such as silicon) [4] but can also be essential in the bcc metals and some intermetallic compounds (TiAl, NiAl) [6].

According to the conventional point of view the velocity of dislocations in the Peierls relief is determined by the balance of the processes of thermofluctuation nucleation of kinks and annihilation due to mutual recombination of kinks and antikinks or their disappearance at the defects [4,5]. However, recently the experimental data have become available [5,7,8] which cannot be described adequately by this simplified scheme. The results [9] of numerical simulation of dislocation migration in the two-dimensional (2D) Frenkel-Kontorova model also have demonstrated that the traditional views should be revised. As it was shown in Ref. [9] the kinks on the dislocations can behave like solitons and, when collising, pass through each other without annihilation in spite of thermal fluctuations and damping. As a result a much higher kink density than that predicted in terms of the traditional approach should be expected. It seems interesting to consider the question on the contribution of dynamical effects as well to the double kink nucleation since it is the process of kink-antikink pair nucleation that determines the temperature dependence of the dislocation mobility [1].

In the present work the process of kink nucleation is thoroughly studied by means of modeling the dislocation movement in the two-dimensional (2D) Frenkel-Kontorova model at the finite temperatures. We demonstrate that, in addition to the well known mechanism of thermofluctuation nucleation of kinks, they may also appear as a result of development of instability of lattice vibrations localized near the dislocation axis.

II. FORMULATION OF THE MODEL

Similar to Ref. [9], we study the dislocation dynamics in terms of the 2D Frenkel-Kontorova (FK) model at finite temperatures. In the generalized 2D FK model [9,10] a layer of atoms, set into the periodic potential relief and interacting with each other by means of elastic forces, is considered. The potential energy of this system has the following form:

$$V=\frac{K}{2}\sum_{\langle n,m\rangle}(\mathbf{u}_n-\mathbf{u}_m)^2+P\sum_n\sum_{\mathbf{g}}[1-\cos(\mathbf{g}\cdot\mathbf{u}_n)], \quad (1)$$

where K is the stiffness of interatomic bonds, $\langle n,m\rangle$ designates the sum over all the pairs of the nearest neighbors, and $\mathbf{g}_1=(4\pi/\sqrt{3})(1;0)$, $\mathbf{g}_{2,3}=(4\pi/\sqrt{3})(\frac{1}{2};\pm\sqrt{3}/2)$ are the reciprocal lattice vectors of minimum length.

In order to consider the damping and thermal fluctuations we introduce the contact with a thermostat using the method of Langevin equations of motion [11]

$$\ddot{\mathbf{u}}_n=-\frac{\partial V}{\partial \mathbf{u}_n}-\gamma\dot{\mathbf{u}}_n+\boldsymbol{\xi}_n(t)+\mathbf{f}_n, \quad (2)$$

where $\mathbf{u}_n$ is the vector of displacement of the nth atom from its equilibrium position, γ is the friction coefficient, $\mathbf{f}_n$ is the external force assumed to be equal for all the atoms, $\xi_{ni}(t)$ is the random Gaussian variable having the properties $\langle\xi_{ni}(t)\rangle=0$, $\langle\xi_{ni}(t)\xi_{n'i'}(t')\rangle=2\gamma T\delta_{nn'}\delta_{ii'}\delta(t-t')$, $(i=x,y)$. The brackets indicate averaging over the realization of random process $\boldsymbol{\xi}_n(t)$. A method of solving the set of stochastic differential equations (2) is described in Ref. [9].

For the numerical experiment the 2D hexagonal lattice with 40×40 atoms with periodic boundary conditions was choosen. At the initial moment the displacements in the crystallite were specified in accordance with the known solution for dislocations in the 1D continual FK model [2]:

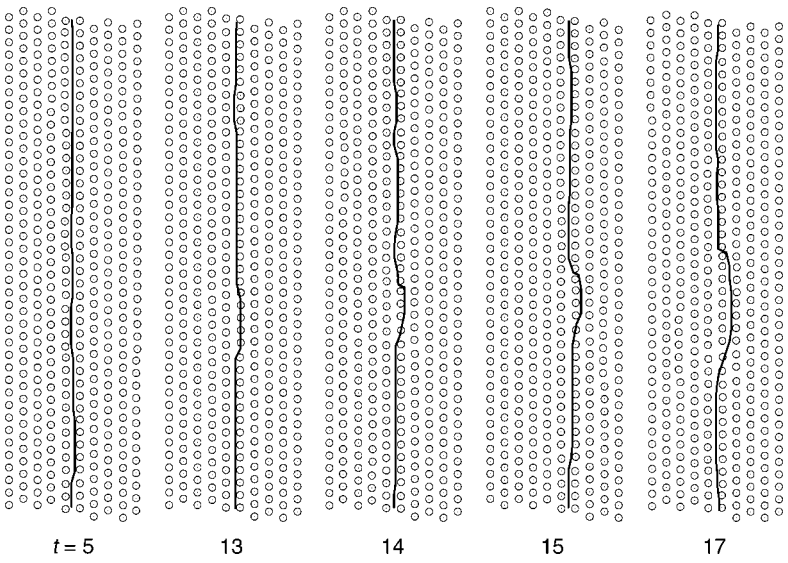

FIG. 1. Configuration of the dislocation line (determined by the condition $|u_y| = 0.5b$) at different times for $P = 0.1$, $T = 0.01$, $\gamma = 0.02$, $f = -0.061$. The rows closest to the dislocation line are $n = 19,20$.

$$u_x = 0, \quad u_y = 1 + \frac{1}{\pi}\arctan\exp\left(-\frac{x}{\lambda}\right), \quad \lambda = \frac{1}{\pi}\sqrt{\frac{K}{P}}. \quad (3)$$

Then the set of equations was integrated numerically for a rather long time ($t \sim 10^2$) at $\mathbf{f}_n = 0$ and the choosen temperature T to find an equilibrium configuration of the dislocation. After that an external force $\mathbf{f} = (0, f_y)$, amounting to 0.75–0.85 of limiting value f_P corresponding to the Peierls stress, was applied.

The most important parameter in the model (1),(2) is the ratio of the height of potential relief P to the stiffness K. We put $K = 1$ (which determines the energy units) and choose $P \approx 0.1$ when, for small displacement $\mathbf{u}$, the forces of atomic interaction with the neighbors and with the substrate layer are comparable. This ratio of parameters leads to the dislocation with $\lambda \sim 1$, which is typical for most of metals (see Refs. [12,13]). The temperature T varied over a wide range from 10^{-3} to 10^{-2} i.e., it was of order of $(0.1–0.01)P$, and the friction coefficient γ varied over the range $(2–5) \times 10^{-2}$, which corresponds to typical values for metals at room temperatures (see, e.g., Ref. [9]).

III. COMPUTATIONAL RESULTS

Figure 1 shows a sequence of dislocation states in the 2D lattice, demonstrating thermofluctuation nucleation of kink-antikink pairs. It is seen that their appearance is preceded by the stage of small amplitude oscillations of the dislocation segment. At a certain time one of these oscillation modes begins to increase, its amplitude reaches the maximum value equal to the distance between the atom rows, and a kink-antikink pair is formed. At subsequent moments of time the kinks move along the dislocation line, reach the crystallite boundaries and, because of periodic boundary conditions, appear on its opposite edges. As was demonstrated in Ref. [9], under the conditions when the termofluctuation kink nucleation is possible, the kinks demonstrate a solitonlike character of motion and, when meeting, pass through each other without annihilation.

In order to understand the mechanism of the pair kink nucleation, let us consider in more detail the picture of atom displacements. An important feature, accompanying the kink nucleation at low values of external force **f** (or of the temperature), is the localization of long-wave lattice oscillations in the vicinity of the dislocation which manifests itself as a correlated motion of atoms in the rows nearest to the dislocation axis. This feature is illustrated by the dependence of the position of center of mass of atomic rows on time [Fig. 2(a)]. Curves 1,2 correspond to the y component (parallel to the Burgers vector) of the average displacement $\langle u_y \rangle$ for the atomic rows with $n = 20$ and 19 (see Fig. 1) nearest to the dislocation axis, curves 3,4 for the atomic rows with $n = 21$ and 18 following the nearest ones. One can see from Fig. 2(a) that the atom row $n = 20$ demonstrates rather regular displacement oscillations $\langle u_y \rangle$ around the average value with a period of tens of characteristic phonon times. The amplitude of these oscillations decreases rapidly with the distance from the dislocation axis, and for $n = 18$ it is practically comparable with the thermal noise level [curve 4, Fig. 2(a)]. Note that the amplitude of the x component of average displacements $\langle u_y \rangle$ (perpendicularly to the Burgers vector) for rows $n = 20$ and 19 is more than by an order of magnitude smaller than $\langle u_y \rangle$. This reduces effectively the dimensions of the problem. The possibility of localization of lattice oscillations on the dislocation was predicted earlier [2] in terms of a simple continual model. Here this phenomenon was found from the numerical experiment on the discrete lattice with allowance for the temperature and damping.

The oscillation stage ends with the nucleation of kink pair whose propagation along the dislocation leads to monotonous decrease in $\langle u_y \rangle$ dependence on t (curve 1, Fig. 3). Thus the analysis of atom displacements reveals that the kink pair nucleation is due to the loss of stability of atom row motion in the effective periodic potential and the onset of an inhomogeneous state similar to the crowdion-anticrowdion pair (see Fig. 3). A similar phenomenon for the 1D FK model was discussed in Ref. [14]. It is this configuration in the row of atoms that corresponds to appearance of the kink-antikink pair on the dislocation line (Fig. 1). Thus, the 2D calculations demonstrate clearly that there is a region of parameters

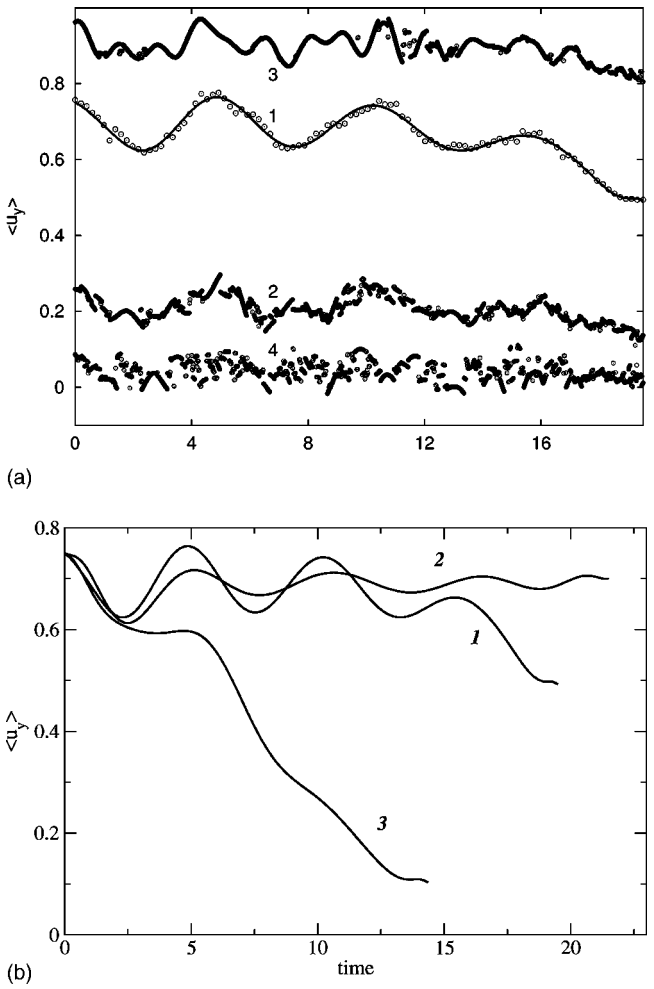

FIG. 2. Time dependence of the center of mass displacement of atomic chains for the rows nearest to the dislocation line with $n=20$, 19, 21, 18 (curves 1–4) at $P=0.1$, $\gamma=0.02$, $T=0.01$, $f=-0.061$ (a) and for atom row with $n=20$, $P=0.1$, $\gamma=0.02$, $T=0.01$, $f=-0.061$ (curve 1), $T=0.08$, $f=-0.07$ (curve 2), $T=0.01$, $f=-0.07$ (curve 3) (b). Solid line is the result of smearing of the computational data to eliminate the thermal noise.

where the scenario of kink pair nucleation on a dislocation is due to the oscillatory instability near the dislocation axis rather than to the classical pattern of thermofluctuation formation and growth of the nucleus. In addition, the kinks on the dislocation in the 2D FK model are found to be similar to crowdions in the 1D FK model. Note that the results obtained not only support this commonly accepted analogy but clarify and extend it.

The observed picture of the kink pair nucleation has an uncommon nonmonotonous dependence in parameters T,**f** (Fig. 4): with the rise on temperature and/or the magnitude of applied force the probability of kink nucleation first drastically reduces (in region II the kinks do not practically appear during the simulation) and with further increase in the parameters are easily formed again (region III). The diagram shown in Fig. 4 is constructed for fixed parameters P and γ; the increase in the damping results in the reduction of the region I. The curves in Fig. 2(b) illustrate the system behavior in three different regions. Curve 1 corresponds to the kink nucleation at low temperature and force applied, described above in detail (region I). Curve 2 corresponds to the intermediate region II where the amplitude of oscillations $\langle u_y \rangle$ decreases rapidly with time to a value comparable with the level of thermal noise. Curve 3 is typical of high temperatures or external forces (region III) when the kink nucleation is again observed. However the ''high-temperature'' kinks differ essentially from the ''low-temperature'' ones; they are much wider so that displacements change slowly at a distance to some lattice parameters [Fig. 3(b)]. Their nucleation is more similar to the classical pattern of fluctuation nucleation and growth of the nucleate, without the stage of preliminary oscillations of the dislocation line (Fig. 1) which is typical of region I.

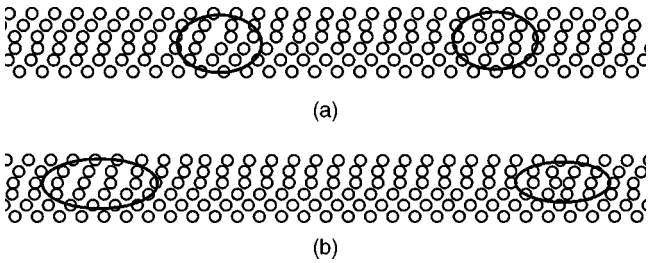

FIG. 3. Crystallite fragments showing the structure of ''low-temperature'' ($T=0.003, f_y=-0.07$), (a) and ''high-temperature'' ($T=0.01, f_y=-0.068$), (b) kinks. The regions of the compression and expansion corresponds to crowdion and anticrowdion, correspondingly.

IV. DISCUSSION

The computer simulations in the 2D FK model described above demonstrate a new mechanism of kink nucleation on a dislocation as a result of development of the instability in the phonon subsystem. Along with the phonon modes spreading within the whole crystallite (bulk phonons) there are also modes localized near the dislocation. In terms of continuum

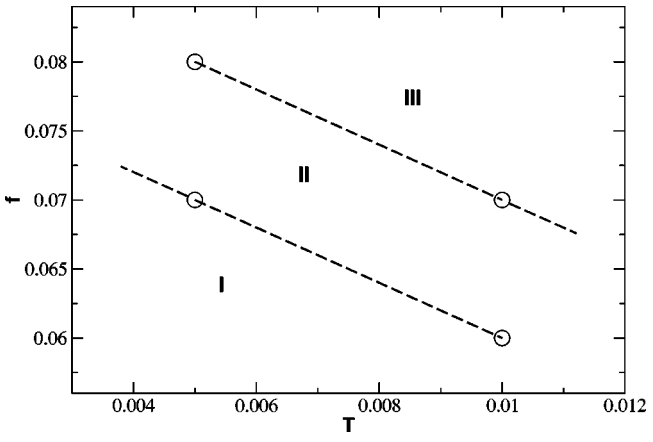

FIG. 4. Regions of the parameter values where the kink-antikink pair nucleation occurs from localized oscillations (I), kinks do not nucleate (II), and they nucleate by the standard thermofluctuation mechanism (III) at $P=0.1$, $\gamma=0.02$. The circles show the parameter values at which the change in the mechanism was observed.

model the possibility of existence of such localized oscillations was discussed earlier (see Ref. [2]). These oscillations are clearly seen in Fig. 2.

At not too high temperatures and forces (region I, Fig. 4) the motion of atoms in the rows nearest to the dislocation line appears to be correlated, which manifests itself in regular oscillations $\langle u_y \rangle$ [Fig. 2(a)]. The change in the behavior of atom motion in the transition to the region II of ''intermediate'' temperatures and forces (curve 2, Fig. 2) is accounted for by the increased damping of localized phonons and loss of coherency, first in the displacements of neighbor atom rows and then inside them. As a result the kink nucleation turns out to be suppressed (note that the growth of damping leads to the same consequences). With further increase in the temperature (curve 3, Fig. 2) the kinks again begin to nucleate but in this case it is a result of development of the instability of ''common'' bulk phonons, which corresponds to the traditional mechanism of thermoflucutation nucleation of the double kink [1]. The transition from region I to region III is accompanied by the change in the kink structure, from narrow kinks [Fig. 3(a)] to the wide ones [Fig. 3(b)]. This indicates the decrease in the secondary Peierls relief [1]. The latter is that shows the loss of coherence in the atom motion in transition to ''high-temperature'' region III.

Let us discuss the significance of the results obtained for understanding the regularities of dislocation motion in the Peierls relief. This motion, generally speaking, occurs due to a complicated collective process with the participation of many kinks. We confined ourselves here to the consideration of the initial stage: nucleation of single kink-antikink pairs. A new phenomenon of fast kink nucleation (for the characteristics times of order of 10–100 inverse phonon frequencies) has been found. In reality, apart from this process a slower thermoactivated kink nucleation process takes place. In the present work we did not study the temperature dependence of the kink nucleation rate. One can assume, however, that for the fast processes considered here, this dependence is weaker than for slow termoactivated processes. Therefore one can expect that the transitions from the low-temperature region to the intermediate-temperature one (suppression of the process of kink nucleation) and from the intermediate- to high-temperature region (restarting of this process) may correspond to inflection points of the temperature dependence of yield stress which have been actually observed in some metals and alloys with a sufficiently high Peierls relief [6,15]. However, this question needs further investigations.

ACKNOWLEDGMENTS

This work is partially supported by the Netherlands Organization for Scientific Research, NWO Project No. 047-008-16, by Russian Basic Research Foundation Grant Nos. 01-02-16108 and 00-15-965-44, and by Russian Science Support Foundation.

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