Fluctuation - induced nucleation and dynamics of the kinks on dislocation. Soliton and oscillation regimes in 2D Frenkel-Kontorova model.

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Numerical simulation of the dislocation motion in 2D Frenkel-Kontorova (FK) model in the thermostat shows an unusual dynamical behavior. It appears that "kink" regime of dislocation gliding takes place in a certain region of parameters of the model but, in disagreement with the common views about the dislocation motion under plastic deformation condition, the kinks appear to be similar to sine-Gordon solitons despite the discreteness of the lattice, damping and thermal fluctuations. At high enough stresses and temperatures the motion of the dislocation is accompanied by its oscillations rather than kink nucleation.

I. INTRODUCTION

The concept of solitons appeared to be very fruitful in various fields of condensed matter physics such as magnetism, charge-density waves, electronic structure of polymers, etc. [1]. Soliton is defined as a nonlinear wave in continuum media with particle-like properties, i.e. conserving its form both at the propagation and at the collisions with other solitons. Generally speaking, the literal transfer of the results of soliton theory to the case of crystal lattice is impossible since the taking into account the discreteness of the lattice may change drastically the character of solutions of nonlinear equations. In particular, the discreteness eliminates the Goldstone mode leading to the pinning of solitons, create the new classes of localized nonlinear oscillatory solutions (breathers), induces the coupling of "soliton" and "phonon" modes and so on [1], [2].

Apart from this, the effects of dissipation, thermal fluctuations etc. are usually important in real situations. There has been recently a growing interest in non-linear effects in the crystal lattice dynamics particularly in the phenomena responsible for plastic deformation (see, e.g., [3]). According to common opinions [3], the gliding of dislocations in crystals with sufficiently high Peierls barrier (in particular, in covalent crystals and semiconductors) is by thermostimulation creation of kink pairs (kink/antikink). In the course of their motion in the opposite sides under the action of external stress the segment of dislocation between the kink and antikink glides into the neighbor Peierls barrier valley. However, while the existence of such kinks is confirmed by direct electronmicroscopic examinations [4], the information on the character of their motion is indirect, i.e. it is obtained from the comparison of results of particular theoretical models [4], [5], [6] with the measurements of dislocation mobility. The common feature of all these models is that the kink is considered as a solitary wave in the Frenkel-Kontorova (FK) model. That is, it is supposed that its shape would persist in the motion [4], [6]. This assumption, strictly speaking, has not been proven since the analytical solutions of soliton type are only available for the ideal continuum model, and the question on their existence in more realistic discrete case is still open.

In the continuum limit the 1D FK model is reduced to the well-known sine-Gordon model [1] which is completely integrable. This means that any initial disturbance of the finite amplitude in this model breaks up into the succession of kinks (solitons), antikinks and breathers (soliton/antisoliton coupled states). In this case the soliton/antisoliton collision may occur by the mechanism of elastic (i.e. without change in the shape) scattering or be accompanied by breather formation. It is unknown to what extent such a behavior might be applied to the discrete case. The existing phenomenological model of kink motion along a dislocation [1], [2] are based on a quite contrary supposition of an unavoidable kink-antikink annihilation in the collision. This statement bases on the hypothesis that such factors as the discreteness of crystal lattice, damping (viscosity) and thermal fluctuations, so important in the actual situation, would destroy the features associated with the complete integrability. Of course, this hypothesis can be either confirmed or refuted only by means of particular numerical calculations which, however, did not give any definite answer to this questions up to now [2]. It should be stressed also that applications of results concerning soliton motion in 1D models to the kinks are doubtful even in the continuum limit since the kinks are "solitons on soliton", i.e. nonlinear excitations of 2D or 3D character. We do not know any analytical results about such excitations in non-one-dimensional continuum models and therefore computer simulation is the only way to investigate them.

Ref. [2] was the first attempt to do this but the nucleation and propagation of kinks were not observed in that calculation. Only recently opportunities appeared of
computer simulations of the dislocation motion in realistic 3D case. Rather complicated picture of the dislocation motion in Al has been demonstrated in \[13\]. However, even when the simplest 2D simulation is not understood now, it is worthwhile to investigate systematically processes of nucleation, propagation and destruction of kinks for a model case.

The present work is devoted to computer simulations of such processes in the framework of 2D FK model. We show that, for certain values of the model parameters, the dislocation gliding is really accompanied by the nucleation and motion of kink-antikink pairs but the dynamics of the latter can be soliton-like. At the same time, for another region of the model parameters well-defined kinks are not observed at all. It means that basic assumptions of conventional phenomenological models of dislocation gliding are at least not evident and the question about their applicability remains.

II. Formulation of the Model and Simulation Method

Consider the common two-dimensional generalization of FK model (2D FK). To take into account the effects of damping and interaction with the thermostat we solve numerically (as well as in \[14\]) the Langevin equations of the following form

\[
\ddot{u}_{ni} = -\frac{\partial V}{\partial u_{ni}} - \gamma \dot{u}_{ni} + \xi_{ni}(t) + f_i, \quad (1)
\]

where \(u_n\) is the vector of \(n\)-th atom displacement, \(i = (x, y)\) are the Cartesian coordinates, \(\gamma\) is the damping factor (the atom masses being equal to 1), \(f_i\) is the constant external force, \(\xi_{ni}(t)\) is the Gauss random force \((<\xi_{ni}(t)>=0)\) with the correlator

\[
<\xi_{ni}(t)\xi_{n'i'}(t')>=2\gamma T\delta_{nn'}\delta_{ii'}\delta(t-t'), \quad (2)
\]

As is known \[14\] such a choice of random force guarantees the Gibbs distribution to be established in the equilibrium at temperature \(T\). The potential energy is chosen as

\[
V = \frac{K}{2} \sum_{<n,m>} (u_{n}-u_{m})^2 + P \sum_n \sum_g (1 - \cos (g \cdot u_n)), \quad (3)
\]

where \(<n,m>\) are the pairs of nearest neighbors in the lattice, \(g\) is three least vectors of reciprocal lattice (we will consider the hexagonal lattice with a parameter \(a = 1\), then \(g_1 = \frac{4\pi}{\sqrt{3}}(-1,0), g_{2,3} = \frac{4\pi}{\sqrt{3}}(\frac{1}{2}, \pm \frac{\sqrt{3}}{2})\)). The first term in Eq.(3) describes the interaction of atoms in the harmonic approximation, and the second one is the simplest approximation corresponding to the sine law for the returning force in 1D FK model. Note that, unlike the present work, Ref. \[12\] considered the square lattice which, in the nearest neighbor approximation, has a certain pathology (the zero shear modulus). In contrast with this, hexagonal lattice in the nearest-neighbor approximation represents rather general isotropic 2D situation. Thus, Eq. (3) can be considered as the most natural generalization of original 1D FK model for 2D case. Depending on specific interatomic interactions and chemical bonds, the substrate potential may be changed in comparison with purely cosine form in Eq. (3). Calculating the substrate potentials for a series of fcc metals \[13\] we found that Eq. (3) may be considered as an adequate enough for substances with almost purely central pairwise interactions (without strong covalency or electron density dependence). In principle, it is not difficult to take into account next terms of Fourier expansion in Eq. (3) but in this work we restrict ourselves only by the consideration of the simplest case.

Initially lattice displacements of atoms \(u_n(0)\) corresponding to the screw dislocation with Burgers vector \(b = (0,1)\) and the axis parallel OY, were set. The displacements for \(t = 0\) were chosen in accordance with the solution of 1D FK as \[1\]

\[
u_n = \frac{2}{\pi} (\pi - tan^{-1} \left( \frac{\pi}{\lambda} \right)) \left( 1 - \frac{x}{\lambda} \right), \quad u_{nx} = 0 \quad (4)
\]

where \(\lambda = \frac{1}{\pi} \sqrt{\frac{2}{f_x}}\). Eqs.(1) were then solved for \(f = 0\), \(T = 0\) and the ”actual” equilibrium distribution of displacement field in the absence of external force was determined. After that external force \(f_y\) \((f_x = 0)\) and temperature \(T\) was introduced, and the evolution of displacement field was studied. The lattice was specified the form of 40x40 cluster of atoms with periodic boundary conditions. Generally speaking, the latter may be dangerous in the simulations of dislocations in realistic models with inverse distance decay of deformation fields and therefore with strong interactions with ”mirror" dislocations. However, the deformation in FK model decay exponentially and long-range part of the dislocation fields is not taken into account.

In order to obtain a reliable information about the evolution of the system investigated, it is necessary to use the so-called "strong" (mean square) methods for integrating stochastic differential equations \[13\], \[17\]. The simpler and more commonly used weak methods (in particular, those used in \[12\]) are actually intended only for the calculation of averaged characteristics such as spectral density and are not appropriate for studying individual trajectories of the system in the thermostat. We used the method proposed in \[18\] and intended for solving the set of stochastic differential equations (the approach used in \[17\] is only directly applicable for the solution of single equation). Specific computational formulas and the details of the method are presented in Appendix.
III. THE RESULTS OF CALCULATIONS

As is seen from Eqs. (1)-(3) the character of solution is determined by four independent dimensionless parameters \( \tilde{\gamma} = \gamma / \sqrt{T} \), \( \tilde{T} = P / K \), \( \tilde{\gamma} = f_0 / K \). Dimensionless damping \( \tilde{\gamma} \) is of order of the ratio of phonon damping to phonon frequencies and is typically of order of \( 10^{-2} \) at room temperature and above. Apart from this, such choose of \( \tilde{\gamma} \) provides strong attenuation of phonon waves at the lengths of order of the crystallite size in our simulations and eliminate essentially artifacts of periodic boundary conditions. Since the phonon damping in the classical region is linear in \( T \) (see e.g. [19]) we put \( \tilde{\gamma} = \gamma / \sqrt{T} \).

The value of the parameter \( \tilde{P} \) determines the transition from continuum case to the discrete one. One can estimate from the expression for \( \lambda \) in Eq. (4) that the width of the kink is of order of interatomic distance at \( \tilde{P} \approx 0.1 \). As it will be seen below it is roughly the “critical” value for the change of a character of dislocation motion. Therefore we investigate in detail the cases \( \tilde{P} = 0.08 \) and \( \tilde{P} = 0.12 \). As for the parameter of external stress it has to be compared with the Peierls stress \( f_p \). The latter is defined as the minimal stress which leads to the motion of the dislocation as a whole at \( T = 0 \). The results of our simulations show that this critical stress turns out to be temperature-dependent decreasing with \( T \) increase. For example, for \( \tilde{P} = 0.08 \), \( \tilde{T} = 0.005 \) the dislocation moves as a practically straight line already at \( \tilde{f} = 0.01 \), whereas Peierls stress for that parameters \( \tilde{P} \) and \( T = 0.002 \) was \( 0.03 \). The accurate calculation of the Peierls barrier in computer simulation is a complicated problem [20]. Since we are interested here in the investigation of the gliding we restrict ourselves only the case \( f < f_p (T) \).

Fig. 1 gives an example of the distribution of displacements around the moving dislocation. Kinks may be seen as inhomogeneities of the distribution along the dislocation axis. However, it is much more suitable to watch them displaying only dislocation line positions. The latter is defined by the condition \( |u_y| = 0.5b \). It corresponds to the center of dislocation since \( |u_y| \) varies continuously from 0 to \( b \), see Fig. 1.

Fig. 2 demonstrates a typical (at least for the values of temperature and damping under consideration) picture of dislocation gliding for \( \tilde{P} = 0.12 \). It shows "soliton-like" behavior of kinks with their thermofluctuation nucleation, propagation without change of their shapes and purely elastic scattering (mutual penetration) of kink and antikink. To our knowledge, this is the first observation of such regime in 2D FK model with the interaction with thermostat.

Figs. 3-4 display some pictures of the gliding for \( \tilde{P} = 0.08 \). The character of the dislocation motion for this value of \( \tilde{P} \) is much more complicated than for \( \tilde{P} = 0.12 \). Depending on the parameters of the model three different regimes of the dislocation gliding are possible. First, kink nucleation similar to Fig. 2 may take place. Second, kinks may appear after preliminary stage of "oscillation" motion when the dislocation glides as a wriggled flexible band or, by another words, kinks arise as a result of evolution of the oscillations of the dislocation segment (Fig. 3). The most important feature here is the demonstration of a possibility of a third regime, namely, rather fast gliding without participation of kinks at all, only due to the oscillations of the dislocation line (Fig. 4). Sometimes the average dislocation velocity without participation of kinks is even higher (compare the motion of dislocation line in Fig. 3 where kinks exist and in Fig. 4 without kinks). Since the oscillating dislocation does not lie in a single Peierls valley the "effective" Peierls barrier for such dislocation segment turns out to be lower than for straight one. Results obtained here shows that the regime of "wriggled flexible band" occurs at large enough temperature and external stress close to the Peierls stress. Similar gliding mechanism due to oscillations has been observed recently in molecular dynamics simulations of the 3D dislocation motion in Al [13]. According to our simulations, the transitions between regimes occur at the change of temperature and damping, e.g., for \( T = 0.002 \) three regimes mentioned above take place for 0.02 \( \leq \tilde{\gamma} \leq 0.03 \), 0.03 \( \leq \tilde{\gamma} \leq 0.04 \), and \( \tilde{\gamma} \geq 0.04 \), correspondingly. General trend is the change of kink regime by the oscillation one at the temperature and/or damping increase. The value of external stress is less important provided that it is lower than the Peierls stress for a given temperature.

Another important feature of that regime is the existence of long-lived coupled kink-antikink pairs similar to discrete breathers [2]. An example of such behavior is seen in the part of Fig. 3 corresponding to 24 \( \leq t \leq 34 \). It is worthwhile to stress that we mean breather-like excitations on the "soliton" (dislocation) and not standard discrete breathers as more or less isotropic localized oscillating in time solution of non-linear equations. Similar breather-like excitations may be observed also for \( \tilde{P} = 0.12 \) but their lifetime is much shorter than for \( \tilde{P} = 0.08 \). Note that the lifetime increases with \( \tilde{\gamma} \) increase for given values of other parameters of the model.

We never observed the kink-antikink annihilation in our simulations; if kinks appear they always behave as solitons at the collisions. It is rather unexpected in comparison with common views [4], [5]. To clarify the situation we investigate kink-antikink collisions generating kink-antikink pairs right in the initial configuration. The results of the simulations shown in Fig. 5 demonstrate that both penetration and annihilation are possible depending on the parameters of the model, the annihilation being take place at rather high values of the damping and temperature (Fig. 5(b)). However, it is that the region of the parameters when, instead of thermofluctua-
tion nucleation of kinks, oscillation regime of the gliding takes place. Therefore we believe that the kink-antikink annihilation is not important process for the dislocation gliding under "normal" conditions when the creation of kinks is of purely thermodiffusion nature. However, it may be important if kinks could create, e.g., by collisions of the dislocation with another defects, etc. This question needs further investigations.

IV. DISCUSSION AND CONCLUSIONS

Summing up the results obtained, it might be stated that the physical picture of the dislocation gliding appeared to be much more complicated that it is supposed in traditional models of dislocation motion in the Peierls relief \[3, 4\]. First of all, we observe (for \(P = 0.12\)) thermodiffusion nucleation of kinks supposed in that models but, in contrast with them, the character of motion of the kinks appears to be purely "solitonic". It is nontrivial since for these values of the parameters the widths of kinks are of order of the lattice constant and the results of continuum models such as sine-Gordon model are definitely not applicable. This implies the annihilation of kinks and antikinks is unlikely in this regime, and their lifetime is anomalously long. It means that under these conditions the thermodynamical equilibrium in the system of kinks and antikinks does not practically establish, and their concentration should be essentially higher than that predicted by the phenomenological models. Note that in the special pulse regime of loading the anomalously high concentration of kinks was observed in Si \[21\] and Ge \[3\]. The explanation proposed in \[3\] is based on the essential effect of impurities. According to the results obtained in the present work this explanation is not the only possible one and high concentration of kinks may be intrinsic property of that materials.

For larger values of width of kinks (\(P = 0.08\)) the character of dislocation motion is very complicated. In contrast with the case \(P = 0.12\) the creation of kinks in this case is not typical thermodiffusion nucleation but rather a result of more or less long evolution of oscillations of the dislocation segment. Both kinks and oscillations of dislocation segments play an important role in the gliding. It is shown that the gliding with rather high velocity may be provided by oscillations only without participation of kinks ("wriggled flexible band" regime). More detailed investigation of these processes depending on the temperature, damping, external stress and the shape of substrate potential relief would allow to correct and improve existing phenomenological models of plastic deformation.

In the conclusion it should be noted that the methods used here can be applied for studying variable loading conditions with a time-dependent external force (ultrasound, pulse loads). The question on the role of impurities \[3\] might be also studied be means of similar simulation. At the same time, we believe that the results obtained may be of more general interest than for physics of plasticity only since until now rather incoherent information about soliton-like excitations in two-dimensional discrete systems are available.

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VI. APPENDIX

Let us represent Eq. (1) as a set of first -order equations in a form used commonly in the theory of stochastic differential equations (SDE)

\[
dv_{ni} = ( -\nabla_{ni} V(u) - \gamma v_{ni}) dt + \kappa d\omega_{ni}(t) \quad (A1)
\]

where \(\kappa = \sqrt{2\gamma \tau}, \ d\omega_{ni}(t)\) is a standard Wiener process. Introducing \(4nm\) dimensional vectors

\[
\vec{\tau} = \left( \begin{array}{c} u \\ v \end{array} \right), \ \vec{d} = \left( -\nabla V(u) - \gamma v \right), \ \vec{\sigma}_r = \left( \begin{array}{c} 0 \\ b_r \end{array} \right)
\]

\(b_{ri} = \kappa \delta_{ri}, \ r = 1, ..., q, \ i = 1, ..., q, \ q = 2nm,\)

one can rewrite Eqs. (A1) in a common form as

\[
d\vec{\tau} = \vec{\sigma}(t, \vec{\tau}) dt + \sum_{r=1}^{q} \vec{\sigma}_r d\omega_r(t) \quad (A2)
\]

To integrate SDE’s (A2) numerically we use the meansquare Runge-Kutta type method of the 3/2- order which leads to the following approximate solution \[18\]

\[
\vec{\tau}_{k+1} = \vec{\tau}_k + \frac{1}{6} ( \vec{\sigma} K_1 + 2 \vec{\sigma} K_2 + 2 \vec{\sigma} K_3 + \vec{\sigma} K_4) + \sum_{r=1}^{q} (\vec{\sigma}_r I_r)_k +
\]

\[
\sum_{r=1}^{q} (\frac{d\vec{\sigma}_r}{dt} I_{0r})_k + \sum_{r=1}^{q} (\Delta_{r} \vec{\sigma} I_{0r})_k + \frac{h^2}{2} L_2 \vec{\tau}_k +
\]

\[\beta_i \]

\[\gamma_i \]
\[
\sum_{r=1}^{q} \left( \frac{d^2 \bar{x}_r}{dt^2} I_{00r} \right) + \sum_{r=1}^{q} (\Lambda_r L_1 \bar{x}_r I_{r00}) + \sum_{r=1}^{q} (L_1 \Lambda_r \bar{x}_r I_{00r}).
\]

Here \( \bar{x}_k \) is the mean-square approximation of the vector \( \bar{x} \) at the instant \( t_k \),

\[
\bar{K}_1 = h \bar{x}(t_k, \bar{x}_k), \quad \bar{K}_2 = h \bar{x}(t_k + h/2, \bar{x}_k + \bar{K}_1/2),
\]

\[
\bar{K}_3 = h \bar{x}(t_k + h/2, \bar{x}_k + \bar{K}_2/2),
\]

\[
\bar{K}_4 = h \bar{x}(t_k+1, \bar{x}_k + \bar{K}_3).
\]

Here \( \bar{K}_i \) is the mean-square approximation of the vector \( \bar{K} \) at the instant \( t_k \).

\[
L_1 = \frac{\partial}{\partial t} + \sum_{i=1}^{\rho} a_i \frac{\partial}{\partial x^i}, \quad L_2 = \frac{1}{2} \sum_{r=1}^{q} \sum_{j=1}^{q} \sigma_{ij} \frac{\partial^2}{\partial x^i \partial x^j}.
\]

\[
\Lambda_r = \sum_{i=1}^{\rho} \sigma_{ri} \frac{\partial}{\partial x^i}, \quad \bar{I}_r = h^{1/2} \zeta_r, \quad \bar{I}_0 = \frac{h^{3/2}}{2} \left( \frac{\eta_r}{\sqrt{3}} + \zeta_r \right),
\]

\[
\bar{I}_{00} = h \bar{I}_r - I_{00}, \quad \bar{I}_{00} = h \bar{I}_r + J_r,
\]

\[
J_r = \frac{h^{5/2}}{2} \left( \frac{\zeta_r}{3} + \frac{\eta_r}{4\sqrt{3}} + \frac{\xi_r}{12\sqrt{5}} \right),
\]

\( h = t_{k+1} - t_k \); \( \rho = 4nm \) is the dimension of \( \bar{x} \) vector; \( \zeta_r, \eta_r \) and \( \xi_r \) are independent normally distributed random variables with zero mean value and dispersion equal to unity.

Generally speaking, this method is \( "h^{3/2}-method" \), i.e. it provides the accuracy of order of \( h^{3/2} \) for \( \bar{x}_k \) for every realization of stochastic process. However it may be proven \( [1] \) that for the case of small enough noise it is even more accurate ("\( h^4 \) method"). We have chosen in our simulations \( h = 0.005 \); in that case the accuracy of the calculations for trajectories as well as of Gibbs distribution at the equilibrium appeared to be restricted only by Monte-Carlo inaccuracy.

[1] Soliton in Action, Ed. by K. Lonngren and A. Scott (Academic Press, New York, 1978); K. Maki, In: Electronic Properties of Inorganic Quasi-one-dimensional Compounds, Ed. by P. Monseau (Academic Publishers, Kluwer, Dordrecht, 1985), p. 125.
FIG. 3. As in Fig. 2, \( t = 10, 13, 16, 18, 20, 22, 24, 26, 28, 30, 32, 34, 37, 40 \), for \( \tilde{P} = 0.08, \tilde{T} = 2 \cdot 10^{-3}, \tilde{\gamma} = 0.035, \tilde{f} = -0.008 \).

FIG. 4. As in Fig. 2, \( t = 7, 10, 13, 16, 19, 22, 25, 28, 31, 34, 37, 40, 43, 46 \), for \( \tilde{P} = 0.08, \tilde{T} = 2 \cdot 10^{-3}, \tilde{\gamma} = 0.045, \tilde{f} = -0.01 \).

FIG. 5. The dynamics of the kink-antikink pair created in the initial configurations. The dislocation line at different times \( t = 4.5, 6, 7.5, 9, 10.5, 12, 13.5, 15 \) is shown. Here \( \tilde{P} = 0.08, \tilde{T} = 2 \cdot 10^{-3} \) and (a) \( \tilde{\gamma} = 0.02, \tilde{f} = -0.030 \) (penetration regime) (b) \( \tilde{\gamma} = 0.03, \tilde{f} = -0.040 \) (annihilation regime).
