Kinks motion and underdamped dc-driven dynamics of atomic monolayers

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Abstract

A multi-step dynamical phase transition from the locked to the running state of atoms in response to a dc external force is studied by molecular dynamics simulations of the generalized Frenkel–Kontorova models in the underdamped limit. We show that the hierarchy of depinning transition recently reported [Braun et al., Phys. Rev. Lett. 78 (1997) 1295] strongly depends on the friction. In the present study we consider (i) a generalized FK model with *highly anisotropic* quasi-one-dimensional rectangular potential, and (ii) an *isotropic* triangular system, where the interactions between neighboring "channels" play an important role in the dynamics. Copyright © 1998 Elsevier Science B.V.

1. Introduction

The nonlinear response of a system of interacting atoms to a dc driving force has recently attracted a great interest (see [1–10] and references therein), since the knowledge of the *microscopic* mechanisms for mobility, friction and lubrication processes is very important for a better understanding of solid friction at *macroscopic level*, as well as in various fields of applied science and technology such as adhesion, contact formation, friction wear, lubrication, fracture, etc.

One generic example represents a layer of atoms adsorbed on a crystalline surface, often treated within the framework of a generalized Frenkel–Kontorova (FK) model [11–13]. When an external dc force is applied to such a system, its response can be very nonlinear and complex. By contrast, the driven motion of a single Brownian particle in the external periodic potential has been studied in detail and is now well understood [14]. If a force F is applied to the particle, the total external potential in the direction x of the force is a corrugated plane with a slope

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F. For small forces the potential has local minima and the particle is *locked*. The local minima disappear at forces higher than $F_{f0} \equiv C\pi\varepsilon/a$, where ε is the amplitude of the periodic potential, a its period and C a numerical factor depending on the shape of the potential. Thus, when the applied force is adiabatically increased, the atom passes from the locked to the *running* state at F_{f0} and, the mobility $B = \langle v \rangle/F$ (where $\langle v \rangle$ is the drift velocity) reaches its maximal value $B_f \equiv 1/m\eta$, where m is the atomic mass and η the friction coefficient. On the other hand, if one decreases the force F adiabatically starting from the running state, the critical force $F_{b0} \simeq 4\eta\sqrt{m\varepsilon}/\pi$ for the backward transition to the locked state is different owing to inertia of the system. Indeed, in the underdamped limit ($\eta \ll \omega_0$, where ω_0 is the frequency of atomic vibration in the external potential), the inequality $F_{b0} < F_{f0}$ holds and one can observe a *hysteresis*: in the *bistable* region $F_{b0} < F < F_{f0}$, the particle is either locked or running depending on its initial velocity. However, since the "forward" critical force F_{f0} is independent of the friction and the "backward" force F_{b0} grows linearly with friction, the width of hysteresis could vanish and, moreover, for a single particle, the bistability disappears at any nonzero temperature.

The problem of *interacting* particles in a periodic potential is much more difficult. If the nonlinear mobility of the overdamped ($\eta \gg \omega_0$) FK model has been studied in a number of papers [1–4,9], investigations of the underdamped case are very limited. In that context, Persson [6] observed *hysteretic* dynamical phase transition, similar to the $T = 0$ one-particle case, in the MD simulation of a two-dimensional system of interacting atoms subjected to a periodic potential. In addition, our recent work [10] on the underdamped generalized FK model revealed strong collective effects in the dynamics of the dc-force driven layer of atoms. When the external force increases, the FK system exhibits a complex hierarchy of first-order dynamical phase transitions from the completely immobile state to the totally running state, passing through several intermediate stages characterized by the running state of collective *quasiparticle* excitations of the FK model known as kinks [10]. All the observed transitions are hysteretic and, it is remarkable, that, by contrast with the case of noninteracting atoms, the hysteresis survives at *nonzero* temperature of the system.

However, the results [10] have been obtained for one value of the friction constant η and, in the present work, we will be interested in the evolution of the observed dynamical transitions when the friction changed. We present the dynamical "phase diagram" of the FK system in the (F, η) plane for a generic atomic concentration (Section 3). Finally, we will consider not only a *highly anisotropic* Frenkel–Kontorova model, but also an *isotropic* triangular system, where the interactions between neighboring "channels" play an important role in the dynamics. We will emphasize that the mobility of the system could vary *nonmonotonically* when the force is increased.

2. The model

The detailed description of the generalized FK model, of the numerical procedure and also the explanation of the choice of model parameters can be found in [10]; here we only outline the main aspects of the model. The atomic motion is governed by the Langevin equation:

$$m\ddot{x}_i + m\eta\dot{x}_i + \frac{\mathrm{d}}{\mathrm{d}x_i}\left[V_{\text{sub}}(x_i, y_i, z_i) + \sum_{j\neq i} V_0 \exp(-\beta_0|\mathbf{r}_i - \mathbf{r}_j|) \right] = F^{(x)} + \delta F_i^{(x)}(t) \tag{1}$$

for the x coordinate of ith atom, and similar equations for y and z. Here, $V_{\text{sub}}(x, y, z)$ is the external substrate potential, $V_0 = 10\,\text{eV}$ the amplitude and $\beta_0 = 0.85\,\text{Å}^{-1}$ the inverse of the range of interaction of pairwise repulsion between atoms, F the dc driving force, and $\delta\mathbf{F}$ a Gaussian random force.

To model the substrate, we used in the simulation a true three-dimensional external potential periodic in the (x, y) plane, and parabolic in the z direction: $V_{\text{sub}}(x, y, z) = V_{xy}(x, y) + \frac{1}{2}m\omega_z^2 z^2$ where ω_z is the frequency of normal vibration of a single atom. For the periodic $V_{xy}(x, y)$ part of the potential, we consider two different cases:

(i) *A highly anisotropic potential with rectangular symmetry of minima* $V_{xy}(x, y) = V_{pr}(x; a_{sx}, \varepsilon_{sx}, s_x) + V_{pr}(y; a_{sy}, \varepsilon_{sy}, s_y)$ *where*

$$V_{pr}(x; a, \varepsilon, s) = \frac{\varepsilon}{2} \frac{(1+s)^2[1 - \cos(2\pi x/a)]}{1 + s^2 - 2s\cos(2\pi x/a)}. \tag{2}$$

The choice of the lattice constants, $a_{sx} = 2.74$ Å and $a_{sy} = 4.47$ Å, of the energy barriers, $\varepsilon_{sx} = 0.46$ eV and $\varepsilon_{sy} = 0.76$ eV, provide a high anisotropy of this potential, which can be viewed as the set of "channels" with the corrugated bottoms, oriented along the x-direction. This potential is typical for the furrowed crystal surfaces and our parameters were chosen for the Na-W(112) adsystem [10]. The parameters $s_x = 0.2, s_y = 0.4$ determine the frequencies of atomic vibration near the minima of potential, $\omega_{x(y)} = \omega_0(1 + s_{x(y)})/(1 - s_{x(y)})$, where $\omega_0 \equiv (\varepsilon_{sx}/2m)^{1/2}(2\pi/a_{sx}) = 1.09$. Thus we have $\omega_x = 1.65, \omega_y = 2.02$.

(ii) *An isotropic substrate potential with triangular periodicity of minima:*

$$V_{xy}(x, y) = \frac{\varepsilon_{sx}}{2}\left[1 - \cos\left(\frac{2\pi x}{a_{sx}a}\right)\cos\left(\frac{\pi y}{a_{sy}}\right) + \frac{1}{2}\left(1 - \cos\left(\frac{2\pi y}{a_{sy}}\right)\right)\right], \tag{3}$$

where we chose the same ε_{sx}, and a_{sx} as in the case (i), and put $a_{sy} = \sqrt{3}/2a_{sx}$. Thus we have a potential with a very isotropic energy barrier ε_{sx}, and $\omega_x = \omega_y = \omega_0 \approx 1.09$. In both cases (i) and (ii) we put $\omega_z = 1.84$. We want to emphasize that our choice of parameters does not claim to be a quantitative interpretation of the concrete adsystem, because the model is oversimplified; however, we do believe on a qualitative description and claim that typical adsystems should exhibit similar behaviors.

In the present work we study the behavior of the system in a wide range of frictions in the underdamped limit $\eta \ll \omega_x$, corresponding to typical adsystems [15]. In the simulation, we first look for the minimum-energy configuration of the system. Then, we adiabatically increase temperature and force; finally, we measure the mobility B for given values T and F (this procedure was described in detail in [10]). Here, in order to emphasize the phase transitions, the system is studied at a very low substrate temperature, $T = 0.0005$ eV.

An important parameter of the generalized FK model is the atomic concentration. For the repulsive interatomic interaction used in the present work, we have to impose the periodic boundary conditions in the x and y directions in order to fix the concentration. We place N atoms into the fixed area $L_x \times L_y$, where $L_x = M_x a_{sx}$ and $L_y = M_y a_{sy}$, so that the dimensionless atomic concentration (coverage) is equal to $\theta = N/M$ ($M = M_x M_y$). The atomic concentration in the FK system plays a crucial role since it defines the number of quasiparticle excitations called geometrical kinks. These excitations can be defined for any background *commensurate* atomic structure $\theta_0 = p/q$, where p and q are relative prime integers [13,16]. If the concentration θ slightly deviates from the background value θ_0, the ground state of the system corresponds to large domains with background commensurate coverage θ_0, separated by localized incommensurate zones of compression (expansion) called kinks (antikinks). As we study finite systems in the simulations, we must choose an appropriate system size to insert N_k kinks into the $\theta_0 = p/q$ commensurate background structure; the integers N and M must therefore satisfy the equation $qN = pM + N_k$ [16]. In the present work we consider the simpler case of a *trivial* (with $p = 1$) background coverage, $\theta_0 = 1/2$, so that the kinks defined on the background of this coverage are called *trivial* kinks [13]. Namely, we choose $\theta = 21/40$, which corresponds to domains of the $\theta_0 = 1/2$ coverage, separated by trivial kinks.
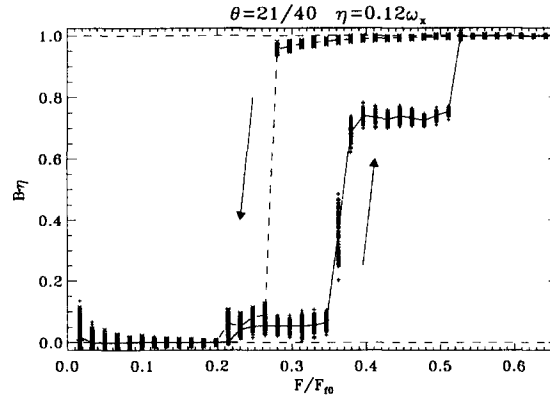
Fig. 1. The mobility B versus external force F for the quasi-one-dimensional FK model when $\theta = 21/40$ coverage. We took $N = 105$ and $M_x = 200$, having thus ten kinks over the length under investigation with an average spacing of $20a_{sx}$ between kinks. The solid (resp. dashed) curve corresponds to force increasing (resp decreasing). The arrows indicate the hysteresis. F is in the units of the constant "forward" critical force for a single particle $F_{f0} = C\pi\varepsilon_{sx}/a_{sx} \approx 0.607$.

3. Frenkel–Kontorova model with rectangular symmetry

In this section, we only consider the quasi-one-dimensional case ($M_y = 1$), since this simplified choice leads only to a minor difference [10] in system behavior in comparison with the true two-dimensional FK system. Note however, that even in this quasi-one-dimensional case the interaction between the atoms, as well as the atomic motion still has the three-dimensional character.

3.1. Nonlinear mobility

The generic evolution of the mobility $B(F)$ for the friction constant $\eta = 0.12\omega_x$ and coverage $\theta = 21/40$ is presented in Fig. 1. During the force-increasing process, one can distinguish several steps in the $B(F)$ dependence, corresponding to a hierarchy of depinnings of kinks [10]. At $F < F_{tk} \approx 0.23F_{f0}$ the system is in the completely immobile state, while at $F > F_{tk}$ the system has a nonzero mobility B_{tk} due to the *running state* of trivial kinks (Fig. 2(a)). It was shown in [10] that the force F_{tk} is related to the vanishing of the periodic Peierls–Nabarro potential ε_{PN} for the trivial kinks under the effect of F. The kinks start to slide at $F > F_{tk} \approx \pi\varepsilon_{PN}/a_{sx}$. The second abrupt increase of the mobility to the value B_m takes place when the force exceeds a threshold $F_{pair} \approx 0.35F_{f0}$, connected with the vanishing of the energy barrier for creation of additional kink–antikink pairs in the system: the number of mass carriers in the system increases leading to the increase of the mobility. The running kinks have the remarkable tendency to come closer to each other, thus bunching into compact groups. This tendency is especially enhanced after the second threshold F_{pair}, where the concentration of kinks is large. The bunched kinks build up dense groups of immobile atoms with $\theta = 1$, while the rest of the system consists of running atoms (corresponding to the running state of force-excited antikinks). This state, very reminiscent of a *traffic jam* (Fig. 2(b)), survives until the last threshold force $F_f \approx 0.53F_{f0}$; after that threshold, all atoms are sliding over the periodic potential and the system reaches the highest possible value of the mobility $B_f = 1/m\eta$. During the force-decreasing process, the system jumps back to the immobile state at the critical force F_b and, the large hysteresis survives at nonzero temperature [10] contrary to the one-particle case.

As was mentioned in Section 1, the "forward" force F_{f0} for a single Brownian particle is independent of the friction, while the "backward force" F_{b0} is linearly proportional to the friction. By contrast, the situation is more

regime of running kinks

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traffic jam regime

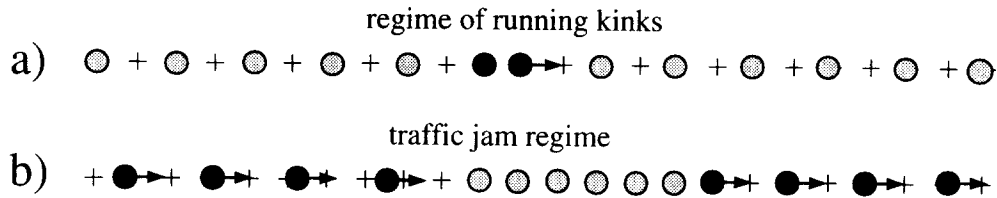b)   +●➞+ ●➞+ ⬤●➞ +●➠+ ◎ ◎ ◎ ◎ ◎ ◎ ●➞+ ●➞+ ●➞+ ●➞

Fig. 2. Illustration of the atomic motion in the regime of running kinks (a) and in the "traffic jam" regime (b). Immobile atoms are denoted with gray circles, running atoms and atoms in the kink regions are denoted with black circles; arrows indicate the direction of atomic motion.
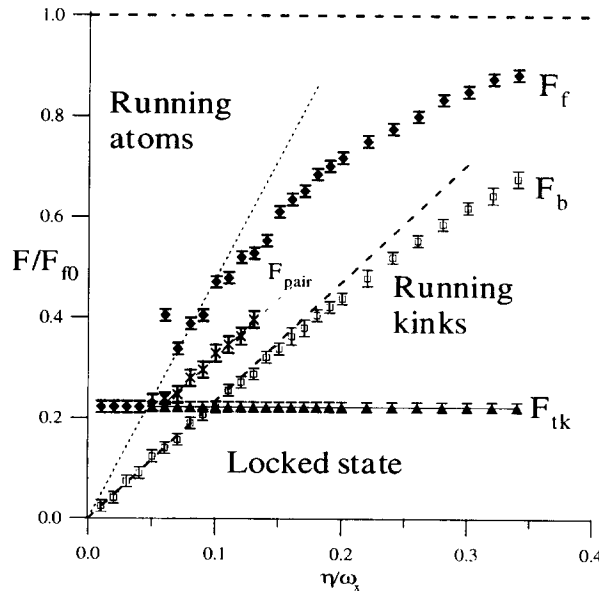

Fig. 3. Dynamical phase diagram in the (F, η) plane for the quasi-one-dimensional FK model at the $\theta = 21/40$, i.e. for the trivial kinks on the background of simple $\theta_0 = 1/2$ structure.

complex in the case of interacting atoms. Fig. 3 represents the dynamical phase diagram in the (F, η) plane, where we plot the critical forces F_{tk}, F_{pair}, F_f and F_b versus the friction coefficient η. Let us consider first the forward transition from the locked to the running state. One can distinguish two regions of friction corresponding to different scenarios of the transition.

(i) At very low frictions, $\eta < 0.05\omega_x$, there is no intermediate stage. When the force increases, the system jumps from the locked to the running state directly at the force F_f, this force being exactly equal to the critical force F_{tk} for the *kink* transition to the running state.

(ii) At larger frictions, $\eta > 0.05\omega_x$, the above-mentioned intermediate stages with running kinks exist. The second difference from the very low friction region is that the "forward" force F_f and the kink–antikink nucleation force F_{pair} are *friction-dependent* (however, we do not plot F_{pair} at higher frictions, because the "traffic jam" regime is not well-defined due to finite-size effects [18]).

The backward transition from the running to the locked state has one interesting feature: F_b grows with η increasing and one can even notice that at not too high frictions, $F_b(\eta)$ exactly matches the law $F_{b0} \simeq 4\eta\sqrt{m\varepsilon_s}/\pi$ for *noninteracting* atoms (dashed line in Fig. 3). If the friction is high enough, F_b is larger than the critical force for

kinks F_{tk} =const. Therefore, at $\eta < 0.1\omega_x$ the system jumps back to the completely *locked* state of atoms, while at $\eta > 0.1\omega_x$ the backward transition has also a multi-step character: when the force decreases, it first occurs a drop of the mobility B from B_f to the kink-mobility value B_{tk} and only at some $F < F_{tk}$ the mobility vanishes finally.

3.2. Phenomenological approach

The most interesting feature of the phase diagram F, η is that the critical forces, separating various intermediate stages during the forward transition, are *friction dependent*, except the first critical force, which corresponds to the transition from the completely locked stage. We may conclude that the kinetic energy of the system in the *preceding* stage defines the transition to the *following* stage.

First, let us consider the lowest interval of frictions, $\eta < 0.1\omega_x$, in the phase diagrams of Fig. 3. The explanation of the dependence of F_f on friction in this region can be done solely with the help of kinetic arguments. Assume the existence of a "critical" kink velocity v_c, above which the *running* kink cannot exist as a stable quasiparticle (such a critical velocity does exist for the running kinks in the frictionless case [17]). Then, at given values of the force F and the friction η, if the kink drift velocity $\langle v_k \rangle = F/m_k\eta_k$ is higher than v_c, the kink should destroy itself as soon as it starts to move: it will immediately cause an avalanche driving the whole system to the totally running state of atoms. In the phase diagram, the region (F, η), where the running kinks are stable, is bounded by the straight line $F \propto v_c\eta$, if one makes the additional assumption $\eta_k \sim \eta$; this simple linear dependence (the dotted line in Fig. 3) is in agreement with the $F_f(\eta)$ data for $\eta < 0.1\omega_x$. Thus, for $\eta < 0.05\omega_x$, when the applied force exceeds the threshold F_{tk}, the stationary drift velocity for the kink is higher than v_c and the system goes directly to the running state of atoms, and $F_f = F_{tk} =$ const in this region. However, at $\eta > 0.05\omega_x$, the kink can move as a stable quasiparticle and the transition to the running state takes place at a higher force $F_f \propto \eta$.

At higher frictions, $\eta > 0.1\omega_x$, F_f starts to deviate significantly from the simple linear law and finally tends to a constant value F_f^*. This behavior may be qualitatively explained if we take into account that the *running* kinks stimulate the transition of the system to the totally running state. Indeed, owing to their nonzero kinetic energy T_{kink}, the running kinks effectively reduce the average energy barrier for the transition of all the atoms to the running state; therefore the effective barrier ε_{eff} should be lower than ε_{sx}. Let us approximate the effective barrier as $\varepsilon_{eff} = \varepsilon_{sx} - T_{kink}$, where $T_{kink} \propto \langle v_k \rangle^2 \propto F^2/\eta^2$. Then, the critical force for the transition to the running state, $F_f = C\pi\varepsilon_{eff}/a_{sx}$, is determined by the following equation,

$$\frac{\alpha}{\eta^2}F_f^2 + F_f = F_f^*, \tag{4}$$

where $\alpha > 0$ is a phenomenological coefficient and $F_f^* \approx F_{f0} \equiv C\pi\varepsilon_{sx}/a_{sx}$. Eq. (4) provides a qualitative agreement with the simulation data: at small η, the forward force $F_f(\eta) = \eta\sqrt{F_f^*/\alpha}$ is proportional to η, while at $\eta \to \infty$ we have $F_f \to F_f^*$. This asymptotic forward critical force F_f^* has been found equal to the critical force for a single atom $F_{f0} = C\pi\varepsilon_{sx}/a_{sx}$ because the dimensionless elastic constant $g_{eff} = a_{sx}^2 V_{int}''(a_A)/2\pi^2\varepsilon_{sx}$ is well below unity. Therefore, the interaction between atoms should not lead to a significant change of the barrier for the transfer of one atom to the running state unless the running kinks contribute to this transition.

This qualitative picture holds also for other intermediate critical forces, and for a more complex atomic coverage like $\theta = 21/31$. In this case (it is described in detail in [18]), the state of running *trivial* kinks is preceded by the state of running *superkinks*, which leads to the dependence of F_{tk} on friction, due to the contribution of kinetic energy of superkinks [18].
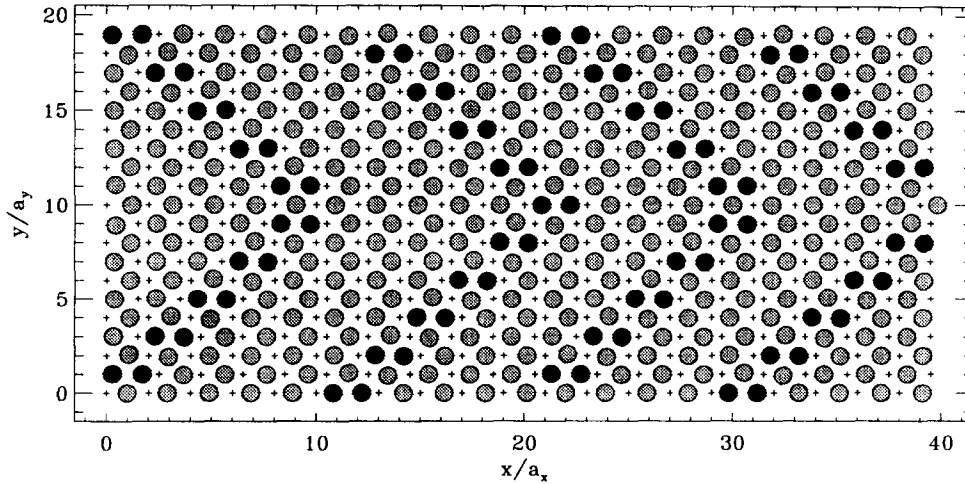
Fig. 4. Atomic configuration with a domain wall of "light" kinks at the $\theta = 21/40$ coverage with *triangular* symmetry of the minima of the external potential (atoms are denoted with gray circles, atoms in the kink regions are denoted with black circles, minima of external potential are denoted with crosses). $M_y = 20$, $M_x = 40$ and $N = 420$.

4. Isotropic FK model with triangular symmetry

Let us consider now the two-dimensional array of atoms placed on a periodic substrate with minima situated on a triangular lattice. To allow some comparisons with the anisotropic rectangular FK model, we have chosen the background coverage $\theta_0 = 1/2$, whose minimum energy configuration was found [19] to be the c(2×2) structure (see Fig. 4). In the 2D case, this structure allows for the existence of different types of kinks in domain walls (DWs). For instance, if the center of a kink in one row is placed in front of an occupied (resp. empty) site in the neighboring row, we will call it a "light" (resp. "heavy") kink. The label is chosen according to the respective rest energies of these two types of excitations. Starting from the minimum energy configuration containing only DWs of "light" kinks illustrated in Fig. 4, we studied the nonlinear mobility in response to an external force F applied along the x direction.

The $B(F)$ dependences plotted in Fig. 5 for two generic values of the friction constant $\eta = 0.15\omega_0$ and $\eta = 0.35\omega_0$ show quite interesting behavior. There exist several intermediate regimes of the mobility between the locked state $B = 0$ and the running state $B = 1$. For the lower friction case, at $F_k \approx 0.18F_{f0}$, one can observe a sharp increase of the mobility whereas, surprisingly, at $F_d \approx 0.26F_{f0}$, the system goes back to a locked state $B = 0$. A nonzero mobility reappears again at $F > F_{\text{pair}} \approx 0.32F_{f0}$ and, one can also observe the existence of a weak "shoulder" in the $B(F)$ dependence. Finally, at $F_f \approx 0.4F_{f0}$, the system goes to the totally running state with $B = 1$. From the other hand, at a higher friction $\eta = 0.35\omega_0$, one can see two clear-cut intermediate plateau in the $B(F)$ dependence: one at $F_k < F < F_{\text{pair}}$ (where $F_{\text{pair}} \approx 0.4F_{f0}$) with the mobility $B \approx 0.2$ and, the second in the interval of forces $F_{\text{pair}} < F < F_f$ ($F_f \approx 0.75F_{f0}$) where the mobility is $B \approx 0.5$; the intermediate *locked* state with $B = 0$ does not appear at this higher friction.

A visual examination of the atomic configurations (see Fig. 6) clearly reveals the nature of the complex atomic motion at the intermediate stages. Fig. 6(a) shows the typical atomic configuration at the first intermediate plateau of the mobility at $F_k > 0.18F_{f0}$. The atoms in the body of c(2×2) are immobile and, they perform slip-stick motion only in the regions of DWs. Therefore this plateau is characterized by the running state of the "light" DWs. Consequently, the critical force F_k can be interpreted as the force at which Peierls–Nabarro barrier for the translation
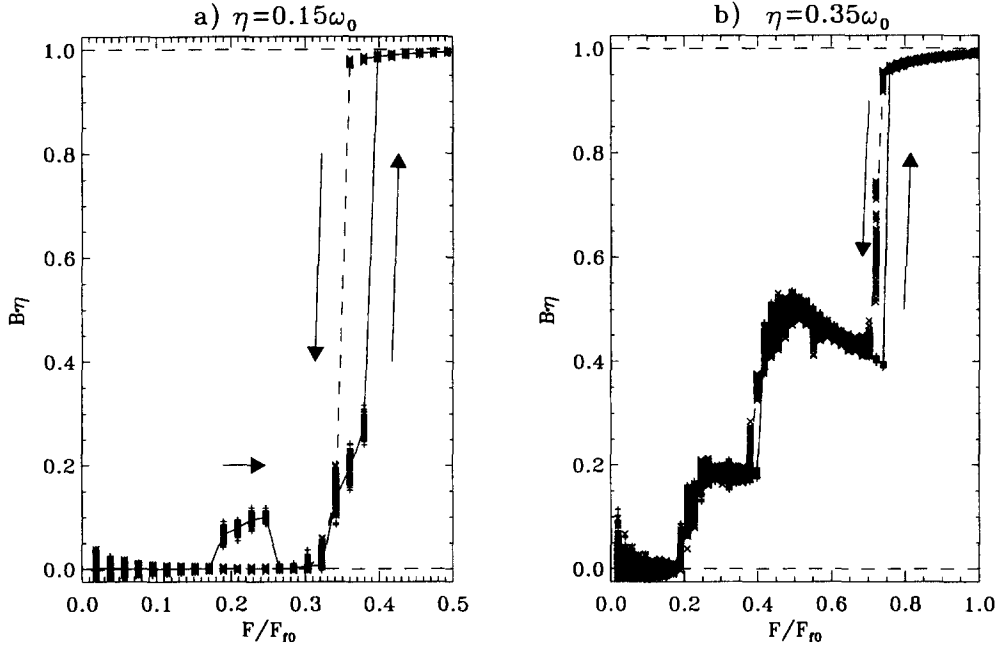
Fig. 5. The mobility B versus external force F for the triangular FK model at the $\theta = 21/40$ coverage. F is in the units of the constant "forward" critical force for a single particle $F_{f0} = \pi\varepsilon_{sx}/a_{sx} \approx 0.527$.

of these DWs has vanished. Moreover, it is interesting to notice that initially tilted (relatively to the direction of the applied force), the domain walls line up perpendicularly to the applied force during their motion.

With a further increase of the applied force the velocity of running DWs also increases and at a critical force F_d, the domain walls become unstable and *destroy* themselves. This results in the *disordering* of the whole system, which loses the c(2×2) structure (see Fig. 6(b)) and goes to a disordered state with zero mobility since the concerted regular atomic motion (running kink DWs) is no longer possible. We emphasize that this state is a *metastable* state (it can be checked by performing "backward" runs, i.e. reducing force to $F = 0$ starting from the disordered locked state of Fig. 6(b)). It is instructive to remind the famous "frustration" problem for the triangular *lattice-gas* (or Ising) model at coverage $\theta_0 = 1/2$ (see e.g. [20] and references therein). Indeed, if the repulsion of adatoms in the lattice-gas model is restricted to nearest neighbors, the ground state at $\theta_0 = 1/2$ is disordered and infinitely degenerated. However, in the continuous model and for a larger range of the interatomic interaction, the ordered ground state does exist (the c(2×2) structure in our case), but is probably still surrounded by metastable disordered "neighboring" states in the energetic spectrum. Thus, with the increase of the force, when the total energy of the system increases due to the kinetic energy of running DWs, the system can be trapped in such a metastable state. By contrast, at a higher friction $\eta = 0.35\omega_0$, the drift speed of domain walls is lower and they can exist in the stable *running* state until the critical force F_{pair} corresponding to a switch to another specific kind of slip-stick motion.

The atomic motion at the next intermediate stage $F_{pair} < F < F_f$ is illustrated in Fig. 6(c). The atoms can move not only in the region of the domain walls, but also in the body of c(2×2) structure. Therefore, similarly to the "traffic jam" regime in the case of the quasi-one-dimensional rectangular FK model (Fig. 2(b)), this picture can be interpreted as the creation of kink–antikink pairs ("light" kinks) inside the c(2×2) structure. At an instant of time, only *half* of the atoms in a single c(2×2) domain are able to move for $F > F_{pair}$; e.g. moving atoms, situated in the
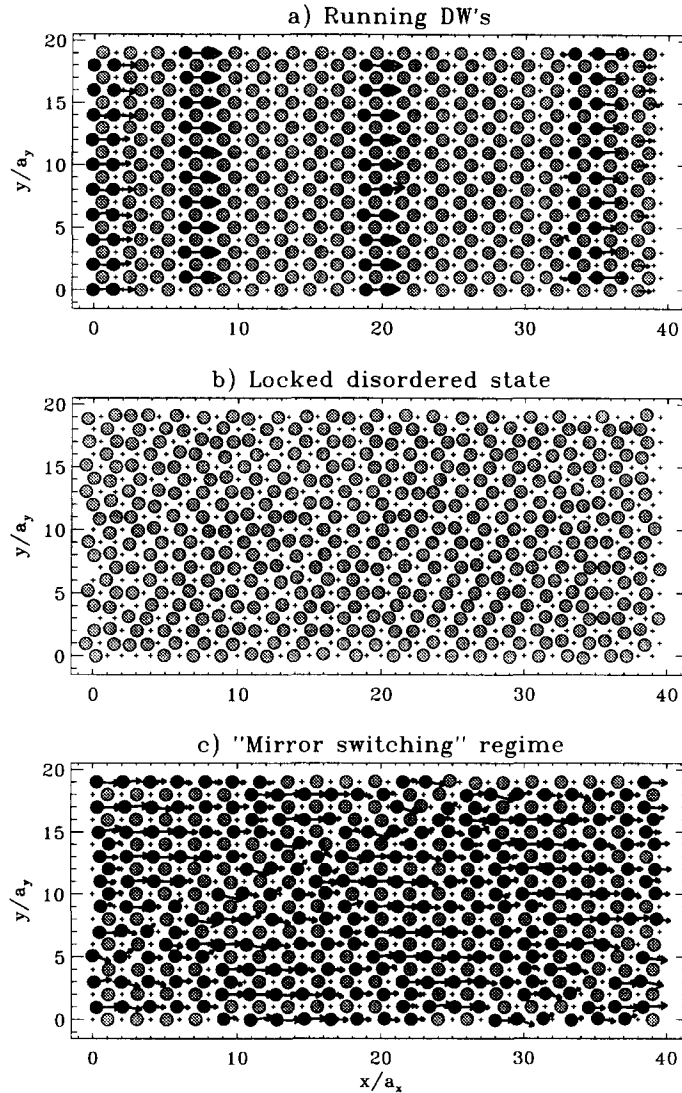
Fig. 6. Atomic patterns at the intermediate stages of the $B(F)$ dependences plotted in Fig. 5: (a) regime of running domain walls; (b) locked disordered state; (c) "mirror switching" regime. Immobile atoms are denoted with gray circles, running atoms and atoms in the kink regions are denoted with black circles, arrows indicate the direction of atomic motion.

center of the c(2×2) unit cell, belong to even rows (Fig. 6(c)). These atoms can move to the neighboring sites inside their cells, changing the symmetry of the given c(2×2) domain to its mirror image. The complementary sublattice is then able to move in the same way reverting its structure to the previous symmetry. This regime can therefore be represented as a periodic change between the two mirror images of a c(2×2) domain; we call it as a "mirror switching" regime (Fig. 6(c)). As roughly half of the atoms are moving, the value of the mobility is $B \approx 0.5$ in this regime. One should also note that, even at $F < F_{pair}$, when an *existing* single DW passes by a given c(2×2) domain (Fig. 6(a)), it also changes the mirror symmetry of this domain. However, at $F > F_{pair}$, the atomic motion can be represented as a spontaneous nucleation of the two possible islands ("odd rows immobile/even rows mobile"-island or vice-versa) inside the background structure with the subsequent coalescence of these islands. Because of the

coalescence process, one can observe a slight decrease of the mobility with force (or simulation time) increasing (see Fig. 5(b)). Indeed, when the size of such islands increases, the number of *completely* locked atoms inside the islands increases too, since at the boundaries between islands (their number decreases during coalescence) all the atoms are rather moving than locked. Of course, the "mirror switching" regime is observed also for initial configuration without kinks, i.e. for the coverage $\theta_0 = 1/2$.

The dynamical phase diagram F, η for the triangular system will be presented elsewhere [19]. Here we emphasize that similarly to the rectangular case, the intermediate critical forces F_f, F_d, F_{pair} are found to be friction-dependent namely they grow approximately linearly with friction η (at the same time the "first" force $F_k = $ const), which confirms our conclusion, that the critical quantity for the dynamical transitions studied is the *velocity* of kinks (or domain walls). In particular, in the friction interval $0.1\omega_0 < \eta < 0.2\omega_0$ the relation $F_k < F_d < F_{pair}$ is fulfilled, leading to the existence of the non-monotonic dependence $B(F)$.

5. Conclusion

In summary, we have studied the dynamical phase transition from the locked to the running state of interacting atoms in a periodic external potential under the action of a dc external force in the underdamped limit of a generalized Frenkel–Kontorova model. This transition proceeds by a complex multi-step scenario, which can be treated as a hierarchy of depinnings of quasiparticle excitations of the FK model (kinks). The interesting feature of the transition is that the critical forces separating different intermediate stages during the "forward" transition are friction dependent, except the first critical force which corresponds to the transition from the completely locked ground state. This reflects the dynamical nature of transitions between intermediate stages, i.e. the main role of the kinetic energy of running kinks for the transition towards the *following* stage.

On the basis of simulation results, we have proposed a phenomenological approach which qualitatively explains the observed friction dependences of the critical forces. According to this approach for low frictions, the critical quantity determining the criterion for the transition to the totally running state of atoms is the drift velocity of kinks at the preceding stage. This approach leads to the simple phenomenological equation (4) for the dependence of the forward critical force on friction. However, for a quantitative description of the simulation results, one has to take into account the resonant interaction of the running kinks with the phonon bath [17,21]. Work along this line is in progress.

We have studied two distinct shapes of the periodic external potential: one is a highly anisotropic (quasi-one-dimensional) potential with a rectangular symmetry of minima, and the other is an isotropic potential with triangular symmetry. For the first one, the generic scenario corresponds to the staircase-like growth of the mobility with the increase of the external force. By contrast, the case of the triangular external potential gives rise to an interesting novel feature of the dynamical phase transition studied. Namely, the mobility can vary *nonmonotonically* with increasing force. Indeed, after the intermediate regime of running DWs with $B \neq 0$, the system can be then trapped in a metastable disordered immobile state ($B = 0$) due to the destruction of the running domain walls of kinks when they reach a critical speed. Finally, we observed for the case of the triangular potential new specific slip-stick stage, called "mirror switching" regime.

Acknowledgements

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