Impurity-kink interaction in the two-dimensional Frenkel-Kontorova model

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The dislocation gliding in crystals with impurities is investigated by computer simulations for the two-dimensional Frenkel-Kontorova model. It is shown that the impurity-dislocation interaction can result in both the stimulation of the double-kink formation (which increases the dislocation mobility) and the trapping of moving kinks by the impurities with the following kink-antikink recombination (which slows down the dislocation motion). The relative importance of these competing mechanisms depend mostly on the temperature as well as the type of impurity. Here we demonstrate that the presence of impurities can increase the dislocation velocity at low temperatures which leads to the solid solution softening. With increasing temperature, a transition from the solid solution softening to the solid solution hardening regime takes place.

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I. INTRODUCTION

The dislocation mobility in crystal lattice periodic potential (the Peierls relief[1]) is one of the key problems in solid state physics which still attracts considerable interest. The Peierls mechanism determines the dislocation mobility and, consequently, the mechanical behavior in covalent crystals (Si, Ge), bcc metals, and some intermetallic compounds. Despite considerable theoretical and experimental efforts[2,3] the microscopic processes which are responsible for the dislocation mobility in the Peierls relief are still a matter of intensive discussions.[4–9]

It is commonly accepted that the dislocation motion in materials with high Peierls relief is accomplished by the propagation of kinks along the dislocation line. It has been assumed that the kink density (and, consequently, the dislocation mobility) is determined by the processes of thermal fluctuation kink nucleation and of the kink-antikink pair recombination. However, this very transparent but simplified concept is insufficient to describe the mechanical properties of real materials[2,3] where the impurity-kink interactions play a crucial role in the kink dynamics. Standard models considering the impurities just as centers of kink-antikink recombination processes[2] seem to be inadequate and do not explain accumulated experimental data.[3,8,10,11] The contradictions between the theoretically predicted equilibrium density of the kinks and that estimated from experimental data initiates a hypothesis regarding the existence of so-called "weak obstacles" controlling the equilibrium density of kinks, however, the nature of these obstacles has not yet been clarified.[3]

The effect of impurities on the mechanical properties of the crystals is rather complex and cannot be reduced only to the deceleration of kinks or to the initiation of their annihilation as it was supposed in the earlier models.[2] In particular, besides the well-known effect of the solid solution hardening (SSH) which is clearly connected with the pinning action of the impurities on the dislocations, in some cases the alloying leads to the opposite phenomenon which is known as the solid solution softening (SSS). For example, the doping by Ga decreases the dislocation mobility in Ge, whereas the doping by As, on the contrary, increases it.[12] The SSS effect is well known for bcc transition metal alloys[13–17] and was also observed in intermetallics[18] and ceramics spinel.[19] It has been demonstrated experimentally in Ref. 14 that the SSS is observable in a low temperature region; with the temperature increase the transition from the softening to the hardening occurs.

It is a common view that the SSS effect results from the enhanced kink nucleation at point defects.[14,20,21] However, the microscopic mechanism of this phenomenon still remains a matter of discussion. In particular, it is not clear why SSS was observed for some additions and not for others and why this effect is dominant in comparison with the usual pinning mechanism. Also, it is not clear what is a specific scenario of the transformation from the SSS phenomenon to the SSH one with the temperature increase.

Despite the recent developments of powerful atomistic simulation techniques, the investigation of kink dynamics and impurity-dislocation interactions is still a difficult problem for theoretical materials science due to the involvement of essentially different space scales—microscopic (for atoms in the dislocation core) and macroscopic (for the long-range elastic fields). Therefore, model investigations of the kink dynamics are helpful. The first attempts of the direct numerical simulations of the kink dynamics without impurities were made in Refs. 9, 23, and 24 in a framework two-dimensional (2D) Frenkel-Kontorova (FK) model. As was shown in Ref. 9, in contrast with traditional assumptions, the kinks on the dislocations can behave like solitons and pass through each other without annihilation in spite of thermal fluctuations and damping. The impurity-kink interaction was considered in a framework of a one-dimensional (1D) FK model[22] and also reveal an important role of dynamic effects in this process, but have not clarified an issue on the double kink nucleation.

Here we investigate the mechanism of the kink-impurity interaction and the effect of this interaction on the steady-state dislocation velocity by the computer simulations for a generalized 2D FK model.[9,23,24] This model allows us to de-

scribe adequately the kink behavior for the values of applied stress and temperatures corresponding to low enough dislocation velocity, that is, much smaller than the sound velocity. We demonstrate that within this model approach both the softening and strengthening of chemical bonds impurities enhance the double kink nucleation and that softening may be replaced by hardening with the temperature increase due to interplay of the kink nucleation and kink trapping processes.

II. FORMULATION OF THE MODEL

Similar to Refs. 9, 23, and 24, we study the dislocation dynamics with the 2D FK model where a layer of atoms interacting by elastic forces put into a periodic potential relief. The potential energy of this system has the following form:

$$\Phi = \frac{k}{2}\sum_{n,m}(\mathbf{u}_n - \mathbf{u}_m)^2 + P\sum_n \sum_{\mathbf{g}} [1 - \cos(\mathbf{g}\mathbf{u}_n)], \qquad (1)$$

where k is the stiffness of interatomic bonds, the sum in the first term is taken over all pairs of the nearest neighbors, $\mathbf{u}_n$ is a displacement vector of the nth atom from its equilibrium position, $\mathbf{g}$ is the three smallest vectors of the reciprocal lattice {we will consider the hexagonal lattice with a parameter $a=1$, then $\mathbf{g}_1=(4\pi/\sqrt{3})(-1,0)$, $\mathbf{g}_{2,3}=(4\pi/\sqrt{3})[\frac{1}{2}, \pm(\sqrt{3}/2)]$}.

In order to consider both the damping and the thermal fluctuations, we introduce the thermal bath using the method of the Langevin equations of motion[25]

$$M\ddot{\mathbf{u}}_n = -\frac{\partial \Phi}{\partial \mathbf{u}_n} - \gamma \dot{\mathbf{u}}_n + \xi_n(t) + \mathbf{f}_n, \qquad (2)$$

where M is an atomic mass, γ is a friction coefficient, $\mathbf{f}_n$ is an external force assumed to be equal for all 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 parentheses indicate averaging over the realizations of random process $\xi_n(t)$. To integrate the stochastic differential equations (2), we use a so-called "strong" mean-square Runge-Kutta type method of the 3/2 order[26] which provides an accuracy of the calculations for individual trajectories as well as for average characteristics (for details see Ref. 9). Despite its oversimplicity, the model defined by Eqs. (1) and (2) allows us to process the nucleation of the kinks and their propagation along the dislocation.[9,23]

Here, we consider the effects of immobile substitution impurities on the dislocation motion; this case corresponds to low temperatures ($T<0.5T_m$, where T_m is the melting temperature) when the diffusion of dopant atoms can be neglected. The impurity atom at the point $\mathbf{R_0}=0$ was introduced by three different ways: (i) by change in the spring stiffness between the node $\mathbf{R_0}$ and its nearest neighbors, $k' \neq k$, (ii) by variations in the amplitude of the substrate potential P, and (iii) by the addition of the impurity potential

$$\Phi_{\text{imp}}(\mathbf{R_{0n}}) = Q\exp\left(-\frac{R_{0n}^2}{2\sigma}\right) \qquad (3)$$

to Eq. (2), where σ is a parameter, varied from 0.1 to 8. For simplicity we assume that the impurity atom has the same mass as the host ones.

In a framework of Fleischer's continuum elasticity approach[27] describing the impurity-kink interaction effects in terms of the size and modulus mismatch between the solute and host atoms, the variation of the spring stiffness $\delta k=(k'-k)/k$ corresponds to a local variation of the elastic modulus in the vicinity of the impurity.[28] In general, the chemical bonding effect in the impurity-dislocation interaction cannot be reduced to a local change of elastic moduli ($\delta k \neq 0$), but also modify a substrate potential. This effect has been recently considered by *ab initio* calculations.[29] The impurity effect on the substrate potential δP simulates the change of the chemical bonding, which cannot be reproduced in terms of linear elasticity theory. Besides that, the potential Φ_{imp} allows us to take into account an additional mechanism of the interaction which is essentially different from those described above.

The most important parameter in the model (1) and (2) is the ratio of the height of potential relief P to the stiffness constant k. We set $k=1$ (which determines the energy units as ka^2) and choose $P \approx 0.1$ when, for a small displacement $\mathbf{u}$, the forces of atomic interactions with the neighbors and with the substrate layer are comparable. This ratio of parameters leads to the dislocation with the core width $\lambda \sim 1$. The time unit corresponds to $2\nu^{-1}$, where $\nu=2\sqrt{k/M}$ is a characteristic local vibration frequency. The temperature T varied over a wide range from 10^{-3} to 2×10^{-2}, i.e., it was of the order of $(0.1/0.01)P$ (according to our simulations the melting temperature T_m for this model is about 5×10^{-2}). A damping parameter γ (in dimensionless units defined above) is of the order of the ratio of phonon damping to phonon frequency. We have chosen $\gamma=0.08$ which corresponds to typical values for metals at room temperatures,[30] $\gamma=0.1/0.01$. We did not take into account the temperature dependence $\gamma(T)$ since the latter does not essentially change the results as is shown in Ref. 9.

For numerical simulations, a 2D crystallite containing 80×80 atoms with periodic boundary conditions was used. Previously, it was shown that even for a smaller crystallite (40×40 atoms) the effect of the periodic boundary condition is negligible. In particular, the chosen value of γ provides a strong attenuation of the lattice vibrations on the length of crystallite and therefore eliminates its possible overheating. Besides, the deformation produced by the dislocations in FK model decays exponentially at large distances and therefore a long-range part of the elastic fields due to "mirror" dislocations may be ignored. The 80×80 atomic crystallite used here is sufficient to reveal statistical regularities in the kink dynamics. We have checked that further increase of its size (from 80×80 to 100×100) does not lead to any essential change of the results. Due to the periodic boundary conditions the dislocation passing out the boundary of the crystallite returns to it through the opposite boundary. These multiple runs of the dislocation are essential to determine the

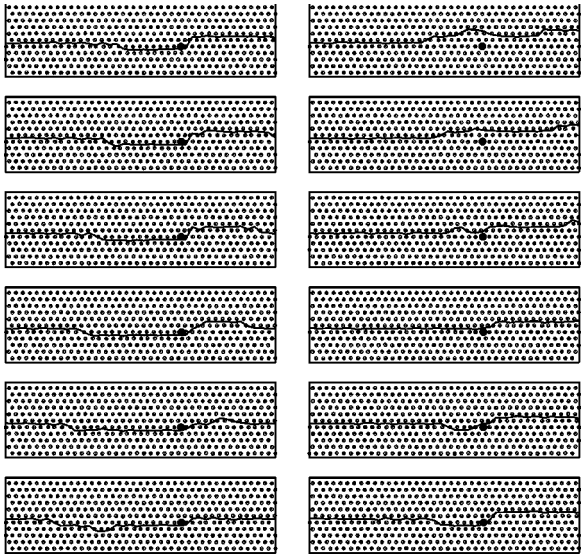

FIG. 1. Pinning (left column) and subsequent passage (right column) of kinks through the impurity simulated by the change of the stiffness $\delta k=-0.5$, $T=0.0075$, $f=0.265$. The consequent snapshots of the central part of 80×80 crystallite correspond to $t=60$, 62, 64, 66, 68 (left column, from bottom to top), 70, 72, 74, 76, 78, 80, and 82 (right column, from bottom to top). The position of the dislocation line is defined by the condition $|u_y|=0.5b$ (i.e., as a center of the displacement profile).

steady-state velocity. We have chosen the time step $\Delta t=0.01$; in this case the accuracy of the calculations for trajectories as well as of Gibbs distribution at the equilibrium appeared to be restricted only by the Monte Carlo inaccuracy.

At the initial moment the screw dislocation with Burgers vector $\mathbf{b}=(0,1)$ and the axis parallel to Oy was introduced in the crystallite by specifying the displacements $\mathbf{u}_n(0)$ in accordance with the known solution for the continuum limit of the 1D FK model,[28]

$$u_x=0, \quad u_{ny}=\frac{2}{\pi}\left\{\frac{\pi}{2}-\tan^{-1}\left[\exp\left(-\frac{x_n}{\lambda}\right)\right]\right\}. \qquad (4)$$

Then the equations (2) were integrated numerically at a given temperature T and $\mathbf{f}_n=0$ for a rather long time ($t\sim 10^2$) to reach the equilibrium configuration of the dislocation. After that, an external force $\mathbf{f}=(0,f_y)$, which is of the order of $0.2-0.3f_P$ was applied, f_P being the limiting value corresponding to the Peierls stress.

III. KINK-IMPURITY INTERACTIONS

Initially, in our simulations the dislocation was introduced in the lattice far enough from the impurity and started its motion after thermal fluctuation nucleation of the kink-antikink pairs, similar to what was observed in Refs. 9 and 23. A typical picture of the kink-impurity interaction for $\delta k<0$ and $\delta P=0$, $Q=0$ (linear kink-impurity coupling) is shown in Fig. 1. In this case the kink loses its mobility being captured by the impurity. For sufficiently small δk the thermal fluctuations can release the kink out of the potential well. At large δk the process of the dislocation depinning is stimulated by the annihilation of the kink trapped by the impurity with antikink, and the impurity happens to be behind the dislocation (Fig. 1, right column).

Earlier we demonstrated that in the 2D FK model without impurities, the kinks and antikinks do not annihilate, as a rule, at the collisions, but pass through each other similar to the sine-Gordon solitons.[9] As we have shown here, the bond weakening impurity with $\delta k<0$ turns out to be a natural center of the kink-antikink recombination. Thus, the interaction between kinks and weakening impurities lead to the decrease of the dislocation mobility due to both kink pinning and enhancement of the kink-antikink annihilation and manifests itself in the SSH.

In the opposite case when $\delta k>0$ we have not observed the pinning of kinks by impurities. This difference in the interaction of the kink with bond weakening and hardening substitute atoms cannot be understood in terms of the variation of the kink effective potential due to impurity[22] or in continuum elastic models.[2] Indeed, in these models the pinning action of the impurity occurs for the cases of both attraction (the trapping on the impurity) and repulsion (the trapping before the impurity). According to our computational results, it seems that the kink pinning occurs for the bond weakening impurity ($\delta k<0$) and does not occur in the opposite case. One can assume that the increase of the kink mobility with strengthening interatomic bonds ($\delta k>0$) results from a lowering of the secondary Peierls relief (i.e., the energy profile for the kink motion), due to a reconstruction of the kink structure near the impurity. It is discussed below in Sec. V in more details.

An initiation of the double kink nucleation by impurities is another previously unknown feature found in our simulations. This process is illustrated in Fig. 2 where the dislocation was initially put near the impurity and then started to move after the nucleation of the kink-antikink pair. In our simulations, the double kink nucleation was found both for the bond weakening impurities (in accordance with the suggestion of Ref. 20), and for the bond strengthening one (Fig. 2) which looks rather surprising.

We have found that the variations of the substrate potential, δP, only (keeping $\delta k=0$ and $Q=0$) has a different effect on the impurity-kink interaction than the stiffness variation. We have observed both the kink trapping for $\delta P>0$ and the initiation of the kink nucleation for $\delta P<0$. These results are in agreement with the suggestion[20] that a weakening of interatomic bonding by impurity should enhance the double kink nucleation due to a lowering of the Peierls relief.

The modification of the substrate potential according to Eq. (3) stimulates the nucleation of kink-antikink pairs near the impurities independently on the sign of Q (Fig. 3). In this case we have not observed the kink pinning, even for small σ when the perturbation of substrate potential $\Phi_{\mathrm{imp}}(\mathbf{R})$ is strongly localized near the impurity and the corresponding forces $-\nabla\Phi_{\mathrm{imp}}$ acting on the kinks are the largest. Despite the absence of the kink trapping the deceleration of the kinks by the potential Φ_{imp} is well pronounced and it is stronger for smaller σ.

It is important to stress that the decelerating effect of impurities on the dislocation motion is not reduced to the kink

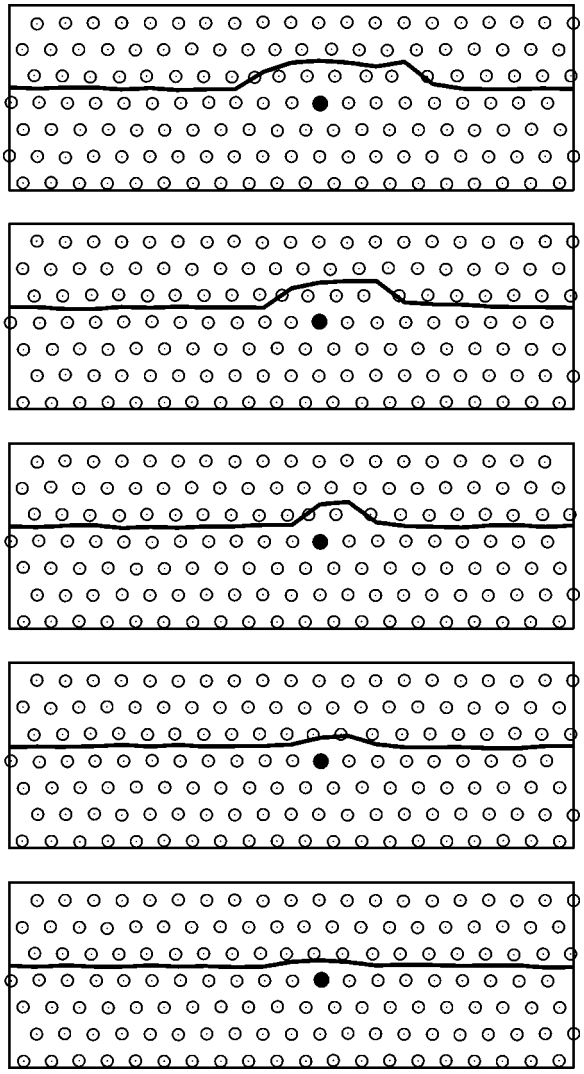

FIG. 2. Dislocation release from the impurity simulated by the change in the stiffness ($\delta k=0.5$) with the formation of the kink-antikink pair; $T=0.0075$, $f=0.265$. The consequent snapshots correspond to $t=35$, 36, 37, 38, and 39 (from bottom to top).

pinning processes, but is also connected with the slowing down of the kink motion which can occur at any signs of the impurity perturbation potential. Besides, the different processes of the impurity kink interaction discussed above are only clearly distinguished for low enough temperatures. With the temperature increase, the interplay between different mechanisms becomes important. To clarify the role of different contributions for different temperature ranges investigations of the dislocation dynamics in the crystallite with array of impurities are necessary. The corresponding results are described in the next section.

IV. DISLOCATION MOBILITY

To investigate the effects of impurities on the dislocation motion in a more quantitative way, we have calculated the temperature dependence of the steady-state dislocation velocity V both in the absence of impurities and for chaotically

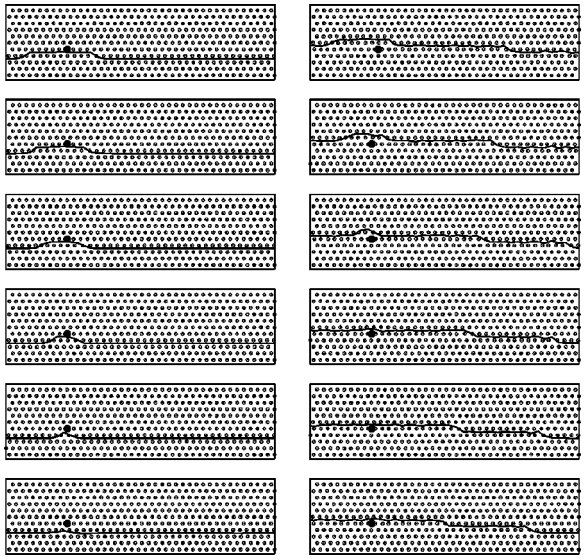

FIG. 3. Formation of double kinks on the impurity with the increase of the substrate potential, $Q=0.8$. Here $T=0.0075$, $f=0.265$, $\sigma=4$. The consequent snapshots correspond to $t=49$, 51, 53, 55, 57, 59 (left column, from bottom to top), 85, 87, 89, 91, 93, and 95 (right column, from bottom to top).

distributed ones (from 20 to 60 impurities in 80×80 crystallite). The value, V, has been determined from the time dependence of the total atomic displacement $u_y(t)$ along the Burger vector, $u_y=\Sigma_i u_y^{(i)}$. The value u_y characterizes the plastic deformation in the crystallite accumulated during dislocation motion. After the finishing of transient processes, with the kink density increase, the dependence $u_y(t)$ reaches a linear-in-time stage that allows us to determine a steady state dislocation velocity as $V=L_y^{-1}du_y/dt$. One should note that the steady-state motion of the dislocation within the model under consideration depends mainly on a propagation of multiple kinks which is accompanied by relatively rare nucleation and annihilation processes. We found that the multiple kinks, in contrast with the solitary ones,[9] can annihilate during collision processes that provides the equilibrium kink density. In this case the, dislocation is high ($V\sim0.1-0.4c$, where the sound velocity c is equal to 1) and effects of impurities are no longer dominant. However, for smaller velocities the kink-impurity interaction is really of crucial importance.

Computational results are shown in Fig. 4. The shape of the $V(T)$ curves for the crystallite with impurities (dashed line) is similar to that without impurities (solid line). One can see that in all cases the presence of impurities leads to an increase of the dislocation velocity (i.e., results in the solution softening) at low temperatures ($T<0.01$). This means that the effect of impurities on the kink-antikink pair nucleation dominates in comparison with the deceleration of kinks even for $\delta k<0$. With the increase in T the effect of impurities on the dislocation velocity practically vanishes for $\delta k>0$ or $\delta P<0$ and at $\delta k<0$ or $\delta P>0$ the velocity of dislocation decreases. In the latter case, a transition from softening to hardening action of impurities occurs as the temperature increases.

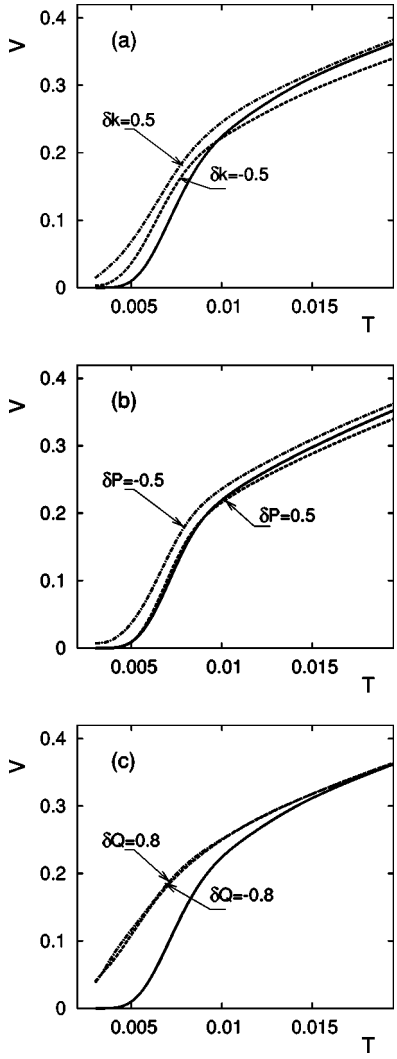

FIG. 4. Temperature dependence of the dislocation velocity at $f=0.265$ averaged over the ensemble of 40 impurities changing the stiffness of bonds δk (a), of the substrate potential δP (b), or Φ_{imp} (c). Solid curve corresponds to the crystallite without impurities.

The temperature dependence of the impurity effect on the dislocation mobility looks rather natural. Indeed, at low temperatures the thermal equilibrium kink concentration is not high enough and the influence of impurities on the rate of nucleation of new kinks is more essential than the decelerating effect on the mobility of existing kinks. This conclusion is confirmed by an increase of the dislocation velocity with impurity concentration for the low temperature region (Fig. 5). With temperature increase, the density of the thermal equilibrium kinks multiply exponentially and the interaction of the impurity with propagating kinks becomes the most important factor in determining the dislocation mobility.

V. DISCUSSION AND CONCLUSIONS

The interaction of the kinks with impurities play a crucial role in the dislocation dynamics and, correspondingly, in mechanical properties of alloys with high Peierls barriers. The present conception of the dislocation-impurity interaction is

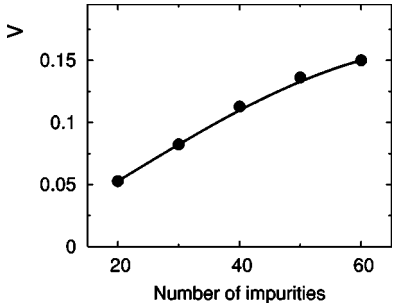

FIG. 5. Dependence of the steady state dislocation velocity on the number of impurities; $T=0.005$, $f=0.265$, $\delta k=0$, $Q=0.8$.

based on the following intuitive ideas summarized in Refs. 2 and 31: first, kinks can be trapped by any kind of impurities and, second, the impurities weakening interatomic bonds facilitate the double kink nucleation. However, as was mentioned above, this concept is not sufficient to explain some recent experimental results.[3,8,10,11] This discrepancy is connected in part with using Fleischer's continuum elasticity theory of the impurity-dislocation interaction which is not reliable enough if the solute atom is inside the dislocation core—exactly where the strongest interaction occurs. Besides, the current concept assumes the quasistatic picture of the impurity-dislocation interaction and ignores dynamic effects which may be important in both kink propagation and nucleation processes.[9,23]

Earlier investigations of the microscopic mechanisms of kink-impurity interactions have been carried out (for review, see, e.g., Ref. 22) in a framework of theory of nonlinear chains (1D FK model). It has been shown that in the one-dimensional case three essentially different scenarios are possible: (i) kinks can pass through the impurity, (ii) they can be reflected by the impurity, and (iii) they can be trapped by the impurity due to a formation of the resonance state between kink (soliton) and a localized breather. These results have demonstrated a complexity of the kink-impurity interaction. At the same time, an applicability of 1D dynamic models to the real kinks is questionable.

Our simulations of the dislocation dynamics in the framework of the 2D FK model at finite temperatures have revealed new important features of the impurity-kink interaction effects. First, for the parameters considered of the model, the presence of impurities results in an enhancement of the kink-antikink pair nucleation for all types of impurities. Although the magnitude of this effect depends on the character of the lattice perturbation near impurities, up to intermediete temperatures the mechanism of the heterogeneous nucleation is dominant (see Fig. 4). On the other hand, the decelerating effect of impurities on the kink mobility is very sensitive to changes in the interatomic bonds. The pinning of kinks occur only for impurities increasing the substrate potential ($\delta P>0$) or weakening interatomic bonds ($\delta k<0$).

An observation of the enhancement of double kink nucleation for both bond-weakening and bond-strengthening impurities is rather unexpected and contradicts an intuitive assumption that a reduction of the Peierls relief is necessary to increase the nucleation rate. This conclusion can be under-

stood on the basis of the results of simulations of double kink nucleation in 2D FK model without impurities.[23] According to Ref. 23, the double kink nucleation may be considered as an appearance of a crowdion-anticrowdion pair caused by an instability of phonon modes localized near the dislocation line. Obviously, a presence of bond weakening (strengthening) impurities stimulates the crowdion (anticrowdion) formation and kink nucleation.

Although this mechanism of double kink nucleation was found here within the 2D model, one can expect that it may be relevant for dislocations with nonsplit (compact) cores. At the same time, if one takes into account the fine structure of the dislocation, the nucleation scenario can change significantly. In particular, it was shown in Ref. 33 that in fcc based alloys where plastic deformation is provided by split dislocations an enhanced kink nucleation can be initiated by a doping which decreases the stacking fault energy and thus influences on the dislocation core structure.

A pinning effect for $\delta k<0$ and transition from the pinning of kinks to their passage through the impurity with δk increase are also not trivial. In particular, in the 1D FK model[22] the kink may be treated as a particle moving in an effective potential with the Peierls periodic part and with the perturbation due to impurity $U_{\mathrm{imp}}\sim \delta k/\cosh^2 y$, where y is the coordinate along the atomic chain. As a result, the kink will be trapped by the impurity independently on a sign of δk.

The observed behavior can be explained if one suggests that some changes in the kink width happens near the impurity which results in sharp variation of the secondary Peierls stress f_P^{II} (i.e., limiting stress for the kink propagation). An estimation of f_P^{II} in the framework of the 1D FK model[22] gives the following result: $f_P^{II}=2\pi^2/[\lambda \sinh(\pi^2\lambda)]$. Since the width of the kink $\lambda\sim\sqrt{k/P}$ [cf. Eq. (4)] decreases the stiffness k or increases the amplitude of substrate potential P leads to an exponential growth of the value f_P^{II} and in a qualitative modification of a character of impurity-kink interactions.

Note, that the effect of impurities on the kink shape is crucial for the kink mobility if the external force f is chosen in the interval $f_P^{II}<f<f_P$. In this case the dynamic regime in kink propagation is dominating; the kinks move with high velocity and are not sensitive to the lattice locking. The effect of impurities results in a relatively weak deceleration of the kinks in this regime. However, the picture changes drastically when the kink shape and, consequently, the secondary Peierls relief f_P^{II} change essentially during kink-impurity collisions.

An observation of the steady stage in the dislocation motion testifies that we reach an equilibrium kink density which is determined by competition between nucleation and annihilation processes. It it worthwhile to emphasize that we observed an annihilation during *multiple* kink-antikink collisions, whereas single kink and antikink pass through without annihilation, and in agreement with our previous simulations.[9] One can say that the steady-stage regime is provided by the thermofluctuation mechanism but, in contrast with traditional assumptions,[31] the motion of individual kinks is closer to the propagation of free particles than to a slow viscous process. This results in a relatively high dislocation velocity V which can be comparable with sound velocity c in our simulations. One should stress, however, that for $V>c/3$ and $T>0.02$ the results appear to be less reliable due to an essential lattice heating during the simulations. Therefore, we should restrict ourselves to the consideration of the region where the dislocation velocity is below $c/3$.

Based on the dependence of $V(T)$ presented in Fig. 4 two regions can be separated, low ($T<0.01$) and high temperatures, correspondingly. In the low-temperature region, the kink density is small and an appearance of new kink-antikink pairs result in a sharp increase of the velocity $V(T)$. At higher temperatures, when the thermal equilibrium kink density is comparable with the impurity concentration a decelerating effect of impurities on the kink mobility due to the pinning processes becomes dominant. One notes that the solid solution hardening turns out to be well pronounced only for $\delta k<0$, when the kink trapping takes place.

Of course, a simplified model considered here cannot describe all the details of the dislocation motion in alloys. First, this approach does not take into account the dislocation core structure (in-plane splitting in fcc metals or three-fold core structure in bcc ones) which may be important for the kink-impurity interactions.[32,33] Besides, the results of the calculations correspond to the dynamic regime of the kink motion whereas under real conditions a viscous kink propagation takes place. Nevertheless, one can expect that the results of our simulations reproduce some general features of the kink-impurity interactions which may be relevant for the SSS or SSH phenomena.

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[1] R. Peierls, Proc. Phys. Soc. London **52**, 34 (1940).
[2] H. Alexander, in *Dislocation in Solids*, edited by F. R. N. Nabarro (North-Holland, Amsterdam, 1986), Vol. 8, p. 115.
[3] K. Maeda and S. Takeuchi, in *Dislocation in Solids*, edited by F. R. N. Nabarro (North-Holland, Amsterdam, 1996), Vol. 10, p. 445.
[4] V. V. Bulatov and E. Kaxiras, Phys. Rev. Lett. **78**, 4221 (1997).
[5] B. Joos and M. S. Duesbery, Phys. Rev. Lett. **78**, 266 (1997).
[6] Yu. L. Iunin, V. I. Nikitenko, V. I. Orlov, and B. V. Petukhov, Phys. Rev. Lett. **78**, 3137 (1997).
[7] W. Cai, V. V. Bulatov, J. F. Justo, A. S. Argon, and S. Yip, Phys. Rev. Lett. **84**, 3346 (2000).

[8] Yu. L. Iunin and V. I. Nikitenko, Scr. Mater. **45**, 1239 (2001).
[9] Yu. N. Gornostyrev, M. I. Katsnelson, A. V. Kravtsov, and A. V. Trefilov, Phys. Rev. B **60**, 1013 (1999).
[10] V. I. Nikitenko, B. Ya. Farber, and Yu. L. Iunin, Zh. Eksp. Teor. Fiz. **93**, 1304 (1987) [Sov. Phys. JETP **66**, 738 (1987)].
[11] R. Jones and A. T. Blumenau, Scr. Mater. **45**, 1253 (2001).
[12] J. R. Patel and A. R. Chaudhuri, Phys. Rev. **143**, 601 (1966).
[13] R. Gibala and T. E. Mitchell, Scr. Metall. **7**, 1143 (1973).
[14] E. Pink and R. J. Arsenault, Mater. Sci. **24**, 1 (1979).
[15] A. Sato and M. Meshii, Acta Metall. **21**, 753 (1973).
[16] K. Okazaki, J. Mater. Sci. **31**, 1087 (1996).
[17] S. Nemat-Nasser and R. Kapoor, Int. J. Plast. **17**, 1351 (2001).
[18] H. Inui, K. Ishikawa, and M. Yamaguchi, Intermetallics **8**, 1131 (2000).
[19] T. E. Mitchell, J. Am. Chem. Soc. **82**, 3305 (1999).
[20] R. J. Arsenault, Acta Metall. **16**, 501 (1967).
[21] H. Suzuki, in *Dislocation in Solids*, edited by F. R. N. Nabarro (North-Holland, Amsterdam, 1979), Vol. 4, p. 1.
[22] O. M. Braun and Yu. S. Kivshar, Phys. Rev. B **43**, 1060 (1991); Phys. Rep. **306**, 1 (1998).
[23] Yu. N. Gornostyrev, M. I. Katsnelson, A. V. Kravtsov, and A. V. Trefilov, Phys. Rev. E **66**, 027 201 (2002).
[24] D. J. Srolovitz and P. S. Lomdahl, Physica D **23**, 402 (1986); P. S. Lomdahl and D. J. Srolovitz, Phys. Rev. Lett. **57**, 2702 (1986).
[25] V. G. van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdam, 1981).
[26] G. N. Milshtein, *Numerical Integration of Stochastic Differential Equations* (Kluwer Academic, Dordrecht, 1995); P. E. Kloden and E. Platen, *Numerical Solution of Stochastic Differential Equations* (Springer, Berlin, 1992).
[27] R. L. Fliescher, Acta Metall. **9**, 996 (1961).
[28] A. M. Kosevich, in *Dislocation in Solids*, edited by F. R. N. Nabarro (North-Holland, Amsterdam, 1979), Vol. 1, p. 33.
[29] O. Yu. Kontsevoi, Yu. N. Gornostyrev, A. J. Freeman, M. I. Katsnelson, and A. V. Trefilov, Philos. Mag. Lett. **81**, 455 (2001).
[30] V. G. Vaks, S. P. Kravchuk, and A. V. Trefilov, J. Phys. F: Met. Phys. **10**, 2105 (1980).
[31] E. M. Nadgorny, *Dislocation Dynamics and Mechanical Properties of Crystals*, in *Progress in Materials Science*, edited by J. W. Christian, P. Haasen, and T. B. Massalski (Pegamon, New York, 1988), Vol. 31, p. 1.
[32] M. Grujicic, Mater. Sci. Eng., A **183**, 223 (1994).
[33] T. E. Mitchell, P. M. Anderson, M. I. Baskes, S. P. Chen, R. G. Hoagland, and A. Misra, Philos. Mag. **83**, 1329 (2003).