Theory of Quantum and Polaron Effects in Depinning of Dislocation Kinks

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A microscopic theory is presented of stress-assisted fluctuational breakaway of dislocation kinks from pinning centers. It is shown that a polaron lattice distortion near a pinned kink essentially affects the magnitude of energy fluctuation required to activate a jump over the pinning barrier. The effect of quantum lattice fluctuations on the low-temperature depinning rate is analyzed. The role played by the kink geometric width in depinning phenomenon is disclosed.

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The study of kinks on dislocations has proved fruitful in theories [1] of plastic flow and strength of crystalline materials. Although various aspects of kinetic behavior of kinks in pure crystals have received considerable attention [2], much work needs to be done to clarify the situation where the kink motion is hindered by local pinning agents (such as solute atoms, impurity clusters, radiation damage, etc.). In this connection, understanding of microscopic mechanisms which control the breakaway of kinks from efficient pinning centers is of fundamental importance.

The phenomenological descriptions [3] of the depinning process rely on an assumption that in a wide range of temperatures T, a kink acted on by a stress τ less than the Peierls stress τ_P breaks away from its pin with an effective rate $\nu=\nu_0\exp[-E(\tau)/T]$, where ν_0 is a rather ill-defined attempt frequency, and $E(\tau)$ is the activation energy (we set $k_B=1$). As regards the stress dependence of $E(\tau)$, it is usually assumed that $E(\tau)=U_0-\nu\tau$, where the pinning barrier height at $\tau=0$, U_0, is decreased by the work $\nu\tau$ done by the stress, and ν is the activation volume of the process, maintained by environmental fluctuations.

One cannot escape the feeling that the aforementioned absolute reaction-rate formula gives an oversimplified description of the breakaway process for at least two reasons: Clearly, the Arrhenius behavior of the rate will no longer be valid at sufficiently low temperatures, when quantum environmental fluctuations are expected to dominate. Moreover, the explicit form of the activation energy involved tells one nothing about the physical mechanism by which the energy is supplied to the activated kink. As is known from the classical work of Eshelby [4], an effective mechanism of energy gain from lattice fluctuations is provided by the kink-phonon coupling. *A priori*, it seems possible that this coupling, if strong enough, may be able to cause an appreciable distortion of the host lattice near a pinned kink. If this is the case, then there is a good reason to suspect that such a polaron effect can essentially modify the simple phenomenological picture of the depinning process.

In view of all this, one concludes that environmental effects on depinning kinetics are only vaguely understood. In an attempt to clarify the situation we propose in this Letter a microscopic theory of the dislocation-kink depinning process. Our approach takes into account the coupling of the kink to phonons, the lattice distortions, and other pertinent processes that have not been appreciated in previous studies.

Consider for definiteness a kink of height a (the lattice spacing) in a parent *screw* dislocation with Burgers vector $\mathbf{b}=(b,0,0)$ directed along the dislocation axis chosen as the x direction. The well-known model [1,4] treats a kink as a one-dimensional quasiparticle constrained to slide along the straight dislocation line. A specific feature which distinguishes the kink from ordinary mobile defectons [5–7] in solids is its geometric width. In the isotropic continuum model of a crystal with elastic modulus G and host atom mass M, the width w of a continual kink ($w\gg a\sim b$) is related to its effective mass μ by [1,4] $w/a\sim M/\mu\sim(G/\tau_P)^{1/2}\gg 1$, if one assumes as usual that the dislocation line tension is $S\sim Ga^2$.

With this background relevant to the foregoing discussion, consider now a kink pinned down by a single, immobile pin located at $x=0$. Since the true interaction between the pin and the kink is not known, we construct a simple model in which an attractive pinning potential $U_{\rm pin}(x)$ is taken to be

$$U_{\rm pin}(x)=\begin{cases}-U_0+\frac{1}{2}\xi x^2, & |x|\le x_0,\\ 0, & |x|\ge x_0,\end{cases}\qquad U_0=\tfrac{1}{2}\xi x_0^2. \tag{1}$$

Here, x denotes the kink center-of-mass position on the dislocation line, the spring constant ξ characterizes the strength of the pin-kink interaction of range x_0, U_0 is the depth of the pinning well, and the zero of energy is taken at the bottom of the kink band [8]. The expression (1) is supplemented by the condition required for the model to be free from self-contradiction: $a\le x_0\ll(\xi_a/\xi)a$, where $\xi_a=Ga\sim M\omega_D^2$ is the standard atomic spring constant in solids, and $\hbar\omega_D=\theta$ is the Debye energy. The left-hand inequality in this condition imposes a natural lower bound

on x_0, while the right-hand one serves to guarantee that the pinning force is much less than the typical interatomic forces in solids (i.e., ensures that the model describes a breakable pin, rather than an anchoring one). In the following the pinning potential is assumed to be sufficiently strong, more specifically that

$$\xi \gg \xi_s \sim (\mu/M)\xi_a , \tag{2}$$

and $U_0 \gg \hbar\omega$, where $\omega = (\xi/\mu)^{1/2}$ is the oscillation frequency in the pinning well. For such a strongly pinned kink the effect of crystalline resistance on its dynamics may be easily ignored [9]. Therefore, the total potential felt by the pinned kink upon application of a constant external stress takes the form $U_t(x) = U_{\text{pin}}(x) - fx$, where $f = \tau ab$. It will prove convenient to transpose the zero of the kink energy to the bottom of the shifted well in this potential and represent the total potential in the following physically equivalent form:

$$U(x) = \begin{cases} \frac{1}{2}\xi(x - x_c)^2, & |x| \le x_0 , \\ \bar{U} - f(x - x_0), & |x| \ge x_0 . \end{cases} \tag{3}$$

In Eq. (3), $x_c = \gamma x_0$, $\gamma = \tau/\tau_m$, and $\bar{U} = U_0(1-\gamma)^2$ is the stress-dependent height of the pinning barrier. In our model $\tau_m = 2U_0/v$ plays the role of the stress required to produce a mechanical breakaway, and the volume associated with the pin is $v = abx_0$.

At this point a comment on the nature of the pinned state in (3) should be made. Strictly speaking, after the stress has been applied, the pinning well becomes metastable because of the possibility of tunnel crossing of the pinning barrier. However, in view of the condition that [1,4] $\tau < \tau_P$, Eq. (2) suggests that $\gamma < \tau_P/\tau_m \sim (\tau_P/G)^{1/2}\xi_s a/\xi x_0 \ll 1$. It then follows that the tunnel transparency of the barrier is extremely small. [More precisely, the WKB tunnel widths of the low-lying quantum levels in the well (3) are exponentially small compared to the characteristic energy parameters $\hbar\omega, \hbar\omega_D$.] Therefore, in the limit $T \ll \hbar\omega$ assumed hereafter, the pinned state is adequately described by a quasistationary state [7], occupying the ground-state level $\varepsilon_0 = \hbar\omega/2$ in the well in (3).

Thus far, we have neglected lattice fluctuations. To pursue their effect on the bare pinned state, one needs to specify the many-body Hamiltonian of the entire kink-phonon system. For the sake of simplicity, here we concentrate our interest on the case of coupling to longitudinal acoustic phonons, and treat the latter in the Debye approximation. Then, guided by the analogy with successful descriptions [10,11] of various one-dimensional quasiparticles coupled to 3D phonons, we write the full Hamiltonian as

$$H = -(\hbar^2/2\mu)(d/dx)^2 + U(x) + (2M)^{-1}\sum_{\mathbf{q}} (\hat{P}_{\mathbf{q}}^2 + M^2\omega_{\mathbf{q}}^2 Q_{\mathbf{q}}^2) + H_{\text{int}} , \tag{4}$$

with H_{int} describing the kink-phonon interaction, which in terms of the set $Q = \{Q_{\mathbf{q}}\}$ of the coordinates for phonons of wave vector $\mathbf{q}$ and frequency $\omega_{\mathbf{q}} = sq$ is $H_{\text{int}} = \sum_{\mathbf{q}} C_{\mathbf{q}} Q_{\mathbf{q}} \exp(iq_x x)$. $P_{\mathbf{q}}$ is the momentum conjugate to $Q_{\mathbf{q}}$, s is the sound velocity in the crystal, and the relevant features of the interaction are encapsulated in the coupling coefficients $C_{\mathbf{q}}$. Using elasticity theory [12], and proceeding along the lines worked out in Ref. [4], we obtain the following expression for $C_{\mathbf{q}}$:

$$C_{\mathbf{q}} = 2i(1/N)^{1/2} Gab q^{-1}(\mathbf{qn}) \operatorname{sech}(wq_x/2) , \tag{5}$$

where $\mathbf{n}$ is a unit vector normal to the dislocation slip plane, N is the number of unit cells in the crystal, and we have assumed in deriving Eq. (5) that the shape of the Peierls potential for the parent dislocation is sinusoidal [1,2,4].

We are now in a position where we can address the quantum states of the Hamiltonian (4). Once again we recall the condition Eq. (2), which now implies that the pinned kink moves faster than the lattice can respond. This makes it possible to present the eigenfunctions of H in the adiabatic manner [5], $\Psi_{kl}(x,Q) = \psi_k(x,Q) \times \chi_l(Q - Q^k)$, where the indices k and l label the adiabatic states of the kink and lattice vibrational states, respectively. An important point to notice is that, due to H_{int}, the lattice must suffer local distortion to conform better to the presence of the pinned kink. One can find $Q^{k=0}$'s, the shifts in the equilibrium positions of the phonon coordinates, pertaining to the ground state $\psi_{k=0}$, by using the prescriptions of standard polaron theory [13]. The result is as follows:

$$|Q_{\mathbf{q}}^0| = (M\omega_{\mathbf{q}}^2)^{-1} |C_{\mathbf{q}}| \exp[-(q_x \bar{x}/2)^2] , \tag{6}$$

where $\bar{x} = (\hbar/\mu\omega)^{1/2}$ is the localization length (quantum size) associated with the pinned kink. This polaron lattice distortion dresses the kink by a cloud of virtual phonons. As a result, the energy of the dressed pinned state reduces to $\bar{\varepsilon}_0 = \varepsilon_0 - 2\Delta$, where $2\Delta = \sum_{\mathbf{q}} M\omega_{\mathbf{q}}^2 |Q_{\mathbf{q}}^0|^2$ is twice the elastic strain energy stored in the self-consistently deformed lattice. With the aid of Eq. (6) one can calculate Δ by transforming the sum over $\mathbf{q}$ into an integral throughout the Brillouin zone. To zeroth order in the quantity $\bar{x}/w \sim (\varepsilon_0/U_0)^{1/2}\xi_s x_0/\xi a \ll 1$, we find that

$$\Delta = \Delta_a (a/w)[\ln(w/a) + 1] , \qquad \Delta_a = (Ga^2 b)^2/\pi M s^2 \sim Ga^3 . \tag{7}$$

This important result, which shows that the lattice relaxation energy is *not sensitive* to the pinning strength, seems puzzling initially. However, this fact is just a manifestation of the extended character of the dislocation kink. One can develop a physical feel for (7) by referring back to our basic equations (5) and (6). It is then seen on quick inspection that only phonons with wave-vector components $q_x \lesssim \min\{w^{-1}, \bar{x}^{-1}\} = w^{-1}$ are expected to interact essentially with the pinned kink. Accordingly, a cutoff at $q_x \sim w^{-1}$ naturally occurs in the Brillouin zone,

which in turn establishes the form of Eq. (7) [14]. From now on we shall assume that the polaron effect is strong, i.e., that $\Delta \gg \theta$. Physically, this condition means that the polaron cloud is created by many vibrational quanta and is capable of sustaining against a single-phonon fluctuational disintegration.

After the strong polaron effect is removed from H, the residual weak interaction which mixes the adiabatic kink-vibrational states is described by the nonadiabaticity operator [6] $\hat{L}$, acting on Ψ such that

$$\hat{L}\Psi_{kl} = (2M)^{-1}\sum_{\mathbf{q}} [2\hat{P}_{\mathbf{q}}\psi_k(x,Q)\hat{P}_{\mathbf{q}}\chi_{kl}(Q) + \chi_{kl}(Q)\hat{P}_{\mathbf{q}}^2\psi_k(x,Q)] .$$

When sandwiched between the different adiabatic states of H, $\hat{L}$ triggers quantum transitions between the kink states, accompanied by a simultaneous multiquantum excitation and redeformation of the lattice. A single activation event contributing to the overall depinning rate may therefore be viewed as a two-stage process involving (i) a fluctuation-induced jump of the kink to an excited level ε_k in (3), and (ii) a successive resonance transition of the kink through the barrier region, via either underbarrier tunnel paths (if $\varepsilon_k < \bar{U}$), or overbarrier ones (if $\varepsilon_k > \bar{U}$). We hope to discuss the role of tunnel paths in the depinning process in a longer paper [15] at a later opportunity; at present we focus on the case where the pinning barrier is jumped over (the criterion for the realization of such a regime will be given below). The jump rate is defined as follows:

$$\nu = \int_{\varepsilon_k > \bar{U}} [\partial\nu(\varepsilon_k)/\partial\varepsilon_k]\, d\varepsilon_k , \tag{8}$$

with the integrand being the (differential) rate at which the kink fluctuationally leaves the pinned state using the overbarrier continuum state ψ_k, in which the kink defecton is effectively decoupled [7,8] from phonons. In the considered case of the strong coupling of the pinned kink to the lattice distortion the integrand of Eq. (8) can be written explicitly as [16]

$$\begin{aligned} &\partial\nu(\varepsilon_k)/\partial\varepsilon_k = (2\pi/\sigma^2)^{1/2} P_{\rm ph} \exp[-(\varepsilon_k - \bar{\varepsilon}_0)^2/2\sigma^2] , \\ &P_{\rm ph} = (\hbar/M)\sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} |P_{\mathbf{q}}|^2 (\bar{n}_{\mathbf{q}} + \tfrac{1}{2}) , \\ &\sigma^2 = \sum_{\mathbf{q}} \hbar\omega_{\mathbf{q}} M\omega_{\mathbf{q}}^2 |Q_{\mathbf{q}}^0|^2 (\bar{n}_{\mathbf{q}} + \tfrac{1}{2}) , \end{aligned} \tag{9}$$

where $P_{\mathbf{q}} = C_{\mathbf{q}}(\varepsilon_k - \varepsilon_0)^{-1}\langle\psi_k(x,0)|\exp(iq_x x)|\psi_0(x,0)\rangle$ is the kink transition-matrix element in the Condon approximation [5,16], $\bar{n}_{\mathbf{q}}$ are the Bose occupation numbers for phonons, and σ measures the half-width of the Gaussian function in (9). By employing Eq. (6), we obtain σ^2 as a function of T:

$$\sigma^2(T) = 2\Delta\theta g(\theta,T_0) \times \begin{cases} T/\theta g(\theta,T_0), & \theta \ll T, \quad (10a) \\ [1 + (T/\theta)\ln(T/T_0)], & T_0 \ll T \ll \theta, \quad (10b) \\ 1, & T \ll T_0, \quad (10c) \end{cases}$$

where $g(\theta,T_0) = [1 + \ln(\theta/T_0)]^{-1}$, and the kink width manifests itself in the characteristic temperature $T_0 = \hbar s/w \sim (\mu/M)\theta$. Qualitatively our result (10) can be divided into three regions in T. Above θ the lattice is sensibly classical ($\bar{n}_{\mathbf{q}} \gg 1$), and σ^2 varies linearly with T. Below θ phonons with energies $\hbar\omega_{\mathbf{q}} > T$ are frozen, and σ^2 is governed both by classical and quantum (zero-point) fluctuations of the lattice. When T is further lowered through T_0, the last essential phonons with $q \sim w^{-1}$ drop into their ground states, and the half-width is controlled by quantum fluctuations.

To find $P_{\mathbf{q}}$, let us observe that, due to the localized character of the harmonic-oscillator wave function ψ_0, the main contribution to the matrix element comes from the region $|x - x_c| \sim \bar{x}$. Using in this region a simple WKB expression for ψ_k, and normalizing it by standard means [17], we get

$$|P_{\mathbf{q}}|^2 = (4\pi\varepsilon_0\varepsilon_k^5)^{-1/2}|C_{\mathbf{q}}|^2 \exp\{-[(q_x + \kappa)\bar{x}]^2\} , \tag{11}$$

where $(\kappa\bar{x})^2 = \varepsilon_k/\varepsilon_0 \gg 1$. With $|P_{\mathbf{q}}|^2$ in hand, the phonon sum $P_{\rm ph}$ can be calculated in just the same way as we obtained Eq. (7). Thus, we have

$$P_{\rm ph} = (\omega_D/6\pi^{1/2})[(Ga^2b)^2\theta T_0/Ms^2\varepsilon_k^3]F(T)(\varepsilon_k/\varepsilon_0)^{1/2} \times \exp(-\varepsilon_k/\varepsilon_0) , \tag{12}$$

where, for $T \gg \theta$, $F(T) = 3T/2\theta$, whereas in the opposite limit, $T \ll \theta$, $F(T) \sim 1$.

To proceed further, we now need to determine the extent to which the approximation of the overall rate by Eq. (8) is valid. Physical intuition would say that the overbarrier jump is preferable for the kink whenever τ is small and/or T is high. Indeed, a detailed study [15] of the contribution of the underbarrier tunnel paths to the overall rate shows that the rate is dominated by overbarrier paths, when $\gamma < \min\{\tau_P/\tau_m, (a^3\varepsilon_0/U_0)^{1/2}\}$, where $a = \sigma^2(T)/\varepsilon_0(U_0 - \bar{\varepsilon}_0) \ll 1$.

Collecting Eqs. (9) and (12) into Eq. (8), and exploiting the above condition in carrying out the integration over ε_k, we arrive at the final result:

$$\begin{aligned} &\nu = \nu_0 \exp\{-[(U_0 - \bar{\varepsilon}_0)^2/2\sigma^2(T)][1 - (\tau/\tau^*)]\}, \quad \tau^* = (U_0 - \bar{\varepsilon}_0)/2\nu , \\ &\nu_0 = (2^{1/2}/6\pi)\omega_D[(Ga^2b)^2\sigma\theta T_0/Ms^2U_0^4]F(T)(U_0/\varepsilon_0)^{1/2}\exp[-(U_0 - \nu\tau)/\varepsilon_0] . \end{aligned} \tag{13}$$

We can now reach rigorous conclusions regarding the temperature behavior of the depinning rate. Combined with (10a), Eq. (13) suggests that in the classical temperature limit above θ the rate may be presented in an Arrhenius form: $\nu = \nu_0 e^{-E^*(\tau)/T}$. The attempt frequency exhibits a $T^{3/2}$ dependence, while the activation barrier height is given by

$$E^*(\tau) = U_0^* - \nu^* \tau, \quad U_0^* = (U_0 - \bar{\varepsilon}_0)^2/4\Delta, \qquad \nu^* = \nu(U_0 - \bar{\varepsilon}_0)/2\Delta. \tag{14}$$

It now becomes apparent that the polaron effect plays a fundamental role in energetics of the kink depinning phenomenon. In particular, it is seen from (14) that even in the simplest case of zero applied stress the actual barrier height U_0^* differs markedly from the bare height U_0. This is because the multiquantum Gaussian fluctuations have to destroy the polaron cloud by an appropriate lattice deformation in their attempts to release the pinned kink.

When the temperature is lowered, Eq. (10b) states that below θ quantum lattice fluctuations do come into action. As expected, now the thermal-fluctuation Arrhenius law ceases to give a correct description of the breakaway kinetics, so that the concept of the effective (temperature dependent) activation energy should be introduced [18]. This conclusion deserves careful attention in view of the possibility of obtaining valuable information about pinning effects from low-temperature internal friction data [19]. Finally, let us observe that in the ultraquantum temperature region below T_0 (for $\theta \sim 0.03$ eV, and $G/\tau_P \sim 10^3$, we estimate $T_0 \sim 10$ K), both ν_0 and σ are controlled solely by quantum fluctuations. We conclude that in this region the depinning rate displays *athermal* behavior.

Finally, using for an order-of-magnitude estimate of the rate the above values, for $Ga^3 \sim 3$ eV, $x_0 \sim a$, $\omega_D/\omega \sim 0.4$, $\tau/\tau_P \sim 0.5$, and $T \sim \theta$, we obtain $\nu^{-1} \sim 10^{-3}$ s.

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[1] J. P. Hirth and J. Lothe, *Theory of Dislocations* (Wiley, New York, 1982); A. Seeger and P. Shiller, in *Physical Acoustics*, edited by W. P. Mason (Academic, New York, 1966), Vol. 3, p. 361.

[2] M. Buttiker and R. Landauer, Phys. Rev. Lett. **43**, 1453 (1979); Phys. Rev. A **23**, 1397 (1981); P. Hanggi, F. Marchesoni, and P. Sodano, Phys. Rev. Lett. **60**, 2563 (1988), and references therein.

[3] See, for example, V. Celli *et al.*, Phys. Rev. **131**, 58 (1963); R. R. Hasiguti, J. Phys. Soc. Jpn. **18**, Suppl. **1**, 114 (1963); T. Ninomiya, R. Thomson, and F. Garcia-Moliner, J. Appl. Phys. **35**, 3607 (1964); A. Sato and M. Meshii, Acta Metall. **21**, 753 (1973); B. V. Petukhov, Fiz. Tverd. Tela (Leningrad) **32**, 2133 (1990) [Sov. Phys. Solid State **32**, 1239 (1990)]; B. V. Petukhov and Yu. I. Polyakov, Kristallografiya **35**, 559 (1990) [Sov. Phys. Crystallogr. **35**, 326 (1990)], and references therein.

[4] J. D. Eshelby, Proc. R. Soc. London A **266**, 222 (1962).

[5] C. P. Flynn and A. M. Stoneham, Phys. Rev. B **1**, 3966 (1970).

[6] Yu. Kagan and M. I. Klinger, J. Phys. C **7**, 2791 (1974).

[7] M. I. Klinger, Phys. Rep. **94**, 183 (1983).

[8] M. A. Strzhemechny, Fiz. Nizk. Temp. **10**, 663 (1984) [Sov. J. Low Temp. Phys. **10**, 348 (1984)].

[9] Indeed, a simple estimate using the fact that the Peierls energy of a second kind [1] U_2 is less [8] than $\tau_P a^3$ ensures that $U_2/U_{\rm pin}(a) < \tau_P a/\xi \sim (\tau_P/G)^{1/2}\xi_s/\xi \ll 1$.

[10] D. I. Pushkarov, Zh. Eksp. Teor. Fiz. **64**, 634 (1973) [Sov. Phys. JETP **37**, 322 (1973)].

[11] A. A. Gogolin, Phys. Rep. **86**, 2 (1982); Zh. Eksp. Teor. Fiz. **92**, 152 (1987) [Sov. Phys. JETP **65**, 85 (1987)].

[12] L. D. Landau and E. M. Lifshitz, *Theory of Elasticity* (Pergamon, New York, 1970).

[13] See, e.g., J. Appel, *Solid State Physics*, edited by H. Ehrenreich and D. Turnbull (Academic, New York, 1968), Vol. 21, p. 193.

[14] It is instructive to consider briefly the abrupt kink limit, $w \to a$. In this limit our model gives $x_0 \to a$, $\xi \to \xi_a$, $\omega \to \omega_D$, while the kink may be regarded as an atomic-scale particle with self-interstitial mass M. Now the integration required to obtain the lattice deformation energy encompasses the entire Brillouin zone and Eq. (7) qualitatively correctly yields $\Delta \to \Delta_a \sim Ga^3$.

[15] L. B. Hovakimian (to be published).

[16] G. Rickayzen, Proc. R. Soc. London A **241**, 480 (1957).

[17] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics-Non-Relativistic Theory* (Pergamon, Oxford, 1977).

[18] G. Alefeld, Phys. Rev. Lett. **12**, 372 (1964); M. Inui, P. B. Littlewood, and S. N. Coppersmith, Phys. Rev. Lett. **63**, 2421 (1989).

[19] See, for example, R. B. Schwarz and A. V. Granato, Phys. Rev. Lett. **34**, 1174 (1975); and the last citation of Ref. [3].