

Quantum-mechanical theory of stress-assisted fluctuational breakaway of dislocation kinks from pinning centers in crystals

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We propose a quantum-mechanical theory of depinning of dislocation kinks. The interaction of the pinned state with the fluctuating host lattice is treated within the framework of the adiabatic approximation. It is shown that the polaron distortion of the lattice near the pinned kink affects essentially the magnitude of energy fluctuation required to activate a jump over the pinning barrier. The effect of quantum lattice fluctuations on the kinetics of breakaway at low temperatures is analyzed. We address also the question of the role of underbarrier tunnel paths in the fluctuation-induced escape of the kink from the pinning well and introduce the concept of a (temperature-dependent) quantum stress, above which the tunneling regime of breakaway becomes operative. The stress and temperature dependences of activation parameters characterizing the depinning process are discussed.

I. INTRODUCTION

It is well recognized that kink excitations play a decisive role in establishing the peculiar dynamical behavior of dislocations in crystals possessing pronounced Peierls potential relief.¹⁻⁴ Being mobile defects, associated with the dislocation core, kinks are regarded by the well-known model^{1,5} as one-dimensional quasiparticles constrained to move along the otherwise straight dislocation line. In the isotropic continuum model of a crystal with host atom mass M and elastic modulus G , the effective mass μ of the continual kink is related to its geometric width w ($w \gg a \sim b$) by the relation^{1,5}

$$\frac{\mu}{M} \sim \frac{a}{w} \sim \left(\frac{\tau_P}{G} \right)^{1/2} \ll 1, \quad (1)$$

where a is the lattice spacing, τ_P is the Peierls stress, b is the Burgers vector, and it is assumed, as usual, that the dislocation line tension is $S \sim Ga^2$.

Owing to the smallness of μ , the continual dislocation kink can be naturally incorporated into the family of light mobile defects (defectons) in solids, the physical properties of which have been thoroughly studied.^{6,7} At the same time, the specific feature which distinguishes the kink from ordinary defectons is its geometric width. In particular, the important role played by the extended nature of a kink in formulating the law of its interaction with elastic crystalline waves has been demonstrated in the classical paper by Eshelby.⁵

In view of the considerable interest, connected with the studies of the Peierls mechanism of plastic deformation and dynamical behavior of kinked dislocations under internal friction conditions, there has been much effort invested in the study of kinetic behavior of kinks in pure

materials. A number of accounts⁸⁻¹⁰ reflect the accumulation of knowledge and the progress achieved in this field of research. At the same time, numerous studies¹¹⁻²² have been exploring more complicated situations, where the motion of kinks in real crystals is hindered by local pinning agents. Of fundamental importance for the further progress in this direction of research is understanding of physical mechanisms which control the process of the breakaway of kinks from efficient pinning centers. It is the purpose of this study to present a description of the kink breakaway phenomenon from the standpoint of a microscopic theory.

The traditional, phenomenological descriptions^{11-17,19,20} 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 τ_P breaks away from its pinnor with an effective rate

$$v = v_0 \exp \left\{ - \frac{E(\tau)}{T} \right\}, \quad (2)$$

where v_0 is a rather ill-defined attempt frequency, and $E(\tau)$ is the activation energy (we take the units such that $k_B = 1$). As regards the stress dependence of $E(\tau)$, it is usually assumed that $E(\tau) = U_0 - v_0 \tau$, where the pinning barrier height at $\tau = 0$, U_0 , is decreased by the work $v_0 \tau$ done by the stress, and $v_0 = T [\partial \ln(v/v_0) / \partial \tau]_T$ is the activation volume of the process, maintained by environmental fluctuations.

Several remarks should be made regarding the aforementioned rate constant (2). It is, of course, reasonable to expect that at sufficiently high temperatures, when the fluctuating environment can be well described classically, the depinning rate can display classical thermal-fluctuation Arrhenius dependence on T . On the

other hand, it is clear that at low enough temperatures, when quantum environmental fluctuations will acquire importance, deviations from the Arrhenius temperature dependence will inevitably occur.

One can further upset the absolute-reaction rate formula (2) by noting that the form of the activation energy involved tells one nothing about the physical mechanism by which the energy is transferred to the activated kink. Since this energy must be supplied to the kink by some crystalline degrees of freedom (e.g., by phonons, electrons, etc.), one should expect $E(\tau)$ to be a sensitive function of parameters directly related to physical properties of that crystalline subsystem which supports the process of activation. In the particular case, where the mechanism of energy gain from lattice fluctuations is provided by the kink-phonon coupling, proper attention must be paid to the relative magnitude of the coupling coefficients. If strong enough, the kink-phonon interaction may be able to produce a noticeable polaronic distortion of the host lattice near the pinned kink. In such a situation the lattice relaxation effects can essentially modify the simple phenomenological picture of the breakaway process.

An essential issue, which a theoretical description of the breakaway process must also address, is determination of conditions under which the kink can fluctuationally leave the pinned state utilizing effectively the under-barrier tunnel trajectories. Following the pioneering paper of Mott,²³ where the question of the importance of quantum tunneling effects for the dynamical behavior of dislocations at low temperatures was addressed, a great deal of attention has been attracted by the problem of quantum dislocation motion through crystalline barriers of various nature. (A good description of these investigations can be found in a number of review papers²⁴⁻²⁶ or in the recent book of Suzuki, Yoshinaga, and Takeuchi⁴). It has been suggested by Alefeld²⁷ that, in view of the condition $\mu \ll M$, tunneling effects for kinks can play an even more pronounced role than for a dislocation itself. The work of Petukhov and Pokrovskii²⁸ has to be mentioned in this connection, where the question of the tunnel penetration of kinks through the Peierls potential was analyzed.

Let us note that in theoretical schemes, developed for the description of the environmentally activated motion of dislocations, the method of stochastic Langevin equations has been commonly used as an effective tool.^{1,29-32} In the present study of the kink breakaway process we shall, however, abandon this method. Instead, wishing to explore the role of the lattice deformations in establishing the physical picture underlying the phenomenon of fluctuational depinning, we are formulating our approach by utilizing methods developed in polaron theory,³³ and theories of nonradiative transitions³⁴ and quantum diffusion in solids.^{35,36} Proceeding in this way, we intend to treat unifiedly both the regimes of over-the-barrier³⁷ and tunneling escape of the kink from the pinned state.

Our paper is organized as follows: Sec. II is devoted to the model description of the pinning potential and to the discussion of the parameters characterizing the pin-dislocation kink interaction. By incorporating the lattice

fluctuations into our analysis, we investigate in Sec. III the effect of the lattice reorganization on the bare pinned state. In Sec. IV the contribution of overbarrier escape paths to the overall depinning rate is found, whereas the tunneling regime of breakaway is studied in Sec. V. We conclude our paper by discussing the stress and temperature dependences of activation parameters that describe the breakaway process.

II. MODEL DESCRIPTION OF THE PINNING POTENTIAL

Consider a kink pinned down by a single immobile pin located at $x=0$. [Let us assume, for definiteness, that the parent dislocation is a screw one, with its Burgers vector $\mathbf{b}=(b,0,0)$ directed along the dislocation axis chosen as x direction]. Since the true interaction between a kink and a pin is not known, we construct a simple model in which an attractive potential of interaction is taken to be

$$U_{\text{pin}}(x) = \begin{cases} -U_0 + \frac{1}{2}\xi x^2, & |x| \leq x_0 \\ 0, & |x| \geq x_0 \end{cases} \quad U_0 = \frac{1}{2}\xi x_0^2 \quad (3)$$

Here x denotes the position of the kink center of mass on the dislocation line, and the spring constant ξ characterizes the strength of the pin-kink interaction. The range of interaction is denoted by x_0 , and the depth of the pinning well is U_0 when the zero of the kink energy is taken at the bottom of the kink band.³⁸ On the parameters, characterizing the interaction, the following condition

$$a \leq x_a \ll \left(\frac{\xi_a}{\xi} \right) a \quad (4)$$

must be imposed, which is necessary for the model (3) to be free from self-contradiction. In (4), $\xi_a = Ga \sim M\omega_D^2$ is the standard atomic spring constant in solids, and $\hbar\omega_D = \theta_D$ is the characteristic Debye energy of the lattice. The left-hand inequality in the above condition imposes a natural lower bound on the range of interaction, whereas the right-hand one serves to guarantee that the (maximal) pinning force acting on the kink is less than typical atomic scale forces in solids (i.e., ensures that the model describes a breakable pin, rather than an anchoring one).

Henceforth, it will be assumed that the pinning potential is sufficiently strong; more specifically, the case will be considered in which the inequalities

$$\xi \gg \xi_s \sim \frac{\mu}{M} \xi_a, \quad (5)$$

$$\left(\frac{U_0}{\hbar\omega} \right)^{1/2} \gg 1 \quad (6)$$

are supposed to hold, where $\omega = (\xi/\mu)^{1/2}$ is the oscillation frequency in the pinning well. For such a strongly pinned kink the effect of the crystalline resistance on its dynamics can be safely ignored. Indeed, taking advantage of the circumstance that the Peierls energy of the

second kind,³ U_P^{II} , is less³⁸ than $\tau_P a^3$, it is easy to verify that

$$\frac{U_P^{\text{II}}}{U_{\text{pin}}(a)} < \frac{\tau_P a}{\xi} \sim \left[\frac{\tau_P}{G} \right]^{1/2} \frac{\xi_s}{\xi} \ll 1. \quad (7)$$

We now turn our attention to the question of the total potential felt by the kink upon application of a constant external stress. Following previous works,^{11-15,17,19,20} we shall exclude the influence of the lattice resistance on the kink motion outside the pinning well; correspondingly, we shall assume that no hopping processes occur during translational kink motion. The condition for such assumptions to be admissible can be written as $\tau > \tau_P^{\text{II}} \sim U_P^{\text{II}}/a^3$. Then, for the total potential under the applied stress we can use the expression $U_t(x) = U_{\text{pin}}(x) - fx$, where $f = \tau ab$.¹⁻⁴ If we now shall transpose, for the sake of convenience, the zero of the kink energy to the bottom of the shifted well in this potential, we then can present the total potential in the following physically equivalent form:

$$U(x) = \begin{cases} \frac{1}{2}\xi(x-x_c)^2, & |x| \leq x_0 \\ \bar{U}_0 - f(x-x_0), & |x| \geq x_0. \end{cases} \quad (8)$$

In Eq. (8), $x_c = \gamma x_0$, $\gamma = \tau/\tau_m$, and

$$\bar{U}_0 = U_0(1-\gamma)^2 \quad (9)$$

is the stress-dependent height of the pinning barrier. It is evident that in our model $\tau_m = 2U_0/v$ plays the role of the stress that would be required to produce a mechanical breakaway, and the volume associated with the pinning is $v = abx_0$. Let us note that the upper limit for the variation of the parameter (dimensionless stress) γ can be found from the requirement that $\tau < \tau_P$. Denoting the ratio τ_P/τ_m by γ_P , one obtains

$$\gamma < \gamma_P \sim \left[\frac{\tau_P}{G} \right]^{1/2} \left[\frac{\xi_s}{\xi} \right] \frac{a}{x_0} \ll 1. \quad (10)$$

Finally, to complete the description of the constructed model, a comment on the quantum-mechanical nature of the pinned state in (8) should be made. Strictly speaking, the applied stress renders the pinning well metastable, since it opens the channel of tunnel crossing of the pinning barrier. In view of the condition (10), however, the Wentzel-Kramers-Brillouin (WKB) tunnel widths of the low-lying quantum levels in the well (8) are exponentially small compared to the characteristic energy parameters $\hbar\omega, \hbar\omega_D$. Therefore, in the limit

$$T \ll \hbar\omega \quad (11)$$

assumed hereafter, the pinned state is adequately described by a quasistationary state,⁷ occupying the ground-state level $\epsilon_0 = \hbar\omega/2$ in the well in (8).

III. QUANTUM STATES OF THE INTERACTING KINK-PHONON SYSTEM

The foregoing discussion has been carried out in the rigid-lattice approximation. Now, in order to incorporate the lattice fluctuations into the present analysis, one has to specify the many-body Hamiltonian of the entire kink-phonon system. For the sake of simplicity, our interest will be concentrated here on the case of coupling to longitudinal acoustic phonons with the Debye spectrum. Then, guided by the analogy with successful descriptions^{39,40} of various one-dimensional quasiparticles, coupled to three-dimensional (3D) phonons, we present the full Hamiltonian in the following form

$$\begin{aligned} \hat{H} = & -\frac{\hbar^2}{2\mu} \left[\frac{d}{dx} \right]^2 + U(x) + (2M)^{-1} \sum_{\mathbf{q}} [\hat{P}_{\mathbf{q}}^2 + M^2 \omega_{\mathbf{q}}^2 Q_{\mathbf{q}}^2] \\ & + \hat{H}_{\text{int}}, \\ H_{\text{int}} = & \sum_{\mathbf{q}} C_{\mathbf{q}} Q_{\mathbf{q}} \exp(iq_x x). \end{aligned} \quad (12)$$

Here the set $Q = \{Q_{\mathbf{q}}\}$ is representing the normal coordinates of phonons of wave vector \mathbf{q} and frequency $\omega_{\mathbf{q}} = sq$, where s is the sound velocity in the crystal. $\hat{P}_{\mathbf{q}}$ is the momentum conjugate to $Q_{\mathbf{q}}$, and the relevant features of the kink-phonon interaction are contained in the coupling coefficients $C_{\mathbf{q}}$. These coefficients can be found using elasticity theory⁴¹ and following the original method of Eshelby.⁵ If the case is considered, where the shape of the Peierls potential for the parent dislocation is sinusoidal,¹⁻⁵ then

$$C_{\mathbf{q}} = 2i \left[\frac{1}{N} \right]^{1/2} Gab \frac{(\mathbf{q} \cdot \mathbf{n})}{q} \text{sech}(q_x w/2), \quad (13)$$

where N is the number of unit cells in the fundamental volume and \mathbf{n} is a unit vector normal to the dislocation slip plane.

We have now reached the point where we are prepared to address the quantum states of the Hamiltonian (12). Recalling the condition, Eq. (5) one can note that the pinned kink moves faster than the lattice can respond. This circumstance makes it possible to separate the dynamical variables of the kink and phonons, using the scheme of the adiabatic approximation.^{7,35} In this approximation one can present the eigenfunction of the full Hamiltonian as $\Psi_{kl}(x, Q) = \psi_k(x, Q) \chi_l(Q - Q^k)$, where the indices k and l label the adiabatic states of the kink and lattice vibrational states, respectively. It should be noted that, due to the kink-phonon interaction, the host lattice has to suffer local reorganization in order to accommodate itself to the presence of the pinned kink. One can find $Q_{\mathbf{q}}^k = 0$'s, the shifts in the equilibrium positions of the phonon coordinates, pertaining to the ground state $\psi_{k=0}$ by using the prescriptions of the standard polaron theory.³³ The result can be presented compactly in the following form:

$$|Q_{\mathbf{q}}^0\rangle = \xi_{\mathbf{q}}^{-1} |C_{\mathbf{q}}\rangle \exp \left\{ - \left[\frac{q_x \bar{x}}{2} \right]^2 \right\}, \quad (14)$$

where $\xi_q = M\omega_q^2$ and $\bar{x} = (\hbar/\mu\omega)^{1/2}$ is the localization length (quantum size) associated with the pinned kink. The effect of this polaron lattice distortion on the bare pinned state is that the latter becomes dressed by a cloud of virtual phonons. As a result, the energy of the dressed pinned state reduces to $\bar{\epsilon}_0 = \epsilon_0 - 2\Delta$, where

$$\Delta = \frac{1}{2} \sum_q \xi_q |Q_q^0|^2 \quad (15)$$

is the elastic strain energy stored in the self-consistently deformed lattice. Making use of Eq. (14), one can find this energy by transforming the sum in (15) into an integral throughout the Brillouin zone. To zeroth order in the quantity $\bar{x}/w \sim (\epsilon_0/U_0)^{1/2} (\xi_s x_0/\xi a) \ll 1$ the result is given by

$$\Delta = \Delta_a \left[\frac{a}{w} \right] \left[\ln \left[\frac{w}{a} \right] + 1 \right], \quad (16)$$

$$\Delta_a = \frac{(Ga^2b)^2}{\pi Ms^2} \sim Ga^3,$$

from which it can be seen that the polaronic distortion of the lattice turns out to be larger in materials where kinks are more heavy. Further insight into the situation can be gained by considering the abrupt kink limit, $w \rightarrow a$. In this limit the kink can be regarded as an atomic-scale particle with self-interstitial mass M , and Eq. (16) qualitatively correctly yields for the lattice deformation energy $\Delta \rightarrow \Delta_a \sim Ga^3$.

It will be assumed in the following that the polaron effect is sufficiently strong. That is

$$\Delta \gg \theta_D. \quad (17)$$

Physically, this condition means that many lattice vibrational quanta participate in the formation of the polaron cloud so that the latter is capable of sustaining against a single-phonon fluctuational disintegration.

IV. CONTRIBUTION OF OVERBARRIER PATHS TO THE DEPINNING PROCESS

After the strong polaron effect is removed from the full Hamiltonian (12), the residual weak interaction which mixes the adiabatic kink-vibrational states is described by the nonadiabaticity operator³⁶ \hat{L} the action of which on the wave function Ψ is given by

$$\hat{L}\Psi_{kl} = (2M)^{-1} \sum_q [2\hat{P}_q \psi_k(x, Q) \hat{P}_q \chi_{kl}(Q) + \chi_{kl}(Q) \hat{P}_q^2 \psi_k(x, Q)]. \quad (18)$$

When sandwiched between the different adiabatic states of \hat{H} , this operator gives rise to a quantum transitions between the kink states accompanied by simultaneous multiquantum excitation and redeformation of the lattice. A single activation event, contributing to the overall rate of breakaway, may be therefore viewed as a two-stage process involving (i) a fluctuation induced jump of the kink to an excited state ϵ in (8), and (ii) a successive resonance transition of the kink through the barrier region by

means of either underbarrier tunnel paths (if $\epsilon < \bar{U}_0$), or overbarrier ones (if $\epsilon > \bar{U}_0$). Correspondingly, the overall depinning rate $\nu(\gamma, T)$ can be presented as a sum of two terms

$$\nu(\gamma, T) = \nu_t(\gamma, T) + \nu_h(\gamma, T). \quad (19)$$

The first term in Eq. (19) originates from the fluctuation-assisted events of tunneling through the barrier region (tunneling regime of breakaway), whereas the second one refers to fluctuationally induced jumps over the pinning barrier (hopping regime of breakaway),

The jump rate $\nu_h(\gamma, T)$ is defined as follows:

$$\nu_h(\gamma, T) = \int_{\epsilon > \bar{U}_0} w_h(\epsilon) d\epsilon, \quad (20)$$

where the integrand is the (differential) rate at which the kink fluctuationally leaves the pinned state using the overbarrier continuum state ψ_ϵ . In the considered case of the strong coupling of the pinned kink to the lattice distortion, the expression for $w_h(\epsilon)$ can be explicitly written as³⁴

$$w_h(\epsilon) = \left[\frac{2\pi}{\sigma^2} \right]^{1/2} \Xi_{\text{ph}} \exp \left\{ -\frac{(\epsilon - \bar{\epsilon}_0)^2}{2\sigma^2} \right\},$$

$$\Xi_{\text{ph}} = \frac{\hbar}{M} \sum_q \hbar\omega_q |R_q|^2 \left[\bar{n}_q + \frac{1}{2} \right], \quad (21)$$

$$\sigma^2 = \sum_q \hbar\omega_q \xi_q |Q_q^0|^2 \left[\bar{n}_q + \frac{1}{2} \right],$$

where

$$R_q = C_q (\epsilon - \epsilon_0)^{-1} \langle \psi_\epsilon(x, 0) | \exp(iq_x x) | \psi_0(x, 0) \rangle$$

is the kink transition matrix element in the Condon approximation,^{34,35} $\bar{n}_q = [\exp(\hbar\omega_q/T) - 1]^{-1}$ are the mean occupation numbers for phonons, and σ measures the half-width of the Gaussian function in (21).

With the aid of the Eq. (14) the temperature dependence of σ^2 can be found to be

$$\sigma^2(T) = 2\Delta\theta_D \begin{cases} \frac{T}{\theta_D}, & \theta_D \ll T, & (22a) \\ \eta(T, T_0) \eta^{-1}(\theta_D, T_0), & T_0 \ll T \ll \theta_D, & (22b) \\ \eta^{-1}(\theta_D, T_0), & T \ll T_0, & (22c) \end{cases}$$

where the characteristic temperature

$$T_0 = \frac{\hbar s}{w} \sim \frac{\mu}{M} \theta_D \quad (23)$$

is equal to the energy of a phonon with wavelength $\sim w$, and the function $\eta(T, T_0)$ is defined through the relation

$$\eta(T, T_0) = 1 + \frac{T}{\theta_D} \ln \left[\frac{T}{T_0} \right]. \quad (24)$$

It can be noticed from Eqs. (22a)–(22c) that the temperature dependence of σ^2 is characterized by three qualita-

tively different regions. Let us consider first the region of high temperatures above θ_D . This is the region where the motion of the lattice distortion about the pinned kink behaves essentially classically. Here the phonon occupation numbers are large ($\bar{n}_q \sim T/\hbar\omega_q \gg 1$), and σ^2 varies linearly with T . Below the Debye temperature, phonons with energies $\hbar\omega_q > T$ are frozen, so that now both the classical and quantum lattice fluctuations determine the T dependence of the half-width. When the temperature is further lowered through T_0 , the last essential phonons with $q \sim w^{-1}$ become frozen and σ^2 is controlled by quantum fluctuations.

To obtain the value of the phonon sum Ξ_{ph} , it is useful to observe that, due to the localized character of the harmonic oscillator wave function ψ_0 , the main contribution to the transition matrix R_q comes from the integration

region $|x - x_c| \sim \bar{x}$. Using the smallness of the parameter $(\epsilon_0/\epsilon)^{1/2}$ for calculating R_q in the WKB approximation,⁴² one can then present the expression for Ξ_{ph} as³⁷

$$\Xi_{\text{ph}} = \frac{\omega_D}{6\pi^{1/2}} \frac{(Ga^2b)^2 \theta_D T_0}{Ms^2 \epsilon^3} F(T) \left[\frac{\epsilon}{\epsilon_0} \right]^{1/2} \exp \left[-\frac{\epsilon}{\epsilon_0} \right], \quad (25)$$

where the asymptotic behavior of the function $F(T)$ is as follows: for $T \gg \theta_D$, $F(T) = 3T/2\theta_D$, whereas in the opposite limit, $T \ll \theta_D$, $F(T) \sim 1$.

Inserting now Eqs. (21) and (25) into Eq. (20) and carrying out the integration over ϵ , we obtain the following expression:

$$v_h(\gamma, T) = \frac{2^{1/2}}{6\pi} \omega_D \frac{(Ga^2b)^2 \theta_D T_0}{Ms^2 U_0^2 \sigma} \left[\frac{\epsilon_0}{U_0} \right]^{1/2} F(T) \Gamma^{-1}(\gamma, T) \cdot \exp \left\{ -\frac{(\bar{U}_0 - \bar{\epsilon}_0)^2}{2\sigma^2} - \frac{\bar{U}_0}{\epsilon_0} \right\}, \quad (26)$$

with

$$\Gamma(\gamma, T) = \left[1 + \frac{\epsilon_0(\bar{U}_0 - \bar{\epsilon}_0)}{\sigma^2(T)} \right]. \quad (27)$$

Physical intuition would say that the overall rate of breakaway can be well approximated by the jump rate, Eq. (26) in the limit of sufficiently low stresses and/or high temperatures. In such a limit one expects that several stress-dependent terms in Eq. (26) can be safely discarded. It is clear that in order to find out the required criterion, one has to explore the role of the underbarrier tunnel paths in the kinetics of breakaway.

V. TUNNELING REGIME OF BREAKAWAY

In choosing an underbarrier path for a fluctuation-assisted escape from the pinning well, the kink is faced with the necessity to pass through the region of the pinning barrier via the quantum-mechanical tunnel process. Hence the contribution of the tunnel path with $\epsilon < \bar{U}_0$ to the breakaway rate can be presented as²⁸

$$w_t(\epsilon) = w_h(\epsilon) \exp \left\{ -D(\epsilon) \right\}, \quad (28)$$

where

$$D_1(\epsilon) = \frac{2}{\hbar} \int_{x_t^{(1)}}^{x_0} |p(x)| dx = 2 \frac{\bar{U}_0}{\hbar\omega} \left\{ \left[1 - \frac{\epsilon}{\bar{U}_0} \right]^{1/2} - \frac{\epsilon}{\bar{U}_0} \ln \left[\left[\frac{\bar{U}_0}{\epsilon} \right]^{1/2} + \left[\frac{\bar{U}_0}{\epsilon} - 1 \right]^{1/2} \right] \right\}, \quad (33)$$

and

$$D_2(\epsilon) = \frac{2}{\hbar} \int_{x_0}^{x_t^{(2)}} |p(x)| dx = \frac{4}{3} \frac{\bar{U}_0}{\hbar\omega} (\gamma^{-1} - 1) \left[1 - \frac{\epsilon}{\bar{U}_0} \right]^{3/2}. \quad (34)$$

$$D(\epsilon) = \frac{2}{\hbar} \int_{x_t^{(1)}}^{x_t^{(2)}} |p(x)| dx, \quad (29)$$

$$p(x) = \left\{ 2\mu[\epsilon - U(x)] \right\}^{1/2}$$

is the WKB barrier penetration factor,⁴² and where, supposing that the condition $(\epsilon/\epsilon_0)^{1/2} \gg 1$ is again satisfied, we can use for $w_h(\epsilon)$ the expression obtained in the previous section. The classical turning points, determining the barrier thickness, are easily found from the condition $p(x_t) = 0$ and Eq. (8) to be

$$x_t^{(1)} = x_c + \left[\frac{2\epsilon}{\xi} \right]^{1/2}, \quad (30)$$

$$x_t^{(2)} = x_0 + \frac{\bar{U}_0 - \epsilon}{f}. \quad (31)$$

By splitting the integration region in (29) into two parts, one can present the barrier penetration factor as a sum of two terms,

$$D(\epsilon) = D_1(\epsilon) + D_2(\epsilon), \quad (32)$$

where

The following observation will now facilitate our task of determining the tunnel breakaway rate $\nu_t(\gamma, T)$. Let us note that the first factor in Eq. (28) is exponentially decreasing with ϵ . This factor is effectively regulated by temperature. The second factor in (29) is exponentially increasing with ϵ and is controlled by the applied stress. Therefore, one encounters a typical saddle-point situation, where the underbarrier path chosen by the kink as the most effective one for an escape will be determined by an "interplay" between the temperature and the applied stress.

To avoid interrupting the main arguments, let us assume that the requirements for the applicability of the saddle-point approximation are fulfilled (we shall return to this essential question below). Then the tunneling breakaway rate can be written as

$$\nu_t(\gamma, T) = \frac{\pi^{1/2}}{3} \frac{(Ga^2b)^2 \theta_D T_0}{Ms^2(\epsilon_0 \epsilon_s^5)^{1/2}} F(T) \frac{\sigma_s}{\sigma} \exp \left\{ -\phi(\epsilon_s) \right\}, \quad (35)$$

where the function in the argument of the exponential has the form

$$\phi(\epsilon) = \frac{(\epsilon - \bar{\epsilon}_0)^2}{2\sigma^2} + \frac{\epsilon}{\epsilon_0} + D(\epsilon), \quad (36)$$

and the effective width of the saddle is characterized by

$$\sigma_s(\gamma, T) = [\phi''(\epsilon_s)]^{-1/2}. \quad (37)$$

The saddle-point ϵ_s , corresponding to the optimal underbarrier escape path, has to be determined from the equation

$$\phi'(\epsilon_s) = 0 = (\epsilon_s - \bar{\epsilon}_0)\sigma^{-2} + \epsilon_0^{-1} + \hbar^{-1}T(\epsilon_s), \quad (38)$$

in which

$$\begin{aligned} T(\epsilon) &= 2 \int_{x_t^{(1)}}^{x_t^{(2)}} \frac{dx}{|p(x)|/\mu} \\ &= \frac{2}{\omega} \left\{ \ln \left[\left[\frac{\bar{U}_0}{\epsilon} \right]^{1/2} + \left[\frac{\bar{U}_0}{\epsilon} - 1 \right]^{1/2} \right] \right. \\ &\quad \left. + (\gamma^{-1} - 1) \left[1 - \frac{\epsilon}{\bar{U}_0} \right]^{1/2} \right\} \end{aligned} \quad (39)$$

has the meaning of the period of oscillation of a classical particle with energy $-\epsilon$ in the inverted potential $-U(x)$.

At this stage of development it will prove useful to introduce a new variable x_s through the following transformation:

$$\epsilon_s = \bar{U}_0(1 - x_s^2). \quad (40)$$

This transformation will now be used for disclosing an important connection that exists between $\nu_t(\gamma, T)$ and $\nu_h(\gamma, T)$. Introducing Eq. (40) into Eq. (35), we find, after some algebra, that

$$\frac{\nu_t(\gamma, T)}{\nu_h(\gamma, T)} = (2\pi^3)^{1/2} \frac{\sigma_s}{\epsilon_0} \frac{\Gamma(\gamma, T)}{(1 - x_s^2)^{5/2}} \exp \left\{ \mathcal{F}(x_s) \right\}, \quad (41)$$

where

$$\begin{aligned} \mathcal{F}(x_s) &= \frac{\bar{U}_0}{\epsilon_0} \Gamma(\gamma, T) x_s^2 \\ &\quad - \frac{\bar{U}_0}{\epsilon_0} \left[x_s - (1 - x_s^2) \operatorname{arctanh} x_s \right. \\ &\quad \left. + \frac{2}{3} (\gamma^{-1} - 1) x_s^3 \right] - \frac{1}{2} \left[\frac{\bar{U}_0}{\sigma} \right]^2 x_s^4. \end{aligned} \quad (42)$$

With the help of the same transformation (40), Eq. (38) for the saddle point can be brought, after being multiplied by \bar{U}_0 , to the following form:

$$\begin{aligned} \frac{\bar{U}_0}{\epsilon_0} [\gamma^{-1} x_s + (\operatorname{arctanh} x_s - x_s)] + \left[\frac{\bar{U}_0}{\sigma} \right]^2 x_s^2 \\ = \frac{\bar{U}_0}{\epsilon_0} \Gamma(\gamma, T). \end{aligned} \quad (43)$$

We can now use the structure of this equation to simplify the expression for $\mathcal{F}(x_s)$. Multiplying Eq. (43) by x_s^2 and inserting it into (42), we get

$$\begin{aligned} \mathcal{F}(x_s) &= \frac{\bar{U}_0}{\epsilon_0} \left[\left[\operatorname{arctanh} x_s - x_s - \frac{x_s^3}{3} \right] + \frac{1}{3\gamma} x_s^3 \right] \\ &\quad + \frac{1}{2} \left[\frac{\bar{U}_0}{\sigma} \right]^2 x_s^4. \end{aligned} \quad (44)$$

Let us now turn our attention to the transcendental equation (43) for x_s . We shall consider it in the limit of low stresses,

$$\begin{aligned} \left[\frac{\gamma}{\gamma_0} \right]^2 \ll 1, \\ \gamma_0(T) = \Gamma^{-1}(0, T) \sim \frac{\sigma^2(T)}{\epsilon_0(U_0 - \bar{\epsilon}_0)} \ll 1, \end{aligned} \quad (45)$$

and seek the solution to it under condition $x_s^2 \ll 1 \ll (\epsilon_s/\epsilon_0)^{1/2}$. Taking advantage of this condition, we can use the asymptotic expansion of the hyperbolic function⁴³ to convince ourselves that the classical particle spends most of the time during its oscillation in the inverted potential in the region $x_0 < x < x_t^{(2)}(\epsilon_s)$. In this way we find that, to the lowest order in γ ,

$$x_s(\gamma, T) = \frac{\gamma}{\gamma_0(T)} \gg \gamma. \quad (46)$$

It now can be seen from the obtained result and Eq. (40) in what manner applied stress and temperature change the location of the optimal escape path under the barrier. While high stress levels and/or low temperatures force ϵ_s to go deeper under the barrier, at small τ and/or high T the optimal path is pushed closer to the barrier's top. Clearly it is this property of ϵ_s to move under the action of τ and T that establishes the actual regime of the breakaway kinetics.

If we now introduce Eq. (46) into the expression for $\mathcal{F}(x_s)$, we can present the leading term of the right-hand

side of Eq. (44) in the form

$$\mathcal{F}(x_s) = \frac{1}{3} \left[\frac{\gamma}{\gamma_Q(T)} \right]^2, \quad (47)$$

where the quantum stress γ_Q is defined as

$$\gamma_Q(T) = \left[\frac{\epsilon_0}{U_0} \right]^{1/2} \gamma_0^{3/2}(T) \ll \gamma_0(T). \quad (48)$$

Using now the same inequalities, under which the expression for x_s was obtained, we can bring the expression for σ_s to the following form:

$$\sigma_s(\gamma, T) \sim (\gamma x_s \epsilon_0 U_0)^{1/2} \sim \gamma \left[\frac{\epsilon_0 U_0}{\gamma_0(T)} \right]^{1/2}, \quad (49)$$

which shows explicitly that, when the applied stress is decreased, the effective width of the saddle (the quantum window for the escaping kink) becomes smaller. With the help of Eq. (49) we can now find that the pre-exponential factor in Eq. (41) becomes proportional to

$$\frac{\sigma_s}{\epsilon_0 \gamma_0(T)} \sim \frac{\gamma}{\gamma_Q(T)}. \quad (50)$$

Looking now at Eqs. (41), (47), and (50), one can notice that in the stress range defined jointly by Eq. (45) and the inequality $\gamma \gg \gamma_Q$, the contribution of underbarrier tunnel paths to the overall rate of breakaway turns out to be overwhelmingly larger than that of the overbarrier paths. In other words, in this stress range the process of breakaway proceeds via fluctuation-assisted tunneling through the pinning barrier. Furthermore, now the form of Eq. (41) indicates that in the range of small stresses, $\gamma \ll \gamma_Q$, the regime of the tunnel breakaway will be replaced by hopping regime. This conclusion, being true in essence, needs some further clarification, and here the criterion for the applicability of the saddle-point method will serve as a guide. In order to write down this criterion, we need the expression for the third derivative of $\phi(\epsilon)$, which takes the form

$$\begin{aligned} \phi'''(\epsilon_s) &\sim (\gamma \epsilon_0 U_0^2 x_s^3)^{-1} \\ &\sim \left[\frac{\gamma_0(T)}{\gamma} \right]^4 [\gamma_0(T) \epsilon_0 U_0^2]^{-1}. \end{aligned} \quad (51)$$

With the help of this formula and Eq. (49) the desired criterion is easily obtained. It is just

$$1 \gg \frac{\phi'''}{(\phi'')^{3/2}} \sim \frac{\gamma_Q(T)}{\gamma}. \quad (52)$$

This result shows that the saddle-point method works only in the stress range above γ_Q , and, what is essential, here it guarantees that $v_t(\gamma, T) \gg v_h(\gamma, T)$. The special attention, paid by Eqs. (47), (50), and (52) to the quantity γ_Q , emphasizes its significance for the present study, and it is, therefore, of direct physical interest to reveal the nature of origination of this characteristic stress. The following remark will be useful for achieving this goal. Above, we have been treating the barrier penetration pro-

cess in the WKB limit, which can be applied, strictly speaking, only to those underbarrier paths, for which the condition $D(\epsilon) \gg 1$ is fulfilled.⁴² Physically, this criterion means that many wavelengths of the tunneling particle are spanned by the barrier region. We can, therefore, still apply qualitatively the WKB approximation in the range of energies, lying close to, but below some critical energy ϵ_c , which has to be determined from the condition

$$D(\epsilon_c) \sim 1. \quad (53)$$

If we now introduce a dimensionless quantity $\alpha_c = (1 - \epsilon_c / \bar{U}_0)^{1/2}$, and assume that $\alpha_c^2 \ll 1$, then, using Eqs. (32)–(34) we can find from Eq. (53) that α_c is given by

$$\alpha_c \sim \left[\frac{\epsilon_0}{U_0} \gamma \right]^{1/3}. \quad (54)$$

After this preliminary remark, let us now see what will happen if the applied stress, being initially in the range above γ_Q , will be gradually decreased. Obviously both the WKB borderline level ϵ_c and the optimal escape level ϵ_s will now move towards the top of the barrier. If we compare the functional dependences of α_c and x_s on γ , we can conclude that the motion of the saddle point to the top is much faster. This means that, eventually, at some characteristic value of the applied stress, the optimal escape level will reach and cross the WKB borderline. It is easy to find, from Eqs. (40), (46), and (54) that this meeting of ϵ_s and ϵ_c will happen at

$$\gamma \sim \gamma_Q. \quad (55)$$

At this characteristic value of the applied stress, the distance remaining between the barrier's top and $\epsilon_s(\gamma_Q)$ will become of the order of

$$\bar{U}_0(\gamma_Q) - \epsilon_s(\gamma_Q) \sim \sigma_s(\gamma_Q) \sim \epsilon_0 \gamma_0(T) \ll \epsilon_0. \quad (56)$$

The foregoing observations, combined with the analysis carried out in Ref. 44, suggest that at low stresses below γ_Q the tunneling regime of escape will lose its importance and the hopping regime will dominate.

Let us now turn our attention to the characteristic features of quantum stress. A remarkable property of $\gamma_Q(T)$ is that this quantity is itself temperature dependent, increasing by about a factor $\eta^{3/2}(\theta_D, T_0)$ between its low-temperature ($T \sim T_0$) and high-temperature ($T \sim \theta_D$) values. Furthermore, at elevated temperatures above θ_D , when the whole phonon bandwidth becomes unfrozen, $\gamma_Q(T)$ begins to display a rapid increase with temperature as $T^{3/2}$. These observations imply that the higher the temperature of the crystal, the higher levels of the applied stress are required for the onset of the tunneling regime of breakaway. Having noticed this, one thus naturally approaches the question of comparison of the characteristic stress $\gamma_Q(T)$ with γ_P . Since it is this latter quantity which determines the upper limit of the actual stress interval in the present study [see Eq. (10)], one concludes that the quantum tunneling window can exist for the escaping kink if only γ_Q will be smaller than γ_P .

Denoting the ratio $\gamma_Q(T)/\gamma_P$ by $\beta(T)$, we can exploit our results obtained above, Eqs. (10), (16), (22), and (48), for writing down an order-of-magnitude estimate for $\beta(T)$ at two characteristic temperatures, T_0 and θ_D , that appear in our study. We find

$$\beta(T_0) \sim \left(\frac{\theta_D}{Ga^3} \right)^{1/2} \frac{\theta_D}{\epsilon_0} \left(\frac{U_0}{Ga^3} \right)^{1/2} \left(\frac{\theta_D}{T_0} \right)^{1/2} \times \left(\frac{Ga^3}{U_0 - \bar{\epsilon}_0} \right)^{3/2} \frac{a^3}{v}, \quad (57)$$

$$\beta(\theta_D) \sim \beta(T_0) \eta^{3/2}(\theta_D, T_0). \quad (58)$$

A number of small and large parameters of our theory are contained in these relations. It is possible to simplify somewhat the latter by noting that

$$\frac{a^3}{v} \frac{\theta_D}{\epsilon_0} \left(\frac{\theta_D}{T_0} \right)^{1/2} \sim \frac{a}{x_0} \frac{\omega_D}{\omega} \left(\frac{M}{\mu} \right)^{1/2} \sim \left(\frac{Ga^3}{U_0} \right)^{1/2}. \quad (59)$$

Using (59), we can continue our order-of-magnitude estimates as follows:

$$\beta(T_0) \sim \left(\frac{\theta_D}{Ga^3} \right)^{1/2} \left(\frac{Ga^3}{U_0 - \bar{\epsilon}_0} \right)^{3/2}, \quad (60)$$

from which it can be noticed that the condition $\beta < 1$ may be fulfilled when

$$\left(\frac{\tilde{U}}{Ga^3} \right)^{3/2} > 1, \quad (61)$$

where

$$\tilde{U} \sim (U_0 - \bar{\epsilon}_0) \left(\frac{Ga^3}{\theta_D} \right)^{1/3}, \quad T \sim T_0, \quad (62)$$

$$\tilde{U} \sim (U_0 - \bar{\epsilon}_0) \left(\frac{Ga^3}{\theta_D} \right)^{1/3} \eta^{-1}(\theta_D, T_0), \quad T \sim \theta_D. \quad (63)$$

An essential circumstance is the appearance of the smallness parameter $(\theta_D/Ga^3)^{1/2}$ in the above relations, Eqs. (57) and (58). To clarify this point, it will be helpful to pass in these relations to the abrupt kink limit [see the discussion after Eq. (16)]. In this limit our model gives $x_0 \rightarrow a$, $\omega \rightarrow \omega_D$, $\xi \rightarrow \xi_a$, $T_0 \rightarrow \theta_D$, $\eta(\theta_D, T_0) \rightarrow 1$, etc. The fundamental crystalline parameters, which survive in this limit are the characteristic Debye energy θ_D and the atomic scale energy Ga^3 , and from Eqs. (57) and (58) we can conclude that qualitatively

$$\beta(T_0) \rightarrow \beta(\theta_D) \sim \left(\frac{\theta_D}{Ga^3} \right)^{1/2} \ll 1. \quad (64)$$

VI. ACTIVATION PARAMETERS

A quantity, which is known to be informative for the purposes of identification of mechanisms by which dislocation segments overcome local or extended lattice barriers under uniform deformation or internal friction conditions, is the activation volume associated with the over-

coming process. It is interesting, therefore, to see what kind of a prediction gives the above presented theory for the stress dependence of the activation volume in the tunneling regime of the kink depinning process. For this purpose we need, together with Eqs. (41) and (47), the stress-dependent terms that are contained in the exponential figuring in the expression (26) for $v_h(\gamma, T)$. Extracting these terms, one can see that the condition $(3\gamma_0)^2 \ll 1$ is sufficient for the activation volume V_Q in the tunneling regime to display growth with the applied stress,

$$V_Q(\tau, T) = va(T) \left[1 + \frac{1}{3} b(T) \frac{\tau}{\tau_m} \right], \quad (65)$$

where the temperature-dependent coefficients of the linear form are given by

$$a(T) = \frac{T}{\epsilon_0} \gamma_0^{-1}(T), \quad (66)$$

$$b(T) = \gamma_0^{-2}(T). \quad (67)$$

We thus see that the sensitive dependence of the optimal escape level on τ and T plays an important role in establishing the stress and temperature dependence of the activation volume in the tunneling regime of breakaway.

Let us now turn our attention to the activation parameters, describing the hopping regime of breakaway. We have concluded above that this regime will take over in the stress range below $\min\{\gamma_Q, \gamma_P\}$. Here we can safely ignore several stress-dependent terms in Eq. (26) and bring the expression for the rate constant to the following form:

$$v = v_0 \exp \left\{ - \frac{(U_0 - \bar{\epsilon}_0)^2}{2\sigma^2(T)} \left[1 - \frac{\tau}{\tau^*} \right] \right\}, \quad \tau^* = \frac{U_0 - \bar{\epsilon}_0}{2v}, \quad (68)$$

$$v_0 = \frac{2^{1/2}}{6\pi} \omega_D \frac{(Ga^2b)^2 \sigma \theta_D T_0}{Ms^2 U_0^4} F(T) \frac{U_0}{U_0 - \bar{\epsilon}_0} \left(\frac{U_0}{\epsilon_0} \right)^{1/2} \times \exp \left\{ - \frac{U_0 - v\tau}{\epsilon_0} \right\}. \quad (69)$$

We can now reach rigorous conclusions regarding the temperature behavior of the depinning rate in the hopping regime. Combined with (22a), Eq. (68) suggests that in the classical temperature limit above θ_D the rate may be presented in an Arrhenius form:

$$v = v_0 \exp \left\{ - \frac{E^*(\tau)}{T} \right\}. \quad (70)$$

The attempt frequency exhibits a $T^{3/2}$ dependence, while the activation barrier height is given by

$$E^*(\tau) = U_0^* \left[1 - \frac{\tau}{\tau^*} \right], \quad (71)$$

$$U_0^* = \frac{(U_0 - \bar{\epsilon}_0)^2}{4\Delta}.$$

This result shows that the fluctuating lattice affects the activation energy of the breakaway process through the

polaron effect.

When the temperature is lowered, Eq. (22b) states that below θ_D quantum lattice fluctuations do come into action. As expected, the thermal-fluctuation Arrhenius law now ceases to give a correct description of the breakaway kinetics. However, one can preserve the formal structure of the Arrhenius exponent, if the actual T in Eq. (70) will be replaced by an effective temperature T_{eff} .²⁵ From Eqs. (22b) and (22c) and (68) we can find that

$$T_{\text{eff}} = \theta_D \begin{cases} \eta(T, T_0) \eta^{-1}(\theta_D, T_0), & T_0 \ll T \ll \theta_D & (72a) \\ \eta^{-1}(\theta_D, T_0), & T \ll T_0. & (72b) \end{cases}$$

We conclude from Eq. (72) that in the ultraquantum tem-

perature region below T_0 the process of breakaway proceeds athermally, and the rate constant exhibits a typical low-temperature plateau.^{27,45}

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