Anomalous mobility of dislocation kink solitons in disordered solid solutions

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Dislocation kink solitons in disordered solid solutions provide an example of quasiparticles showing anomalous kinetics—i.e., the nonlinear dependence of the displacement x on the time t, $x \sim t^{\delta}$ ($\delta < 1$). To describe the dynamic phase transition from the ordinary linear to anomalous regime, the dynamics of a quasiparticle in an energy landscape that performs a correlated random walk on the energy scale was theoretically studied. The phase diagram was characterized by the calculated temperature dependence of the threshold driving force F_{th} below which the average velocity of quasiparticles vanishes. The exponent δ of the kinetic equation for the anomalous phase, $x \sim t^{\delta}$, was determined by simple statistical arguments using the concepts of the "optimal fluctuation method." The dependence of the threshold driving force F_{th} on the concentration of solute atoms and statistical properties of a random energy landscape relevant to disordered solid solutions was calculated. The correlations between steps of the random potential were shown to modify the concentration dependence of F_{th}, thereby providing a qualitative explanation of experimental data on the dislocation pinning in solid solutions.

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I. INTRODUCTION

The problem of mobility of various kinds of particles in a disordered media has recently received considerable attention in the physics and mathematics communities [1–16] (see also references therein). As shown for these systems, a specific phase transition accompanied by a change in the mode of particle motion is possible due to a broad random scatter of the delay times at the fluctuation barriers. Thus, the drift of a particle changes from usual linear in time to sublinear, the latter being characterized by a slower increase in the displacement x with time t, $x \sim t^{\delta}$ ($\delta < 1$). The study of this phenomenon has stimulated interest in the basic concepts of the theory of irreversible processes. In mathematical papers, as well as in some physical publications, the existence of an extended slowly decreasing delay time spectrum is often only postulated. A deeper understanding of the factors responsible for the anomalous behavior can be reached by obtaining the true spectrum from the basic principles of statistical physics.

Keeping in mind the applications to physical systems, it is reasonable to begin with a study of the energy landscape determining the potential relief of the particle motion. In a disordered medium, there are random variations in the potential relief giving rise to barriers that trap the particle. A broad scatter of delay times at traps is associated with a high sensitivity of the thermally activated escape rate to variations in the barrier height. The use of methods of statistical physics allows calculations of the explicit dependence of the kinetic characteristics on the parameters governing the phenomenon for a particular system. In the present paper, this approach is employed to analyze the motion of dislocation kink solitons in disordered solid solutions.

A generally tacitly assumed prerequisite for the normal linear motion mode is the so-called "self-averaging" of the time of overcoming obstacles after passing a sufficiently large number of random barriers along a long path length of the particle. In this case, the total time of motion, t, consisting mainly (neglecting the time of free motion between the barriers) of a large number of delays at individual random obstacles, τ_i, $t = \Sigma_1^N \tau_i$, is approximately equal to $N\langle\tau\rangle$, where N is the number of obstacles in the path of the particle and $\langle\tau\rangle$ is the average delay time at one obstacle. There is also the rigorous mathematical formulation of this prerequisite based on the law of large numbers (see, e.g., [17]). However, the average delay time exists only if the delay time spectrum $P(\tau)$ decreases rather rapidly at long τ, not slower than $1/\tau^{\delta}$ with $\delta > 1$. In most cases, where the scatter of the delay time is caused by a superposition of local barriers or wells, this condition is fulfilled. As a consequence, it follows from the proportionality of the time of motion and the number of obstacles, N, which is, in turn, proportional to the path length x, that the spatial homogeneity is restored after the statistical averaging. As a result, the linear kinetic dependence of the particle displacement x on the time t, $x = \langle V\rangle t$, takes place, where $\langle V\rangle$ is the average velocity. On the contrary, if the average delay time diverges due to a slow decrease of the delay time spectrum, the self-averaging is violated and the time of motion is of the order of the longest delay time at the strongest obstacle along the path length, $t = \Sigma_1^N \tau_i \sim \tau_{\max}$. In this case, the spatial homogeneity is not restored after the statistical averaging and a dynamic phase transition from the kinetics linear in time to nonlinear kinetics would be expected.

For long delay times to be sufficiently probable, special factors enhancing the role of fluctuations are required. Such factors were revealed in [7,11] for kink-soliton-type quasiparticles (see, e.g., [18,19]), as exemplified by dislocation kinks [20] in crystals with randomly distributed impurity atoms. While linear topological defects in crystal lattices, dislocations, are responsible for the mechanical properties of crystalline materials, kinks in a dislocation line, at the second level of hierarchy, are responsible for the dynamics of dislocations in themselves. Being the earliest studied and most evident example of systems exhibiting the dynamic phase transition from the linear to nonlinear drift, the dislocation kink is by far not unique. Numerous examples from various fields of physics, chemistry, biology, geology, etc., were documented [1–16]. The so-called dislocation pinning may

be mentioned as a practical application of the considered phenomenon. A considerable retardation of the kink motion at a load lower than a certain threshold value F_{th} influences the mobility of a dislocation as a whole. For the stable operation of semiconductor devices, it is of great importance to prevent or, at least, retard the dislocation motion in (see, e.g., [21]). The range of subthreshold loads provides a "window" within which it is possible, to a considerable extent, to avoid the movement and multiplication of dislocations. The temperature dependence of the threshold load was used [22] to predict safe regimes of the thermal treatment of silicon wafers at their processing. In [23], the evolution of kink pairs on dislocations in Ge single crystals under a two-level intermittent load was studied and experimental evidence was obtained for the theoretically predicted anomalous nonlinear kink drift.

The calculations of F_{th} were carried out in [7,11] for low concentrations c of foreign atoms, $c \ll 1$, disregarding their mutual interactions. A generalization of the previous calculations accounting for the role of interactions of atoms within the dislocation core is required for the description of experiments on solid solutions with a wide variation of components. This is especially important for the characterization of the anomalous mobility governed by fluctuations with strong deviations from the average density of solute atoms. Hence, a consideration of the anomalous kinetics in a new wide class of correlated random potentials is necessary. This is the aim of the present paper. The image of a dislocation kink will be used for clarity. However, after the derivation of the model potential, one may forget about the specific character of the dislocation kink for the rest of the paper. The derived class of random potentials is rather general and can be used for the description of different one-dimensional systems.

II. RANDOM WALK ALONG THE ENERGY SCALE

Due to the periodicity of the crystal lattice, there is a set of periodically repeated energetically favorable positions for a dislocation, which are aligned along crystallographic directions. A dislocation kink connects branches of a dislocation located in neighboring valleys of the periodic crystalline relief. The dislocation transition from one valley to another proceeds via a lateral displacement of the kink, as shown in Fig. 1 (for details, see [20]). This determines the important role of kinks in the dislocation dynamics.

Randomly distributed foreign atoms violate the equivalence of dislocation states in different valleys of the crystalline relief. The energy of the dislocation core walks along the energy scale in the course of kink displacements, being shifted up and down (the shifts are of the order of the binding energy u of a foreign atom to the dislocation core) when the core randomly receives or loses the foreign atom (see Fig. 1). Therefore, there are not only local interactions between the moving kink and encountered foreign atoms, but also an additional contribution to the energy of the "dislocation+kink" system, which is proportional to the random difference $\Delta N(x)$ between the numbers of foreign atoms in the conjugated valleys along the kink path length x. Actually, the energy of the total dislocation+kink system plays the role of the potential in which the kink migrates. This potential is characterized by a partial "memory" of encountered foreign atoms. The random contribution to the energy integrated along the path length is a source of high randomness of the energy landscape in which the kink migrates (see Fig. 2), and it results in a fundamental distinction between the kink dynamics and the ordinary dynamics of localized particles. For dilute solid solutions, the mean distance between solute atoms is long and their mutual interactions may be ignored. In this case, the "steps" of the random walk potential along the energy scale may be considered as independent. This is the random potential with well-known statistical properties [7,24]. The scope of fluctuations in the energy landscape increases with the kink displacement x as $u\sqrt{x/\bar{l}}$, where $\bar{l}$ is the mean distance between foreign atoms along the valley of the crystal lattice. This is the physical reason for the appearance of a noticeable probability of high barriers and long delay times.

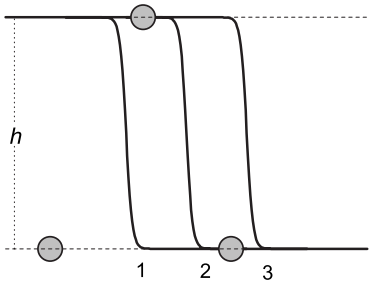

FIG. 1. A dislocation kink moving through randomly distributed solute atoms (represented by circles). The lateral displacement of the kink leads to a shift of the dislocation to another valley of the crystal lattice by the lattice period h. The kink transition via the subsequent positions 1-2-3 leads to either increase or decrease in the dislocation energy depending on the location of a foreign atom passed by the kink in a particular valley.

From the point of view of applications, the statistical properties of the random potentials reveal themselves differ-

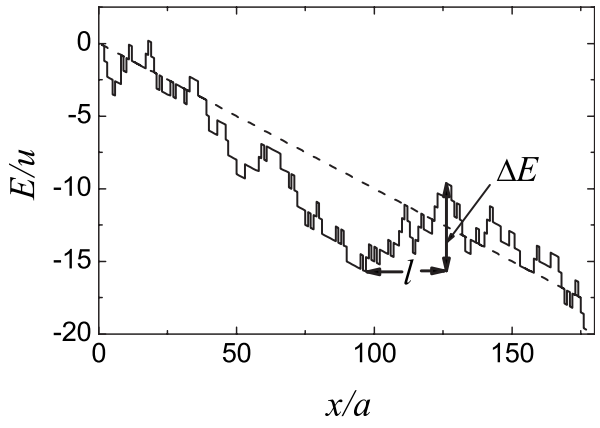

FIG. 2. A particular realization of the energy landscape formed by a superposition of the contributions of the randomly fluctuating density of solute atoms and the driving force. The height ΔE and the size l of the strongest barrier to the kink motion are marked.

ently in different parameter ranges. For example, at high temperature $kT > u$, the random walk potential, which performs discrete steps when the kink encounters foreign atoms, acts similarly to the continuous so-called "Brownian potential," which "diffuses" with the "diffusion coefficient" $D_E = cu^2$ along the energy scale. For this case, the exact solution describing the density of probability $P_2(t) = dP(t)/dt$ of delay times was calculated in [7] (see also [4]). In the notation of the present paper, it takes the form

$$P_2(t) = \frac{\exp[-\tau_1'/t]}{\tau_1'\Gamma(\delta)[t/\tau_1']^{1+\delta}}, \tag{1}$$

where $\delta = FakT/(cu^2)$, $\tau_1' = a(kT)^3/(D_k F c u^2)$, k is the Boltzmann constant, T is the temperature, a is the lattice period along the dislocation line, D_k is the kink diffusivity, $\Gamma(\delta)$ is the gamma function, and F is the driving force. In the case of a dislocation kink, the driving force $F = \sigma bh$, where σ is the corresponding component of the applied stress, b is the Burgers vector magnitude of the dislocation, and h is the height of the kink equal to the distance between the periodic valleys of the crystalline relief in the slip plane [20].

In [24], the theory of anomalous kinetics was extended to low temperatures $kT < u$. In the low-temperature range, the characteristic parameters of the anomalous kinetics δ and the threshold driving force F_{th} in solid solutions were demonstrated to considerably differ from the Brownian case. Due to this sensitivity of the anomalous kinetics to detailed parameters of the random potential, one may expect that, if the solid solution is not dilute, the correlations between subsequent "steps" in the random walk along the energy scale would be taken into account.

III. MODEL DESCRIPTION

Let us consider a solid solution $A_{1-c}B_c$, where c is the concentration of B-type atoms per site of the crystal lattice in the matrix of A-type atoms. The solid solution is supposed to be disordered with a "frozen" random distribution of atoms over the crystal lattice sites. The energy of the dislocation core depends on the amount and, due to the difference in interactions with the core of various combinations of solute atoms, on the configurations of both types of atoms along the dislocation line. The interactions between solute atoms are supposed to belong to short-range interactions. This means that their contribution to the energy of the dislocation core changes only when these atoms occupy the neighboring lattice sites. Let us denote the configuration of atoms within the first of the kink-connected valleys by the symbol Γ_1 and the configuration within the second valley by the symbol Γ_2. The corresponding energies of the dislocation states are denoted as $E\{\Gamma_1\}$ and $E\{\Gamma_2\}$. In terms of this model, the energies of dislocations located in different valleys of the crystal lattice are supposed to be statistically independent. As to the energy of the dislocation core itself, its modification by both isolated solute atoms (in our case, B atoms) and their complexes composed of any number of neighboring atoms along the dislocation line should be taken into account.

The change in the energy of the dislocation segment $E\{\Gamma\}$ caused by B atoms may be written as a sum of the bond energies of the neighboring atoms counted from the A-A-type bond energies. Let us ascribe the energy u_{AB} to A-B- or B-A-type bonds (assumed, for simplicity, to be equal) and the energy u_{BB} to B-B-type bonds. The configuration Γ can be characterized by a set of the random occupation numbers of sites $\{n_i\}$ by solute atoms (B type). If the ith site is occupied by a solute atom, then $n_i = 1$ (with the probability c); otherwise, $n_i = 0$ (with the probability $1-c$). Obviously, the total number n of solute atoms in the dislocation segment of length $l = aN$ is equal to $n = \Sigma_1^N n_i$. Here N is the number of sites in the segment. The change in the energy of the dislocation segment $E\{\Gamma\}$ due to the presence of solute atoms can be written using the occupation numbers in an explicit form

$$E\{\Gamma\} = 2u_{AB}\sum_{i=1}^{N} n_i + (u_{BB} - 2u_{AB})\sum_{i=1}^{N-1} n_i n_{i+1}. \tag{2}$$

With the relationship between the parameters $u_{BB} = 2u_{AB}$, the quadratic over n_i contributions to $E\{\Gamma\}$ are absent. This more simple random potential has been studied earlier [7,24]. In the presence of the quadratic terms over n_i, we shall refer to $E\{\Gamma\}$ as the random potential involving "interactions" between solute atoms in solid solution. The parameters $u_{BB} < 2u_{AB}$ and $u_{BB} > 2u_{AB}$ will model the attraction and repulsion, respectively, between B atoms at dislocations.

IV. AVERAGE TIME OF RANDOM BARRIER OVERCOMING

To calculate the time τ required for a kink to overcome a barrier formed by a fluctuation of the density of solute atoms, the following general formula for the time of the thermally activated transition of a particle through a potential barrier [25] can be used:

$$\tau = \frac{x_1}{D_k}\int_0^\infty \exp\left(\frac{\Delta E(x)}{kT}\right)dx. \tag{3}$$

Here, D_k is the diffusivity of the particle (in the case under consideration, of the kink), x_1 is the coefficient of the length dimension associated with the range of prebarrier state localization, and $\Delta E(x)$ is the profile of the potential hindering the particle displacement. In the case under study, $\Delta E(x) = E\{\Gamma_2\} - E\{\Gamma_1\} - Fx$ is the energy difference of the dislocation segments in the valleys of the crystalline relief between which the transition occurs. In addition, the work of the driving force F is taken into account. When the obstacle to be overcome is formed by a single solute atom [according to Eq. (2), it creates a step of the height $2u_{AB}$], the metastable prebarrier state is localized at the size $x_1 = kT/F$ and the delay time τ_1 calculated according to Eq. (3) is equal to

$$\tau_1 = \frac{(kT)^2}{D_k F^2}\exp\left(\frac{2u_{AB}}{kT}\right). \tag{4}$$

The average velocity of the kink, $\langle V \rangle$, accounting for the contribution of delays at isolated solute atoms can be calculated as

$$\langle V\rangle = \frac{V_0}{1 + V_0\tau_1/\bar{l}}, \tag{5}$$

where V_0 is the velocity of free motion between obstacles. As follows from Eq. (5), for sufficiently high concentrations of solute atoms, $\langle V\rangle \approx \bar{l}/\tau_1$, and the velocity of the kink is mainly limited by the obstacles to be overcome. However, obstacles can also be of a combined type, resulting from a random accumulation of solute atoms. Their contribution drastically changes the kink dynamics and violates the mode of motion linear in time and characterized by a finite nonzero velocity.

Let us calculate the average delay time at a barrier formed by an arbitrary fluctuation of the density of solute atoms. For this purpose, let us average the random integrand in Eq. (3):

$$\langle\tau\rangle = \frac{x_1}{D_k}\int_0^\infty \left\langle \exp\left(\frac{E\{\Gamma_2\} - E\{\Gamma_1\}}{kT}\right)\right\rangle \exp\left(-\frac{Fx}{kT}\right)dx. \tag{6}$$

The averaging is performed by summing over all possible distributions of B atoms over the lattice sites accounting for the corresponding probability determined by their concentration c. Possible statistical variations of x_1 in the preexponential factor are neglected. Although the averaged energies $E\{\Gamma_1\}$ and $E\{\Gamma_2\}$ in different valleys of the crystal lattice coincide due to the statistical homogeneity of the solid solution, the averaging of the nonlinear exponential terms results in the effective dragging force exerted on kinks.

When calculating the averaged exponential in Eq. (6), it is reasonable to use the transfer matrix method elaborated for the Ising model (see, e.g., [26]). Due to the supposed statistical independence of the energies $E\{\Gamma_1\}$ and $E\{\Gamma_2\}$, the average of interest is split into the product of the averages $\langle\exp(E\{\Gamma\}/kT)\rangle$ and $\langle\exp(-E\{\Gamma\}/kT)\rangle$. Let us introduce an auxiliary quantity Z_N^ν, which is a sum of the terms $\exp(E\{\Gamma\}/kT)$ calculated over all configurations Γ accounting for their statistical weights for a definite state of the last link. There are two such states labeled by the index ν, $\nu=0$ and $\nu=1$. The value of ν coincides with the occupation number of the last site by a B atom.

The quantities Z_N^ν obey recurrence relationships for dislocation segments with a length differing by one link:

$$Z_{N+1}^0 = (1-c)Z_N^0 + cZ_N^1\exp(-u_{AB}/kT), \tag{7}$$

$$Z_{N+1}^1 = (1-c)Z_N^0\exp(-u_{AB}/kT) + cZ_N^1\exp(-u_{BB}/kT). \tag{8}$$

Introducing the transfer matrix $V_{\nu\mu}$, the elements of which are clear from Eqs. (7) and (8), it is possible to rewrite the recurrence relationships as

$$Z_{N+1}^\nu = \sum_\mu V_{\nu\mu}Z_N^\mu. \tag{9}$$

The N-fold application of Eq. (9) enables us to express Z_{N+1}^ν via the first-link state vector Z_1^ν and the product of transfer matrices

$$Z_{N+1}^\nu = \sum_\mu (V^N)_{\nu\mu}Z_1^\mu. \tag{10}$$

The dependence Z_N^ν on N for large N, as is known from matrix theory, is given by the factor λ_1^N, where λ_1 is the largest eigenvalue of the transfer matrix. Indeed, for large N the effect of the boundary conditions becomes negligible and V^N depends on N in the same way as this matrix trace $\mathrm{Tr}(V^N)=\lambda_1^N+\lambda_2^N$ with the predominant contribution of the largest eigenvalue λ_1.

The largest eigenvalue of the matrix V is easily determined and equal to

$$\lambda_1 = \frac{1}{2}\left(1 - c + c\exp\left(\frac{u_{BB}}{kT}\right) + \left\{\left[1 - c - c\exp\left(\frac{u_{BB}}{kT}\right)\right]^2 + 4c(1-c)\exp\left(\frac{2u_{AB}}{kT}\right)\right\}^{1/2}\right). \tag{11}$$

Therefore, we obtain

$$\langle\exp(E\{\Gamma\}/kT)\rangle \approx \lambda_1^N. \tag{12}$$

To calculate the second average of interest, $\langle\exp(-E\{\Gamma\}/kT)\rangle$, it is sufficient to change signs at u_{AB} and u_{BB} in Eq. (11),

$$\langle\exp(-E\{\Gamma\}/kT)\rangle \approx \lambda_1'^N,$$

where

$$\lambda_1' = \frac{1}{2}\left(1 - c + c\exp\left(-\frac{u_{BB}}{kT}\right) + \left\{\left[1 - c - c\exp\left(-\frac{u_{BB}}{kT}\right)\right]^2 + 4c(1-c)\exp\left(-\frac{2u_{AB}}{kT}\right)\right\}^{1/2}\right). \tag{13}$$

Collecting all factors providing the dependence of the integrand in Eq. (6) on $N \approx x/a$, we obtain

$$\exp\{(x/a)\ln(\lambda_1\lambda_1') - Fx/kT\}. \tag{14}$$

Hence, the integral converges for $F > F_{\mathrm{th}}$, where

$$F_{\mathrm{th}} = \frac{kT}{a}\ln(\lambda_1\lambda_1') = \frac{kT}{a}\ln\left[\frac{1}{4}\left(1 - c + c\exp\left(\frac{u_{BB}}{kT}\right) + \left\{\left[1 - c - c\exp\left(\frac{u_{BB}}{kT}\right)\right]^2 + 4c(1-c)\exp\left(\frac{2u_{AB}}{kT}\right)\right\}^{1/2}\right)\right.$$
$$\left.\times\left(1 - c + c\exp\left(-\frac{u_{BB}}{kT}\right) + \left\{\left[1 - c - c\exp\left(-\frac{u_{BB}}{kT}\right)\right]^2 + 4c(1-c)\exp\left(-\frac{2u_{AB}}{kT}\right)\right\}^{1/2}\right)\right], \tag{15}$$

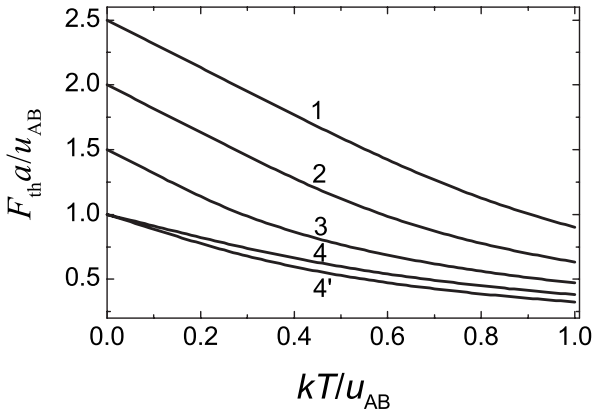

FIG. 3. The temperature dependence of the threshold driving force F_{th} for the concentration of B atoms, $c=0.2$, and for different bond energy ratios $z=u_{BB}/2u_{AB}$: $z=1.25$ (curve 1), $z=1$ (curve 2), $z=0.75$ (curve 3), $z=0.5$ (curve 4), and $z=0.2$ (curve 4′).

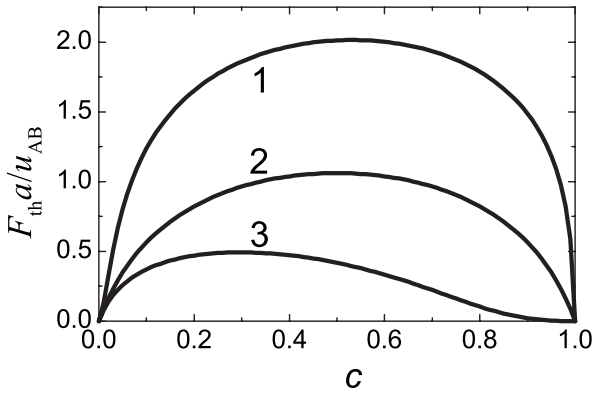

FIG. 4. Plot of the threshold driving force F_{th} at the temperature $T=0.75u_{AB}/k$ vs the concentration c of B-type atoms for different bond energy ratios $z=u_{BB}/2u_{AB}$: $z=1.25$ (curve 1), $z=1$ (curve 2), and $z=0.75$ (curve 3).

and diverges for $F \leqslant F_{th}$. The latter means increasing to infinity the average time of overcoming barriers against the kink migration formed by the fluctuations of solute atoms density and, hence, the vanishing of the average kink motion velocity. For $F > F_{th}$ and $F \to F_{th}$, the average time of the transition over a barrier given by Eq. (6) increases as $\langle \tau \rangle \sim 1/(1-F_{th}/F)$. Correspondingly, in this case the average kink velocity is approximately equal to

$$\langle V \rangle \approx \frac{\bar{l}}{\langle \tau \rangle} \approx \frac{\bar{l}}{\tau_1}\left(1 - \frac{F_{th}}{F}\right). \tag{16}$$

This is direct evidence for the mobility threshold indicating an appreciable retardation of the kink motion for $F < F_{th}$.

The relationship between the parameters $u_{BB}=2u_{AB}$ corresponds to the additive contribution of solute atoms to the total energy, Eq. (2), which means the absence of interactions between these atoms. In this case, the energy $u=2u_{AB}$ may be attributed to a site containing a B atom instead of attributing different energies to atomic bonds. This simplifies the calculations, and Eq. (15) takes the form

$$F_{th} = \frac{kT}{a} \ln\left\{1 + 2c(1-c)\left[\cosh\left(\frac{2u_{AB}}{kT}\right) - 1\right]\right\}, \tag{17}$$

which is consistent with the earlier result [7,23].

It should be noted that F_{th} remains unchanged upon the simultaneous change in the signs of u_{AB} and u_{BB}. Positive values u_{AB} and u_{BB} will be used for illustrating the calculations. In addition, F_{th} is invariant with respect to which matrix (consisting of either A or B atoms) is recognized as the basic one and, correspondingly, to which atoms are considered as foreign. The arbitrary choice of the matrix formed by A atoms may be changed to the matrix formed by B atoms. The expression for the threshold force F_{th} appears to be the same for the $B_{1-c'}A_{c'}$ solid solution after the substitution $c \to c'=1-c$, $u_{AB} \to u'_{AB}=u_{AB}-u_{BB}$, $u_{BB} \to u'_{BB}=-u_{BB}$.

Expression (17) predicts a noticeable increase in F_{th} with decreasing temperature. The same is true for the general case described by Eq. (15) and illustrated in Fig. 3. The equation $F=F_{th}(T)$ determines a line of the dynamic phase transition with destruction of the mode of motion linear in time. Figure 3 illustrates a modification of the phase diagram due to interactions between solute atoms for a set of varying parameters. The threshold driving force increases with increasing u_{BB}, and, on the contrary, it decreases with decreasing u_{BB} compared to the noninteractive case $u_{BB}=2u_{AB}$. The limiting value of F_{th} for $T \to 0$ is equal to u_{BB}/a, if $u_{BB} > u_{AB}$, and to u_{AB}/a, if $u_{BB} < u_{AB}$.

Let us mention some qualitative features of the concentration dependence of the threshold driving force, which are of interest for a comparison with experimental data. In the absence of interactions between solute atoms, the concentration dependence of the threshold driving force F_{th} described by Eq. (17) is of a domelike form symmetric with respect to the transposition of the components—i.e., to the substitution $c \to 1-c$. Since F_{th} corresponds to the resistance of fluctuations of the density of solute atoms to the kink motion, it has the largest magnitude for the intermediate concentration of solutes, $c \sim 1/2$—i.e., for the maximum heterogeneity. However, the symmetry of the concentration dependence F_{th} given by Eq. (17) is a special case and may not be fitted to experimental data. To describe the asymmetric resistance force, it is necessary to consider a more general case. The symmetry of the curve $F_{th}(c)$ is violated if the interactions between atoms of different sorts are taken into account, as is illustrated in Fig. 4.

A remarkable peculiarity of the concentration dependences presented in Fig. 4 is the sharp increase of F_{th} in the range of small c. It follows from Eq. (15) that $F_{th} \approx 2c\frac{kT}{a}\left[\cosh\left(\frac{2u_{AB}}{kT}\right)-1\right]$ for $c \to 0$, so that the slope of the concentration dependence at low temperature $kT \ll 2|u_{AB}|$ may be very steep. In the range $c \to 1$ it follows from Eq. (15) that $F_{th} \approx 2(1-c)\frac{kT}{a}\left[\cosh\left(\frac{2(u_{BB}-u_{AB})}{kT}\right)-1\right]$. Therefore, the concentration dependence F_{th} for $c \to 1$, $z=u_{BB}/(2u_{AB}) > 1$, is even steeper than for small c (the curve 1) and is more flat at $z < 1$, (curve 3). As the result, maximum of the concentration dependence for $z > 1$ is shifted to the side of large c, whereas for $z < 1$ it is shifted to the side of small concentration, thereby creating the curve asymmetry.

This behavior can be compared with the experimental dependence of the yield stress for the $Ge_{1-c}Si_c$ solid solution on the concentration of Si atoms [28]. The yield stress, which is determined by the resistance to the dislocation motion, correlates with the friction force exerted on kinks, which may be characterized by F_{th}. This provides insight into the well-defined domelike shape of the experimental concentration dependence of the yield stress. A certain asymmetry of the concentration dependence of the yield stress may be attributed to a weak repulsion between silicon atoms within the dislocation core.

V. STATISTICAL PROPERTIES OF THE GENERALIZED RANDOM POTENTIAL

The fluctuation contribution to the energy of the dislocation core, Eq. (2), gives rise to a random potential for the kink motion, whose statistical properties depend on relationships between parameters. In the particular case of noninteracting solute atoms $u_{BB}=2u_{AB}$, the potential values at different crystal sites are uncorrelated. The correlation is introduced into the generalized random potential of solutes, Eq. (2), by interaction of solutes. As shown above, this correlation leads to a quantitative change in the boundary $F=F_{th}$ of the normal linear (in time) phase of the kink motion, which is accompanied by the appearance of a new qualitative feature, the asymmetry of the concentration dependence of the threshold driving force F_{th}.

It is worthy of note that the calculated quantity $\langle \exp[\beta(E\{\Gamma_2\}-E\{\Gamma_1\})]\rangle$ ($\beta=1/kT$) is in fact the generating function for the energy distribution. It allows the calculation of the average of any powers (cummulants) of random contributions to the energy of the dislocation core. As an example, after a straightforward calculation we obtain

$$\langle (E\{\Gamma_2\}-E\{\Gamma_1\})^2\rangle = \frac{d^2}{d\beta^2}\langle \exp[\beta(E\{\Gamma_2\}-E\{\Gamma_1\})]\rangle|_{\beta=0} = 2ND_E, \tag{18}$$

where $D_E=c(1-c)\{c(3c+1)u_{BB}^2+4(1-3c+3c^2)u_{AB}^2-4c(3c-1)u_{AB}u_{BB}\}$ is a "diffusivity" of the random potential along the energy scale in the course of the kink motion (the path length expressed in lattice periods, N, plays a role of the time by analogy with the ordinary spatial diffusion). In addition, it determines the high-temperature behavior of the threshold driving force. As follows from Eq. (15), $F_{th}\approx D_E/(akT)$ when $T\to\infty$.

VI. ANOMALOUS KINETICS OF KINKS

The qualitative pattern of the anomalous mobility in the subthreshold interval of loads, which was established for noninteracting foreign atoms [7,27], can be extended to the general case under consideration. The change in the characteristics of the kink motion due to the vanishing of its average velocity is governed by the contribution of long delay times at barriers formed by random accumulation of solute atoms. It turns out that, at $F<F_{th}$, the total contribution of abundant delays at typical or most common barriers [around the maximum of the spectrum $P(\tau)$] is smaller than the contribution of one the strongest barrier at the path length. As a result, the path length distribution is unambiguously related to the asymptotic of the probability of long delay times. In this case, the evolution of the path length distribution with time is represented by the so-called Lévy distribution (see, e.g., [4,15]). The typical dependence of the displacement x on time t, which provides less detail and is described only by the characteristic scale of the Lévy distribution function, is of prime interest for most applications. There is an analogy with the ordinary diffusion, for which the time dependence of the typical displacement, $x\sim t^{1/2}$, can be found without of the complete solution of the diffusion equation. Similarly, the time scaling of the displacement for the anomalous migration of a particle can be determined in a simple qualitative way. Let us demonstrate this, remembering that, in the considered case, the time spent in passing a certain length is determined by the strongest barrier along the length.

If the probability to encounter a barrier with a delay time longer than t is $P(t)$, then the displacement during the time t will be of the order of the mean distance between such barriers, $x\sim 1/P(t)$. For example, the delay time spectrum $P(t)$ for dilute solid solutions is given by $P(t)=\int_t^\infty P_2(t')dt'$ with $P_2(t)$ of Eq. (1). Since only the behavior of the spectrum $P(t)$ at long delay times is of actual interest, for $P(t)$ it follows from Eq. (1) that $P(t)\sim 1/t^\delta$ and $x\sim 1/P(t)\sim t^\delta$ with $\delta=FakT/(cu^2)$. This result, the sublinear regime of the drift for $\delta<1$, was extended by different methods to different random walk models in [4,6,10,11,24,27] (see also references therein). The exponent δ is the most important parameter controlling the path length distribution. This exponent is different for different models and, in particular, it depends on the type of the random potential correlations [13,14]. Detailed calculations for the thermally activated motion of particles in random potentials showed [4,6,7,11,12,24,27] that the exponent δ depends linearly on the temperature so that it can be represented as $\delta=T/T_g$ [in Eq. (1), $T_g=cu^2/(kaF)$]. Since the condition for the transition with changing motion regime is $\delta=1$, the temperature $T=T_g$ has the meaning of the dynamic phase transition temperature.

It can be shown that the linear temperature dependence of δ holds for a wide class of random potentials, including the potential (2) under consideration, and it has a simple physical origin. Since the condition of the transition from the normal to anomalous regime is known [see Eq. (15)], δ can be determined without additional calculations. The use of a qualitative representation of the arrangement of fluctuation barriers controlling the process in terms of the "optimal fluctuation method" [29] provides a useful insight into the physics of the phenomenon.

Let us consider a strong barrier, which is created by a large fluctuation in the density of solute atoms (see Fig. 2) and provides a long delay time. The strong barrier consists of a large accumulation of solute atoms and comprises a large number of sites of the crystal lattice, $N\gg 1$. Hence, N is a large parameter of the theory, enabling simplification of the calculations. Since only the energy at the maximum of the potential relief giving the activation energy is of interest, let us characterize the random accumulation of solutes by the

following two parameters: a distance $l=aN$ between the minimum of the prebarrier potential and the maximum and an increment of the random potential E_a between these points. The external driving force reduces the barrier height to

$$\Delta E = E_a - FaN. \tag{19}$$

Thermal activation requires for the escape from the well, so that the delay time of a kink is estimated by the Arrhenius formula as

$$t = \tau_* \exp\left(\frac{N(\varepsilon_a - Fa)}{kT}\right). \tag{20}$$

Here, considering the energy of the solute accumulation at large $N \gg 1$ to be an extensive quantity, the density of energy per a lattice site, $\varepsilon_a = E_a/N$, is introduced; τ_* is the preexponential factor, which is of no importance for further considerations and is, in the first approximation, a constant. The distribution function $P(t)$ of the delay times is determined by the probability to encounter a well with a given escape time t. This condition fixes one of the involved random parameters—for example, N:

$$N = \frac{kT \ln(t/\tau_*)}{\varepsilon_a - Fa}. \tag{21}$$

The energy density ε_a depends also on intensive quantities, such as the concentrations of solute atoms in the first and second valleys on the accumulation size scale, c_1 and c_2, respectively. These concentrations do not affect the linear dependence of N on T and should be chosen in such a way as to represent the most often occurring accumulations of solute atoms with the required properties—i.e., from the condition for the maximum probability P over c_1 and c_2. The probability to meet this accumulation can be expressed as $P \sim \exp(S)$, where S is the entropy. The condition for the maximum of S over c_1 and c_2 leads to the equations in the optimal values of c_1 and c_2, allowing, in principle, for a determination of the complete arrangement of density fluctuations of solute atoms controlling the kink mobility. However, this detailed information is not necessary for the determination of the quantity of interest: the delay time spectrum. Since the entropy is also an extensive quantity and is additive over the accumulation size, we have $S \sim N$. Then Eq. (21) shows that the entropy $S_{\max}$ of the optimal fluctuation is proportional to $T \ln(t/\tau_*)$. This allows a representation of the probability P in the form

$$P(t) \sim \exp(S_{\max}) \sim \left(\frac{\tau_*}{t}\right)^{T/T_g}. \tag{22}$$

As is easily seen, the scale factor T_g in Eq. (22) coincides with the temperature of the dynamic phase transition from the ordinary linear to the anomalous migration regime. Actually, the quantity T_g characterizes the probability of long delay times of a kink during its motion along the dislocation. A large value of T_g means a slowly decreasing probability of long delay times and, consequently, a long average delay time $\langle \tau \rangle$:

$$\langle \tau \rangle = \int_0^\infty t \frac{dP(t)}{dt} dt = \int_0^\infty P(t) dt. \tag{23}$$

Moreover, the probability $P(t)$ decreases for $T \leqslant T_g$ so slowly that the integral in Eq. (23) diverges and the average delay time becomes infinite. The mobility becomes anomalous and, in this case, the mean displacement $x(t)$ is determined by the average distance between barriers with the delay time exceeding t:

$$x(t) \sim \frac{\Delta l}{P(t)} \sim \Delta l \left(\frac{t}{\tau_*}\right)^{T/T_g}. \tag{24}$$

Thus, the displacement of a kink increases with time more slowly than in the case of the ordinary linear drift under the driving force. The scale parameters Δl and τ_*, which are of secondary interest, are not determined in the framework of this simple approach. To obtain rough estimates, one may use values typical of minimal barriers formed by isolated solute atoms, $\Delta l \sim \bar{l} \sim a/c$ and $\tau_* \sim \tau_1$.

Since the condition for the transition to the anomalous kinetics $T=T_g$ corresponds to the average delay time $\langle \tau \rangle$ approaching infinity, it coincides with the previously found condition determining the threshold value of the driving force, Eq. (15), and vice versa, if the driving force is given, the phase transition temperature T_g can be found from the equation

$$F = F_{\text{th}}(T_g), \tag{25}$$

where the function $F_{\text{th}}(T)$ is given by Eq. (15). Therefore, Fig. 3 represents also the dependence of T_g on the driving force F and other parameters. At low driving forces $F \ll F_{\text{th}}$, the phase transition temperature behaves as $T_g \approx D_E/(kFa)$ with D_E determined under Eq. (18).

Formula (24) gives the desired generalization of the kinetic law of the kink motion in the correlated random potential under consideration with an explicit indication of the temperature dependence of the exponent $\delta = T/T_g$. The phase transition temperature T_g depends, besides the driving force F, on the mean concentration of solute atoms c and the bond energies u_{AB} and u_{BB}. The dynamic phase transition from the normal linear drift of kinks $x \sim t$ for $T > T_g$ to the anomalous sublinear regime of motion $x \sim t^\delta$ with $\delta = T/T_g$ for $T < T_g$ is illustrated in Fig. 5.

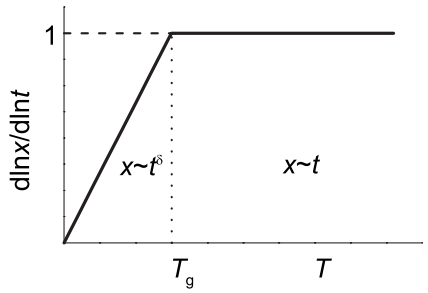

FIG. 5. A schematic illustration of the dynamic phase transition as the motion regime changes from the normal (linear in time) drift $x \sim t$ to the anomalous sublinear drift $x \sim t^\delta$ ($\delta < 1$).

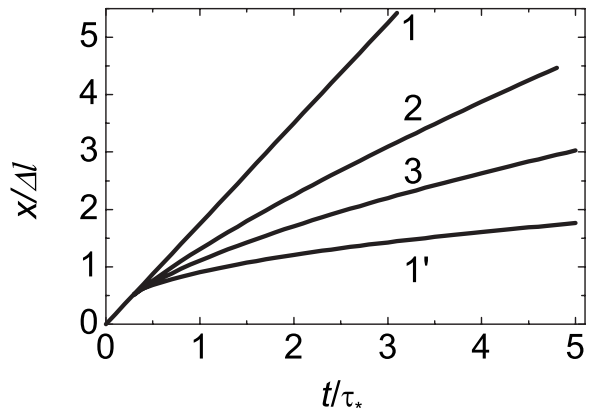

FIG. 6. The dependence of the displacement x on the time t for different driving forces F and the bond energy u_{BB}: $F=1.75u_{AB}/a$, $u_{BB}=2u_{AB}$ (curve 1); $F=1.6u_{AB}/a$, $u_{BB}=2u_{AB}$ (curve 2); $F=1.5u_{AB}/a$, $u_{BB}=2u_{AB}$ (curve 3); and $F=1.75u_{AB}/a$, $u_{BB}=2.5u_{AB}$ (curve 1′). The temperature and the solute concentration are equal to $T=0.75u_{AB}/k$ and $c=0.3$, respectively. For the parameters corresponding to curves 1–3, the threshold driving force is $F_{\text{th}}=1.69u_{AB}/a$; for the parameters of curve 1′, $F_{\text{th}}=2.19u_{AB}/a$. Δl and τ_* are the scale parameters of Eq. (24) in the text.

Figure 6 shows the modification of the kinetic dependences when the driving force F decreases below the threshold value F_{th}. Curves 2, 3, and 1′ calculated according to Eq. (24) (curve 1′ was calculated taking into account interactions of solute atoms) show a much slower sublinear increase in the displacement x with time t compared to the linear dependence described by curve 1.

VII. CONCLUSION

In the present paper, the theory of the dislocation kink motion in a random potential landscape formed by randomly distributed atoms of a disordered solid solution was developed. The total energy of the dislocation+kink system plays a role of the potential, in which the kink migrates. The statistical properties of the energy of the dislocation core are described with consideration of short-range interactions between solute atoms, which can either enhance or reduce random potential fluctuations depending on the sign of the interaction. This system can be modeled by a one-dimensional quasiparticle migrating in a potential, which performs a correlated random walk along the energy scale in the course of the displacement of the quasiparticle. It was shown that a dynamical phase transition from the linear in time to anomalous sublinear regime of the quasiparticle motion in this potential takes place if the driving force is less than a certain threshold value F_{th}. The kinetics of overcoming the barriers formed by solute density fluctuations along the kink path determines the threshold driving force F_{th} and its temperature and concentration dependences. It should be noted that the earlier developed theory, which ignores the correlations in the random potential, is applicable only to a description of the symmetric concentration dependences of the threshold driving force, whereas the present theory allows a description of the general behavior of more realistic systems.

Due to the fluctuation nature of the kink retardation, the calculated increase in the threshold driving force appeared to be strongest in the intermediate concentration range of a solid solution corresponding to the maximum of the material disorder and it approaches zero for any pure component. This behavior provides an explanation for the pronounced dome-like shape of the experimental concentration dependence of the yield stress in the $Ge_{1-c}Si_c$ solid solution [28].

The quasiparticle kinetics in the anomalous regime is controlled by the spectrum of extremely long delay times related to seldom strong fluctuations of the random potential. The statistics of such fluctuations can be efficiently characterized by clear arguments of the "optimal fluctuation method" devised in the theory of disordered systems. In the present paper, these arguments were used for obtaining the distribution of long delay times of quasiparticles at traps formed by fluctuations of the density of solid solution atoms. The temperature T_g of the dynamic phase transition with vanishing of the average velocity of the quasiparticle motion was calculated depending on the parameters of the system. The kinetic law of the quasiparticle motion, $x(t)\sim t^{T/T_g}$, for the anomalous range $T<T_g$ was substantiated. As is seen from the derived formulas and presented figures, the correlations in the random potential noticeably modify the characteristics of the anomalous kinetics of quasiparticles. This may be attributed to the crucial role of strong fluctuations of the random potential caused by large deviations of the density of solute atoms from its mean value.

Finally, let us mention that the extension of the theory to the more general correlated random potential enables applications to a wider class of various systems, such as steps at crystal facets, domain boundaries in two-dimensional phases on a substrate, biological macromolecules, etc.

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