Transition from solid-solution softening to hardening in the plasticity of crystalline materials as a manifestation of quasi-localization of dislocation kinks

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The mechanical properties of materials are highly sensitive to the content of impurities and point defects due to their interaction with plastic deformation carriers-dislocations. This opens up the possibility to some extent control the mechanical properties of materials through alloying and creating solid solutions. In a number of crystalline materials, in addition to the well-known solid-solution strengthening in the region of a low concentration of solution atoms, the opposite behavior is also observed — an increase of plasticity, or softening. In the present work, the mechanism of competition of these effects is revealed and it is shown how the boundary of behavior change can be used to estimate the microscopic parameters of materials. The theory predicts trends in the dependence of plasticity on the concentration of alloying elements, stress, temperature, strain rate, and a number of material parameters.

Keywords: competition of solid-solution hardening and softening, dislocation kinks, random processes.

1. Introduction

The effect of solid-solution hardening of crystalline materials, explained by coupling of plastic deformation carriers — dislocations — to local distortions of the crystal lattice by foreign atoms is widely known [1,2]. However, materials with a high potential relief of the crystal lattice, called the Peierls barriers, also feature the seemingly paradoxical opposite effect of plasticity increase upon doping [3] both with interstitial atoms and substitution atoms. Such materials include metals with a body-centered crystal (BCC) lattice, some semiconductors, ceramics, intermetallides and others [1,3–5], plasticity of which was found to be controlled by dislocations' overcoming of the crystal relief. Thereat, foreign atoms do not create additional obstacles for dislocations, but facilitate their motion. The most popular explanation of this absence of additivity of dislocation impediment mechanisms is a local reduction of the main barriers, generated by the crystal lattice, by solution atoms [3,5,6]. Crystal relief height in a pure crystal is characterized by the so-called Peierls stress — the minimum stress which eliminates barriers for dislocation displacement between crystal lattice valleys [7]. The presence of foreign atoms complicates the potential relief of the crystal lattice. The plasticity increase effect, or softening, is observed at low concentrations ≤ 1%, and gives place to hardening in the region of higher concentrations [3,8]. The softening to hardening transition has not been studied well enough so far, and the present paper is dedicated to studying its mechanism.

Dislocations in such materials move by the well-known way of formation and propagation of kinks, which are topological solitons [1,4,7,9]. The properties of these peculiar quasi-particles manifest themselves on the macroscopic scale, in particular, in a strong temperature dependence of deformation stresses; this is explained by the fact that kink formation is a thermally-activated process taking place in a small volume with a linear size of about tens of lattice constants [1,4]. The competition of softening and hardening effects can be ascribed to a manifestation (on the macroscopic scale) of different influence of solution atoms on different stages, thus promoting the kink formation and preventing their propagation [8,10–12].

The influence of impurity atoms can be both individual in highly dilute solid solutions and by way of collective fluctuations which contain randomly approached groups of atoms. Concentrated solid solutions are sometimes described in the approximation of the so-called „mean field" by way of a homogeneous renormalization of the Peierls stress. However, when studying a softening to hardening transition which takes place at low concentrations of solid solutions equal to about one percent or less, the solution atoms or their randomly approaching groups form local perturbations, which are distant from each other, and the mean field approach is physically not justified. As is well known for thermally-activated processes in general, an essential role in the kink formation is played by local perturbations causing heterogeneous distortions of the dislocation configurations, which reduce the barrier for kink pair nucleation. Certain important effects occurring in concentrated solid solutions, such as interaction of

impurities or the formation of cross-kinks [12–14], will not be considered.

When impurities in a crystal lattice are chaotically located, the energetics of such important configurations as ordinary and paired dislocation kinks has a random distribution. Thus, a description of the softening to hardening transition requires a statistical approach. The need for a statistical approach has been admitted by many authors [12,15]. Thereat, a nontrivial problem of obtaining of „statistically valid" results for comparison with experiments arises. The problem is solved relatively simply in case of the so-called „self-averaged" characteristics, for instance, those meeting the conditions of the central limit theorem in the theory of probabilities of sums of many random values with an identical distribution, fluctuations of which are small as compared to average values [16]. However, in the dislocation dynamics one also has to deal with the characteristics having other properties, which will be discussed later. Interpretation of this type of experimental data depends on the „averaging method", on which different authors often have different opinions and obtain different results.

The dislocation dynamics even in simplified models is characterized by a large number of various parameters: Peierls stress, intrinsic energies of kinks, potentials of kinks' interaction with each other and with impurity atoms, applied force, temperature, impurity concentration and several others. Presentation of results of modelling of this dynamics in such a multidimensional space of parameters is usually selective. That's why it is important to have an analytical description of the dynamics, which compactly concentrates the tendencies of influence of all the essential factors, and this is the goal of the present paper.

The potential relief for kink motion in crystals with chaotically distributed impurities or other point defects, as demonstrated in [10,12], is a random function which chaotically wanders on the energy scale. A similar approach was also used in paper [17], where applicability of this model named the „Wiener Process with drift" was substantiated by numerical modelling.

The present paper will be dedicated to the study of a generalized kink mechanism of dislocation motion with account of heterogeneous influence of randomly fluctuating fields of solution atom concentration.

2. Formation of kinks on fluctuations of solid solution concentration

The position of a straight-line dislocation in a crystal lattice valley at stresses below the Peierls stress is metastably steady and motion requires a thermal fluctuation which throws a part of the dislocation over the Peierls barrier. A thermofluctuation nucleus of dislocation displacement from one valley of the crystal relief to a neighboring one in case of stresses much lower than the Peierls stress, which is studied in the present paper, is a separated kink-antikink pair. The kink width in this case is much smaller than the

size of the whole pair and the kink with the antikink can be approximately interpreted as structureless sharp boundaries of the pair nucleus. The nucleus top is a dislocation segment located near the minimum of the neighboring valley of the crystal relief. The energy of a pair of kinks in the impurity-free material is [7]:

$$E_{kp}(l) = 2E_k - Fl - E_i(l). \qquad (1)$$

Here E_k is the energy of one kink or antikink, l is the distance between pair components, $F = \sigma bh$ is the driving force acting on the kinks, which is generated by external stress σ, b is the value of the dislocation Burgers vector, h is the distance between crystal relief valleys. $E_i(l)$ is energy of kink interaction in an approximation of the elasticity theory, inversely proportional to the distance between kinks $E_i(l) = \alpha/l$. Proportionality coefficient α according to [7] is approximately $Gb^2h^2/8\pi$, where G is the material shear modulus. Equation (1) has a high degree of universality, since its functional form and consequences do not depend on a specific dislocation model, which affects only its constituent constants E_k and α, parameterization of which is a separate problem. The minimum energy of activation of kink pairs in a pure material is given by the minimum of function $E_{kp}(l)$ with the optimal pair size $l_0 = \sqrt{\alpha/F}$ and is equal to $E_0(F) = 2E_k - 2\sqrt{\alpha F}$. The frequency of thermoactivation nucleation of a kink pair on a dislocation unit length in this case is $\Gamma = \Gamma_0 \exp[-E_0(F)/kT]$, where T is temperature, k is the Boltzmann constant, Γ_0 is the pre-exponential factor unimportant for further study. In the absence of significant second-order Peierls relief, kinks freely propagate from the nucleation place to the sample surface or till collision with neighboring kinks.

Let us discuss solid solutions and generalize the given expressions in the case of presence of foreign atoms, chaotically distributed in a material, which are hereinafter called solution atoms or impurities for short. It is to be recalled that a description of the dynamics of dislocations in pure (perfect) materials did not require control of the whole population of dislocation atoms separately; collective kink modes could be used as elementary objects. This was facilitated by homogeneity of pure materials. A disordered distribution of impurity atoms disrupts the homogeneity of materials. Nevertheless, it is also possible to avoid the need for manipulation of chaotic configurations of impurity atoms in the totality. This possibility is provided by the fact that the defining role is played by extremely strong fluctuations, which are distant and isolated due to this. This allows for introducing an intermediate description level and manipulating (as the main characteristics) the functions of time distributions of the same elementary acts of overcoming of kink nucleation and migration barriers.

An elementary act of the dislocation dynamics is its motion to one crystal lattice constant regardless of the structure of the dislocation core which can span several lattice constants, be split etc. Without aiming at obtaining a quantitative description of the process energetics in different

specific materials, but aiming only at representing the physics and the typical tendencies of dependences on the essential parameters, a dislocation can be considered in the conventionally generalized form as a certain linear object in an extended periodic potential relief. A frequently used visual image of such a system is a string on an inclined wash-board [18].

Let us denote the average linear density of impurities along the crystal pattern valley as ρ. The first approximation takes into account only one row of adjoining impurities, whether they are substitutional impurities at lattice sites or interstitial impurities in the row of neighboring interstices which most strongly interact with a dislocation at the given position. This approximation is based on the fact that a decrease of interaction energy in a thermally-activated process even by a relatively small value of the order of thermal energy kT makes such interaction secondary.

However, the important factor for the thermally-activated motion of dislocations is not the average density of impurities, but heterogeneities of the impurity-induced potential relief. Let us consider the influence of a fluctuation cluster of impurities, which leads to a density of impurities in the first valley of the pattern which exceeds their density in the second valley by value $\rho(x) = \rho_2(x) - \rho_1(x)$. The potential of a pair of kinks, centered at points x_1 and x_2, which generalizes expression (1), is

$$E(x_1, x_2) = 2E_k + E_i(\Delta x) - F\Delta x - Nu. \qquad (2)$$

Here $\Delta x = x_2 - x_1$, $E_i(\Delta x)$ is the kink and antikink attraction energy (for specific calculations in the present paper we taken the already mentioned kind of interaction $E_i(\Delta x) = -\alpha/\Delta x$), which is frequently used in applications,

$$N = \int\limits_{x_1}^{x_2} \left[\rho_2(x) - \rho_1(x)\right] dx$$

— difference of the amount of impurities at the segment (x_1, x_2) in the second and first valleys of the pattern $(\rho_2(x), \rho_1(x)$ are the corresponding densities of the amount of impurities, the difference of which is of purely fluctuation nature), u is the dislocation and impurity center interaction energy. Mesoscopic phenomenological models were initially developed based on the elasticity theory to describe the interaction of an impurity with a dislocation in terms of a difference of atomic radii or elastic moduli of the impurity and matrix. However, the experimental results for BCC-metals show that these factors cannot be considered as the main ones, accountable for the observed behavior (see, for instance, [19]). This is not surprising, since the strongest interaction occurs when an impurity atom is inside a dislocation core, where the elasticity theory is not applicable and short-range chemical forces are significant. Moreover, the impurity and dislocation interaction is not represented by continual functions, and in the present paper, like in [10,12], it will be more simply characterized by the single parameter u which is of microscopic nature. The sign

of u does not matter, because it can be changed by changing the notation of numbers of crystal relif valleys.

The chaotic nature of distribution of solution atoms leads to the formation and motion of kinks in a randomly fluctuating potential relief. Accordingly, height of the kink nucleation barrier is a random value which depends on location. That's why the activation energy and nucleation time of a pair of kinks should be characterized by distribution functions determined by the statistics of implementation of a particular impurity configuration.

Assuming the impurity distribution to be completely chaotic, the probability of implementation of any impurity fluctuation $\rho(x)$ will be described as

$$P\{\rho(x)\} = \exp\left[\Delta S\{\rho(x)\}\right],$$

where

$$\Delta S\{\rho_1(x), \rho_2(x)\} = -\int \left[\rho_1(x) \ln \frac{\rho_1(x)}{e\rho} + \rho_1 \right.$$
$$\left. + \rho_2(x) \ln \frac{\rho_2(x)}{e\rho} + \rho_2\right] dx \qquad (3)$$

is a change of entropy of a perfect solid solution due to the formation of the given fluctuation (see, for instance, [20], in (3) and then entropy is determined, according to [20], as a dimensionless quantity — a logarithm of statistical weight of state).

The probability of formation of a pair of kinks with any activation energy E_a is determined by statistical weight of impurity configurations which lead to the corresponding modification of the kink nucleation barrier. This probability sharply decreases with a decrease of activation energy E_a as compared to $E_0(F)$, since stronger and stronger fluctuations of the impurity distribution are required. Thereat, the determining contribution is made by a certain optimal fluctuation which is the most frequent one of all fluctuations which lead to the desired barrier height. The problem of finding the optimal shape of impurity fluctuation, i.e. the one leading to the maximum entropy change at the required activation energy E_a was solved in [21,22], and the obtained results will be used here.

The optimal configuration of impurity density has a symmetrical form, the right part of which is shown in Fig. 1. Up to the point of the maximum potential of a pair of kinks, impurity density ρ_0 is homogeneous, which renormalizes the driving force to the value of $F + \rho_0 u$. The maximum potential at this value of the effective driving force is achieved in $x_1 = \frac{1}{2}\sqrt{\alpha/(F + \rho_0 u)}$ and has the value of $E_a = 2E_k - 2\sqrt{\alpha(F + \rho_0 u)}$. If the cluster ended in x_1, then the potential would be $2E_k - u\rho_0 x_1 - F2x - \alpha/2x$ with a excluded addition to the driving force. That is, it would grow up to point $x_0 = \frac{1}{2}\sqrt{\alpha/F}$ and its potential there would be equal to $2E_k - 2\sqrt{\alpha F} - u\rho_0 x_1$, which exceeds the suggested one. To avoid this contradiction, the impurity cluster should be continued by a smoothly decreasing impurity density $\rho(x) = [\alpha/(2x^2) - 2F]/u$, which leads to a
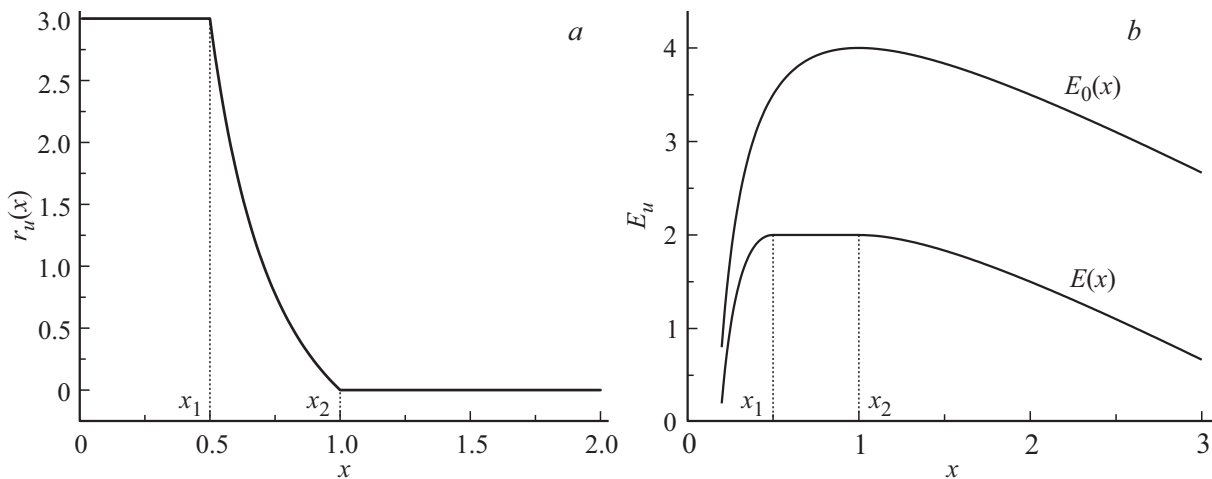
Figure 1. *a*) Example of the shape of an optimal cluster of impurities, leading to a modification of the barrier for formation of a pair of kinks shown in Figure *b*). Parameters $\Delta E/u = 2$; $F\alpha/u^2 = 1$, lengths are measured in units of x_0, impurity density in units of $u/2\alpha$.

potential plateau (2). The cluster stops at $\rho(x) = 0$ in point $x_2 = x_0 = \frac{1}{2}\sqrt{\alpha/F}$. A decrease of the activation energy is

$$\Delta E = 2E_k - 2\sqrt{\alpha F} - E_a = 2\left[\sqrt{\alpha(F + \rho_0 u)} - 2\sqrt{\alpha F}\right].$$

Fig. 1 shows a decrease of the barrier for nucleation of a pair of kinks to the given value of E_a by a fluctuation of impurities which has the highest implementation probability. With the described cluster shape, the change of entropy (3), which determines this probability, is equal to

$$\Delta S_{\text{opt}} = -(r_0 r_u)^{1/2}$$

$$\times \left\{ (1+z)^{1/2}\ln\left(\sqrt{r_0^2 + 1} + r_0\right) + \int_0^1 \frac{\sqrt{x+z}\,dx}{\sqrt{x^2 + w}} \right\}.$$

$$(4)$$

Hereinafter dimensionless parameters are used for convenience

$$r_0 = \rho_0/2\rho = (F_a/r_u)\left[(2E_{ku} - E_u)^2/4F_a - 1\right],$$

$$r_u = 2\alpha\rho/u, \quad F_a = \alpha F/u^2, \quad E_{ku} = E_k/u, \quad E_u = E_a/u,$$

$$z = 1/[(2E_{ku} - E_u)^2/4F_a - 1], \quad w = 1/r_0^2. \quad T_u = kT/u.$$

The calculated entropy determines distribution function $P_a \approx \exp[\Delta S_{\text{opt}}]$ of the value of activation energy for the formation of kink pairs E_a depending on various parameters, as illustrated in Fig. 2. Since the activation energy determines the barrier overcoming time $t_a \propto 1/\Gamma = 1/\Gamma_0 \exp(E_a/kT)$, the obtained expression also yields a distribution of kink pair formation times. A contribution by other, non-optimal fluctuations may change the pre-exponential factors in the calculated distribution function, but this minor circumstance will be neglected in the first approximation.

It is well known that, though the frequency of kink pair nucleation on a dislocation unit length $\Gamma = \Gamma_0 \exp[-E_0(F)/kT]$ in a pure material is determined

by pair energy $E_0(F)$, the dislocation motion speed contains an activation energy equal to half this value $V_d = V_{d0}\exp[-E_0(F)/2kT]$. The reason for this can be easily understood from simple scale considerations. The number of kink pairs nucleating on a dislocation unit length N_{kp} increases proportionally to time t as $N_{kp} \approx \Gamma t$, so that the average distance between them is approximately equal to $L_{kp} \approx 1/\Gamma t$. The path length of a kink having velocity v within time t is $L_k = vt$. The kink lifetime, determined by collisions and annihilation with kinks from neighboring pairs, is found from the condition of equality of path length L_k and distance between the kinks nucleated by the given time L_{kp}, from which it follows that $t_a = 1/\sqrt{v\Gamma}$ and $V_d = a/t_a = (a\sqrt{v\Gamma_0})\exp[-E_0(F)/2kT]$.

The scaling relation must be modified if there are impurity clusters which reduce the kink nucleation barrier and decelerate the kink propagation. The correlations given below are simplified without specification of different pre-exponential factors.

The number of kink pairs which freely nucleated by time t on length L should include the pairs which formed on impurity clusters $(L/l_{1a})P_a(t)$, where l_{1a} is the scale multiplier of the order of the critical pair size, time t is related to the activation energy by Arrhenius relation $t \sim (1/\Gamma_0)\exp(E_a/kT)$. Though such clusters are rare, their contribution can be comparable and even prevailing due to an increased kink generation velocity. Expression $P_a(t) = \exp(\Delta S_{\text{opt}})$ with the above-mentioned ΔS_{opt} (4) will be used for $P_a(t)$.

The second stage of the process of dislocation's crossing of a barrier is the propagation of kinks from the nucleation place, which is also affected by impurities. The time of kink travel to distance L includes the free motion time L/v and the total time of delays on impurity barriers. Probability $P_s(t)$ of meeting an impurity cluster with overcoming time t or longer was calculated in [10,23] and is equal to $P_s(t) = (t_0/t)^\delta$, where t_0 is a characteristic time of an
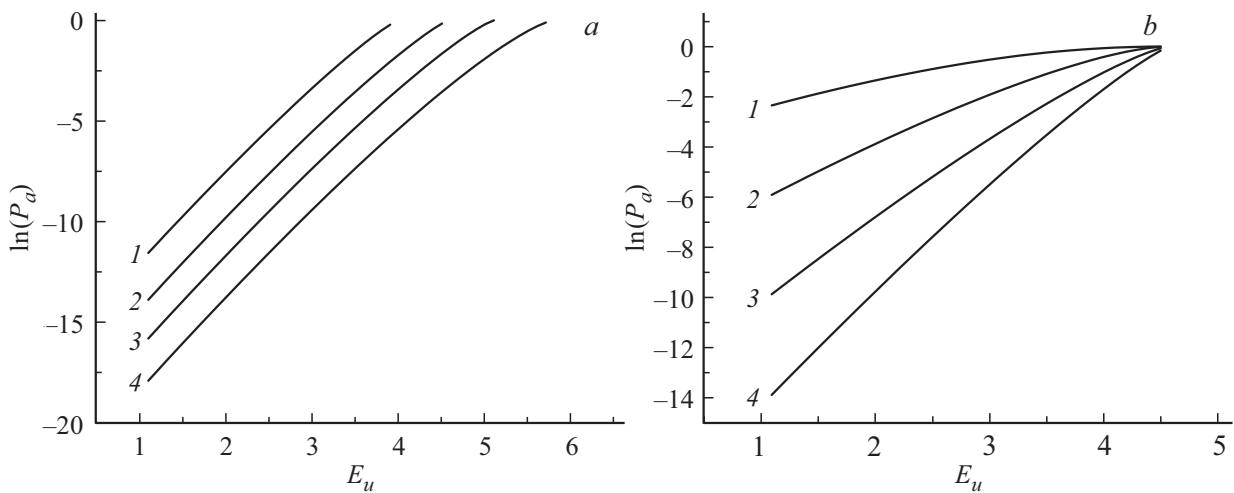
Figure 2. The logarithm of distribution function $\Delta S_{opt} = \ln P_a(E_u)$ vs. activation energy E_u of the formation of a pair of kinks on a fluctuation cluster of impurities at $E_k = 3u$, *a*) dimensionless concentration of impurities $2\rho\alpha/u = 0.001$ and different values of dimensionless driving force: $F\alpha/u^2 = 1$ — curve *1*, 0.5 — curve *2*, 0.2 — curve *3*, 0.01 — curve *4*; *b*) $F = 0.5(\alpha/u^2)$ and different values of dimensionless concentration of impurities: $2\rho\alpha/u = 1$ — curve *1*, 0.1 — curve *2*, 0.01 — curve *3*, 0.001 — curve *4*.

elementary act, $\delta = (kT/u)\varphi$, and φ is found from the relation

$$\left[\exp(\varphi) + \exp(-\varphi) - 2\right]/\varphi = F/\rho u = 2F_a/r_u. \quad (5)$$

However, until the average delay time $\langle\tau_s\rangle = \int_0^\infty P_s(t)dt$ is finite, which occurs at $\delta > 1$, the influence of impurity clusters on kink scattering is not significant. A contrary situation will be considered in the next section.

By equating the average distance between the nucleated kink pairs to the average path length, we obtain a modified equation for the time of dislocation's passing across the Peierls barrier t_a

$$1/\left[\Gamma t + P_a(t)/l_{1a}\right] \approx vt. \quad (6)$$

The solution of this equation is illustrated in Fig. 3, *a* by descending lines. It can be seen how the presence of impurities reduces the energy of kink pair formation in this parameter region as compared to an impurity-free material. The sharp decrease of the barrier overcoming energy is due to the prevalence of kink nucleation on impurity clusters which facilitate the transition.

3. Deceleration of kink scattering by fluctuation cluster of impurities

Hardening of materials is traditionally attributed to the hooking of dislocations to local perturbations of the crystal lattice, induced by impurity atoms or their clusters [24,25]. The Peierls barrier is ignored in this case. However, the kink mechanism in materials with a high crystal relief with not too high impurity concentrations retains, although modified, and a different mechanism of dislocation deceleration is

implemented; it is related to the influence of impurities on kink propagation from their nucleation place.

It was shown in [10,23] that the influence of impurities on the dynamics of dislocation kinks can lead to a kinetic phase transition with a change of the motion pattern and a transition to nonlinear drift or, otherwise, to the so-called anomalous kinetics. Such a transition was associated with an increased role of extremely strong fluctuations of a chaotic impurity relief due to the formation of slowly decreasing asymptotics of times of kink delays on them with an increase of the impurity atom concentration. This prediction was experimentally confirmed in [26]. A survey of the numerous papers on anomalous kinetics in different systems is given in [27,28]. In this case the kink path length x depends on time nonlinearly as $x \approx x_0(t/t_0)^\delta$, where $\delta < 1$. If the value of φ determined from equation (6) is less than u/kT, that is, $\delta < 1$, the probability of long delay times decreases so slowly that the average delay time $\langle\tau_s\rangle = \int_0^\infty P_s(t)dt$ diverges and kink motion has an anomalously slow nature called quasilocalization. With δ becoming 1, the motion law changes to standard linear drift. Thus, the condition $\delta = 1$ determines the boundary of a drastic change of motion modes of kinks and the whole dislocation. Quasilocalization of kinks with an increase of impurity concentration causes a slower motion of dislocations and, on the macroscopic scale, a transition to material hardening.

Substituting the free path length of the kink in equation (6) by the length of shift at nonlinear drift, we obtain a modified equation for the transition time

$$1/\left[\Gamma t + P_a(t)/l_{1a}\right] \approx x_0(t/t_0)^\delta. \quad (7)$$

The solution of equation (6) is shown in Fig. 3, *a* by curves, which descend with an increase of the average impurity concentration in the material, for different temperature
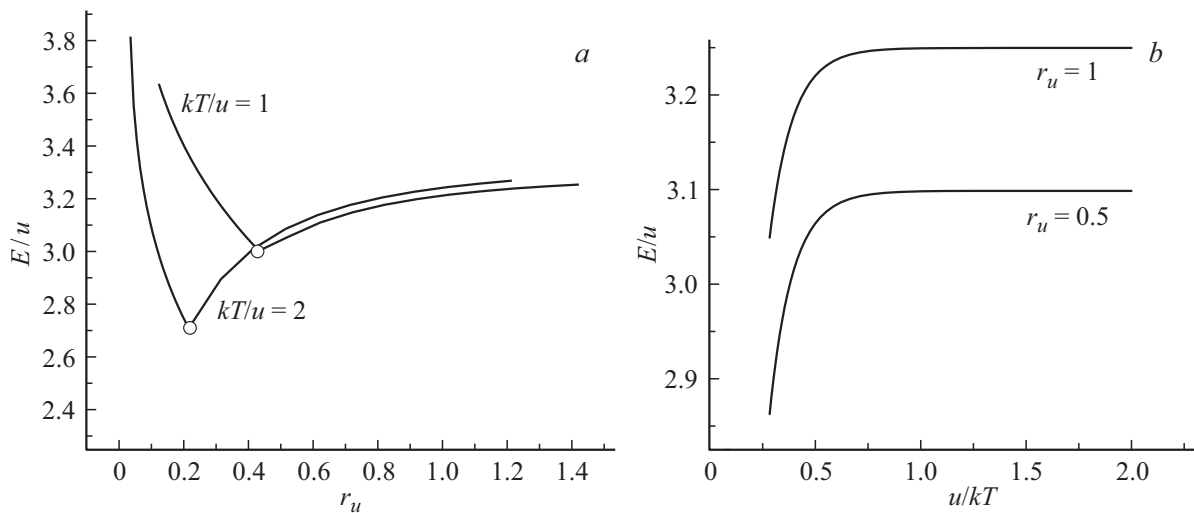
Figure 3. Energy of kink pair formation with driving force $F_a = 0.1$ vs. a) average impurity density for different temperature values; b) reciprocal temperature for different values of average impurity density. Parameter $E_k = 3u$, $r_u = 2\alpha\rho/u$ is the nondimensionalized impurity density. The circles in the left figure show the points of change of dislocation motion modes.

values. The solution of equation (7) is shown by ascending lines. This solution in the right Fig. 3, b is shown as a function of reciprocal temperature. The energy of kink pair formation found from equations (6) and (7) has an effective nature, because the optimal impurity clusters, which determine it, depend on various parameters in a complicated way. In particular, it can be seen that the energy of kink pair formation is not dependent on temperature anymore when temperature decreases. This is explained by the fact that kinks nucleated freely in the wide parameter region considerably less frequently than on impurity clusters. In this case, equation (7) reduces to the following one without temperature

$$S + \varphi E_u = 0. \tag{8}$$

Equation (6) corresponds to a situation when the influence of impurities facilitates the kink nucleation, thus accelerating the motion of dislocations. On the contrary, equation (7) or (8) corresponds to a situation when the influence of impurities particularly affects the deceleration of kinks, thus slowing down the motion of dislocations. After finding E_u from these equations, it is easy to estimate the time of dislocation displacement to the neighboring valley of the crystal relief $t_a = 1/(l_{1a}\Gamma_0) \exp(E_a/kT)$ and to calculate the average dislocation motion speed $V_a = h/t_a = h(l_{1a}\Gamma_0) \exp(-E_a/kT)$. Fig. 3, a clearly demonstrates the transition from the influence of impurities (at their relatively low concentration), which accelerates the dislocation motion, to the decelerating influence at their higher concentration due to the activation of the quasilocalization mechanism of kink deceleration.

The condition of matching of the scales of nucleation L_a and propagation L_v of kinks $L_a \approx L_v$ determines the typical time of dislocation passing across the Peierls barrier from the whole spectrum of kink pair

formation times. It is remarkable that when the calculated value of E_a does not depend on temperature, the $V_a = h/t_a = (h/t_{a0}) \exp(-E_a/kT)$ relation corresponds to the Arrhenius law, fulfillment of which was difficult to foresee in advance within the framework of the calculated mechanism.

4. Determination of energy of interaction between an impurity atom and a dislocation as per experimental data

The main microscopic parameter in the theory is the energy of interaction between an impurity atom and a dislocation u. The theory formulae allow for estimating its value as per the experimental data. According to the given considerations, the boundary of transition from softening to hardening corresponds to a change of the kink motion mode from linear to non-linear drift, in which the condition $\delta = 1$ is met. Substituting the corresponding value of $\varphi = u/kT$ into relation (5), we find u as

$$u = kT \ln \left(F/\rho kT + 2 \right)/2 + [(F/\rho kT + 2)^2/4 - 1]^{1/2}. \tag{9}$$

Let us give as an example the determination of the energy of interaction between an impurity atom and a dislocation as per the experimental data [29] for a solid solution of Ru atoms in NiAl. This material pertains to intermetallides where the crystal relief is high and kinks are relatively abrupt, which satisfies the applicability conditions for the outlined theory. The transition boundary corresponds to stress $\sigma = 3.98 \cdot 10^8$ Pa, Ru atom concentration in percent $\rho = 6.89 \cdot 10^{-3}$, experiment temperature $T = 293$ K. Substituting these values into formula (10), we obtain

the interaction energy $u \approx 0.17$ eV, which, considering the above-mentioned reservations with regard to quantitative estimations of the theory, gives rather a reasonable order of magnitude.

5. Conclusion

The paper gives a theoretical description of the influence of chaotically distributed impurity atoms on the dynamics of dislocations in crystalline materials within the framework of a modified kink mechanism. The influence of impurities on both essential stages of dislocation motion: thermofluctuation formation of kinks and their propagation along the dislocation length is considered. This influence is differently directed and leads to competition of the effects of dislocation motion acceleration and deceleration. At the macroscopic level this corresponds to competition of crystal softening and hardening, as observed in many materials having a high crystal pattern: in semiconductors and ceramics, metals with the BCC-structure, intermetallides and others where the kink mechanism of dislocation motion is implemented [3]. The theory is analytical, which allows for sufficiently clear tracing of tendencies of influence of the numerous material parameters. A comparison of the theory with the experimental data allows for estimating the order of magnitude of the microscopic parameter of interaction between impurity atoms and dislocations, as illustrated by the data of [29] for a solid solution of Ru in NiAl.

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Conflict of interest

The author declares that he has no conflict of interest.

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