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DISLOCATION DYNAMICS IN DISORDERED CRYSTALS WITH HIGH PEIERLS BARRIERS

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Résumé
On étudie le mouvement suramorti d'une corde dans un potentiel périodique, sous l'action d'une force extérieure et en présence d'un faible désordre. On tient compte de la non linéarité de la propagation de décrochements dans le champ de forces aléatoires. Les résultats obtenus sont utilisés pour décrire le déplacement d'une dislocation dans un cristal imparfait.

Abstract
The motion of an overdamped string in a periodic potential under the action of an external driving force in the presence of weak disorder is investigated. The non-linearity in the kinks propagation in the random force field is taken into account. The results obtained are used to describe the dislocation motion in crystals with defects.

We consider the thermal activation large-amplitude excitations of the overdamped elastic string and the influence of the disorder on the propagation of a string in a periodic potential. The problem which has to be solved is the following. Let the string initially lie in the x direction in the Peierls valley. A thermal fluctuation can throw a segment of the string into the next valley, favored by the applied external force F. If the segment is long enough to exceed the size of the critical nucleus then the kink-antikink pair will expand under the action of the external driving force and the string will transit into the next valley. The nucleation rate and the average velocity of the displacement of the string have been calculated by P.A. Kosantsev and V.L. Pokrovsky [1] and by M. Bütter and R. Landauer [2]. It has been shown that string velocity is determined by the nucleation rate J and the kink propagation velocity u. Disorder leads to two important effects: the first one is that the random fields of impurities cause the local fluctuational lowering of the Peierls barrier, giving rise to a higher nucleation rate in the corresponding region. The second effect consists in the lowering of the kink propagation velocity by random fields. The total effect will be determined by the competition between the phenomena described. This problem was attacked in numerous works (see for example, [3,4]).

It has been experimentally revealed that the doping of crystals can give rise to the increase of the dislocation velocity (Patel and Chandhuri [5], Erofeev et al. [6], Erofeev and Nikitenko [7]) and the theoretical analysis (Petukhov [8]) is in qualitative agreement with these results.

It should be noted, however, that two fundamental circumstances, leading to important physical consequences, were beyond the framework of the previous theories. First, the distribution of point defects along the string was assumed to be a Poisson distribution; we believe that the random field generated by point defects has
to be described rather by a Gaussian distribution function. In fact the essential length scale is the size of the critical nucleus which is much greater than the mean spacing between impurities. Therefore a large number of impurities appears to be involved in the process of nucleus creation and one can easily see that the fluctuating addition to the nucleation energy turns out to have a Gaussian distribution function. It should also be mentioned that the fact that the dislocation interacts with defects located below and above slipplane leads to the increase of the effective impurity concentration (it is especially the fact when the long-ranged interaction with charged impurities is considered).

Second, the random field the kink sees during its propagation has to be considered as a random force field rather than as a random potential. To prove that, let the kink travel a distance $x$ along the string. This means that the segment of the string of length $x$ has jumped into the next valley and consequently the string gains extra energy resulting from the random field of defects $V(x)$:

$$
\delta U(x) = \int_0^x \delta V(x')
$$

where $\delta V(x) = V_f(x) - V_i(x)$ is the difference between random fields in the initial $V_i(x)$ and in the next $V_f(x)$ valley. Hence $\delta V(x) = 0$, where the bar denotes averaging over random fields. We see that the random force acting on the kink in point $x$ is

$$
f(x) = -\frac{\delta U(x)}{\delta x} = -\delta V(x)
$$

and has the statistical properties coinciding with a random potential:

$$
f(x) f(x') \equiv \delta V(x) \delta V(x').
$$

The propagation of a one-dimensional particle in a random force field differs essentially from the motion in a random potential. As has been shown by Sinai [3] the diffusion law now becomes

$$
x \sim \ln^2 t
$$

where $x$ is the square root of the mean square displacement of the particle. We also shall show below that the displacement under the action of a driving force can demonstrate nonlinear dependence on time $t$:

$$
x \sim t^\alpha, \quad (x \ll 1)
$$

(this result has been obtained for discrete model by H. Kesten et al. [10]). In this case the term of kink velocity makes no sense. The dim of one paper is to investigate the overdamped string motion taking into account the Gaussian distribution of the random field and nonlinearity in the kink motion.

We shall assume that the phonon friction and secondary Peierls relief are accounted for by the kink undisturbed velocity $U$. We consider the motion through the weak random field: $[f(x)]^2 \equiv \gamma \ll V_p^2$ and $\gamma^{1/2} \ll E_k$, where $E_p \sim \sqrt{\rho V_p}$ is the single-kink creation energy, $V_p$ is the height of the Peiersl barrier and $\rho$ is the dislocation tension. Furthermore we consider moderate temperatures such that $\beta E_p \gg 1$ where $\beta = 1/T$ and moderate external forces $F \ll V_p(F=\sigma b)^3/2$ (where $\sigma$ is the external stress and $b$ is the Burgers vector). The assumptions enlisted correspond to be experimental conditions usually employed to observe the dislocation motion: in Si and Ge the Peiersl barrier is estimated to be of order $V_p \sim 1-2$ eV and the impurity potential $V_i \sim 0.1$ eV and taking into account the defect concentration we see that $\gamma \sim V_i$ is really much smaller than the Peiersl barrier. Furthermore the small random modulation of the secondary Peiersl barrier due to long-ranged defects one can consider as the very weak impurity with an effective linear concentration of about an impurity per atom, and, thus, the effective spacing between impurities is really much smaller than the critical nucleus size which is of order $(10+15)b$.

It should be noted in addition that the same problem was studied by Guyer and Miller [11] but they have considered the annealed disorder, which is hardly adequate for describing the motion of dislocations in a crystal with defects. We should like to stress that we investigate an alternative and conventional case, namely quenched disorder.

As usual the size of the critical nucleus is determined by minimized the nucleus energy $E(1)$ with respect to the nucleus length $l$.

$$
E(1) = 2E_k - \frac{\alpha E_k}{1} - F l - \int_0^l dx \delta V(x) \tag{1}
$$

One can easily obtain that the critical length remains unchanged

$$
\eta = b(\frac{\alpha E_k}{F})^{1/2} \tag{2}
$$

if $\gamma \ll E_k^{1/2} F^{3/2}$. Hereafter we assume this...
relation to be satisfied. As the external force decreases the length of the critical nucleus increases and the contribution to nucleation energy from the random field increases too. When the fluctuational part of energy exceeds $2E_k$ the configuration of nucleus will be mainly determined by the random field. At this moment we are facing with the problem of dislocation motion in disordered crystals without Peierls barrier. This problem is investigated in detail in another publication [12].

The basic point of our calculation is the formula for mean transition time from one valley to the next one for an arbitrary point of the string:

$$\bar{\tau} = \int_0^\infty dt \exp \left\{ - \int_0^t \psi(y) dy \right\} \times$$

$$\exp \left\{ - \int_{z_0}^{z_0+\eta} dy \psi(y) \right\}$$

which one can easily obtain making use of Kolmogorov's method [3]. Here $J_0 \exp \left\{ - \int_{z_0}^{z_0+\eta} dy \psi(y) \right\}$ represents the nucleation creation rate with the position of, say, the left end of the nucleus at point $z$, $J_0$ is the nucleation rate in the pure system, $\psi(x)$ is the random potential normalized with respect to temperature, $\tau(z)$ is the time for the kink to travel from the point $z$ to the 0. The kink displacement $x$ and time $t$ are normalized with respect to the kink size $\xi_0$ and $\tau = \xi_0/u$, $u$ is the bare kink velocity, the value of $x$ is defined by $t = \tau(x)$.

In fact let us find the probability for an arbitrary point of the string to remain at the initial valley up to the moment $t$. If $J(z)$ is the nucleation rate at point $z$ then $\exp(-J(z)t)$ is the probability for the nucleus not to appear up to time $t$. Consequently if the point $z$ were the only nucleation point, the probability for the point 0 to remain at the initial valley would be given by $\exp\{-J(z)(t-\tau(z))\}$. Then as the nucleus can appear at any point of the string, the total probability for the point 0 to keep its position up to time $t$ will be $w(t) = \prod_{z=0}^{x} \exp\{-J(z)(t-\tau(z))\} = \exp\{-\int_0^x \tau(z)(t-\tau(z)) dz\}$.

Now the density of transition probability of point 0 is $d\frac{d}{dt}(1-w(t))$. Making use of this density of probability to calculate the mean transition time and averaging over all the positions of the initial point we obtain (3). Assume for simplicity that the nucleus has a rectangular form, then

$$\tau(z) \equiv \exp \left\{ \int_0^z \psi(y) dy \right\}$$

Make the assumption that the main contribution results from integration over large values of $t$ and that we can neglect $\tau(z)$ in comparison with $t$. After that

$$\bar{\tau} = \int_0^\infty dt \exp \left\{ -J_0 t \int_0^x dz \exp\{-\int_{z_0}^{z_0+\eta} \psi(y) dy\} \right\}$$

The large values of $t$ also implies large distances $x$.

Hence

$$\int_0^x dz \exp\{-\int_{z_0}^{z_0+\eta} \psi(y) dy\} \sim x \Phi,$$

$$\Phi = \exp \left\{ -\int_0^x \psi(x) dx \right\}$$

and

$$\bar{\tau} = \int_0^\infty dt \exp \left\{ -J_0 t x \Phi \right\}$$

In the last formula $x$ is in fact the average displacement in time $t$. We will now show that

$$x = t^{\frac{1}{1-\gamma}}, \quad \gamma = 2F/\beta \gamma, \quad \text{if} \quad 2F/\beta < 1, \quad x = 1, \quad \text{if} \quad 2F/\beta > 1 \quad (8)$$

This result can be simply derived in the following way. When traveling through a one-dimensional random force field the particle simultaneously performs a random walk along the axis of energy and the typical gain or loss in energy corresponding to the displacement $x$ is

$$[\beta^2(x)]^{1/2} = Fx \sim \gamma^{1/2} x^{1/2} - Fx. \quad (9)$$

Hence the time for the particle to travel the distance $x$ is just the time for the particle to scramble out of the Gaussian potential well with depth given by (9) and can be estimated as

$$t \sim \exp \left( \frac{\beta \gamma^{1/2} x^{1/2}}{\gamma^{1/2}} - \beta Fx \right) \quad (10)$$

This estimate is valid until $\gamma^{1/2} x^{1/2} \gg Fx$. If $\gamma^{1/2} x^{1/2} > Fx$ the particle will diffuse obeying the following law
If however the distances become sufficiently large the energy gain from the external field \( F \) exceeds the fluctuational loss in energy. The size \( x_0 \) and depth \( E_0 \) of the Gaussian well which the particle still sees is determined by the minimization of the activation energy (9):

\[
x_0 = \frac{\gamma}{4F^2}, \quad E_0 = \frac{\gamma}{2F}.
\]

When the typical distances become much larger than \( x_0 \), the particle will be retarded only by sufficiently large fluctuations of the random field, exceeding \( E_0 \). These comparatively rare fluctuations are believed to have Poisson distribution. Consequently the distance which provides the emergence of the fluctuation \( E > E_0 \) with a probability close to unity is estimated from

\[
x \exp \left( -\frac{E}{E_0} \right) \sim 1.
\]

The latter condition means that the typical value of the potential barrier appearing in the distance \( x \) is

\[
\bar{E} \sim E_0 \ln x
\]

and the retarding time corresponding to the distance \( x \) the propagating time through \( x \) is

\[
t \sim \exp \left( \beta \bar{E} \right) = x^{\beta^2/2F}
\]

for \( \beta \bar{E} > 1 \) and \( t=x \) for \( \beta \bar{E} < 1 \). Inverting this formula we obtain (7)-(8).

Substituting (7)-(8) into (6) one can easily perform the integration and find

\[
\overline{\tau} \approx \frac{1}{1 + x} \Gamma \left( \frac{1}{2 + \frac{1}{x}} \right) \left( J_0 \Phi \right) \frac{1}{1 + x}
\]

It is possible now, using (7), to check the assumption which has been used in deriving (6) and make sure that the contribution from \( \tau(z) \) is negligible when integrating over \( z \) in (3).

Calculation of the average \( \Phi \) is very simple at high temperatures \( \beta^2 \gamma < 1 \), when the density of thermal activated kinks exceeds the density of kinks generated by defects:

\[
\Phi = \exp \left( \frac{1}{2} \beta^2 \gamma \eta \right)
\]

It can be shown that, at low temperatures, \( \beta^2 \gamma < 1 \), the accumulation of kinks in Gaussian wells occurs and our model is not applicable. The temperature scale describing the transition from high to low temperature is

\[
T' = \frac{\gamma \eta}{2E_k}.
\]

Making use of (15) we find

\[
v \sim (t)^{-1} \sim \exp \left( -\frac{\beta^2 \gamma}{1 + x} \frac{E_k}{l^2} \right) + \frac{\beta^2 \gamma}{1 + x} \frac{E_k}{\sqrt{F}}
\]

\[
T >> T'
\]

In our consideration we have neglected the diffusive motion of the kinks. This is justified as long as the distance \( x_0 \) a kink would diffuse during its mean lifetime is much smaller than the characteristic distance \( \bar{x} \) it travels (the characteristic averaged distance), \( \bar{x} \) is found from (7) and (14) and is given by

\[
\bar{x} \sim (J_0 \Phi)^{-1} \sim \exp \left( \frac{FE_k}{\gamma \eta} \right), \quad T >> T'
\]

Thus our results are valid for

\[
\exp \left( -\frac{2FE_k}{\gamma \eta} \right) >> \frac{E_k^2}{\gamma}.
\]

In the temperature range \( T' < < T' \), as we have previously mentioned, an accumulation of kinks takes place and the term "kink" does not make sense. At these temperatures as well as in the case of sufficiently long critical nucleus the configuration of the dislocation is mainly determined by the random field of defects rather than by Peierls' relief. Hence if \( T' < < T' \) or \( F < \gamma^{2/3} E_k^{1/3} \) we face the problem of dislocation motion in disordered crystals with low Peierls barrier. This problem has been investigated in detail elsewhere [12], and the following result for the dislocation velocity has been obtained:

\[
v \sim \exp \left( -\lambda / \tau^{\alpha} \right).
\]

Here \( \alpha \) and \( \beta \) are the scaling parameters which are determined by the kind of disorder involved (random force or random potential). So, one can see that, at suffi-
ciently small external stresses, the linear dependence of the dislocation velocity on the external stress takes an exponential behaviour, and the transition point $F_0$ can be interpreted as a starting stress. We would like to note that the result (20) is also applicable to the dynamics of interfaces in various disordered media, for example, the motion of domain walls in random antiferromagnets can be described by formula (20).

The essential feature of our result (17) is the possibility of notable variations of the activation energy with the external stress. In fact if at small initial stress, $x$ is much smaller than unity and increases up to $x=1$ as the external stress increases. One can attribute this behaviour to a decrease of activation energy by half.

It should also be stressed that nonlinear motion of kinks is realized only if the distance the kink is displaced before recombination is sufficiently large. For example the characteristic length for the beginning of the logarithmic diffusion law is (under the usual experimental conditions) of order $(10^{-10^{2}})$.b.

In conclusion we would like to note that the results obtained can be applied to describing the dynamics of interfaces in two-dimensional systems (for example the crystals surface) under the action of a moderate external driving force in the presence of disorder. These results also are directly applied to the dynamics of one-dimensional commensurate charge density waves with the order of commensurability $m > 2$.

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References