Mesoscopic Variance of Dislocation Displacements in Crystalline Materials

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Abstract

It is shown that a large variance of dislocation displacements found experimentally and its long relaxation to a steady value in semiconductor materials can be explained by the stochastic nature of the dislocation-kink formation. This stochastic nature results in the development of dislocation line roughness described by the scaling relations, including the mesoscopic time and space scales. Mapping the problem onto the well-examined polynuclear growth model provides a comprehensive description of the self-similar evolution of dislocation shapes and enables to estimate dislocation dynamics parameters.

Keywords: Dislocation dynamics; stochastic kink pair formation; statistical properties of dislocation profile;

1. Introduction

Dislocation motion in relatively pure materials is controlled by an intrinsic potential relief of the crystal lattice (the Peierls relief) and proceeds by thermally activated nucleation of kink pairs and their subsequent spreading along the dislocation line [1-3]. There are a large number of investigations of the dislocation mobility in various materials, which are performed both by the method of selective chemical etching of surface and transmission methods, including observations of the dislocation motion in situ [2,4-6] et al. The problem of studying the dynamics of kinks themselves is much more complicated because of their small (microscopic) size. Such investigations have been extremely rare to date [7]. Therefore, additional possibilities of indirect study of elementary acts of dislocation motion provided by observations at the mesoscopic level, for which there are well-developed techniques, are of interest for controlling the kink mechanism. In the majority of experimental studies, one restricts oneself to measurements of the averaged motion velocity of the dislocation as a whole, thus disregarding a significant portion of the information accessible to analysis. Theoretical description of additional characteristics of the dislocation dynamics principally accessible to investigation is the purpose of the present study.

2. Kink mechanism

In the simplest form, the kink model of the dislocation motion under load looks as follows. An isolated kink represents the step of a height \( h \) equal to the distance between valleys of the periodic crystalline relief. The kink-
antikink pairs are produced with some rate $J$ per unit of dislocation length at random sites under the action of external stress and thermal fluctuations. Later, the kink and antikink move in opposite directions with the drift velocities ± $v_k$. The initial size of the pair, as well as the kink widths, is considered negligible small. We disregard also the interaction between kinks and antikinks outside the critical size of the pair nucleation except the annihilation at the collision.

When studying the kink mechanism, researchers consider two modes. One mode is inherent to short dislocation segments, the average time $1/JL$ of displacement of which at the lattice period $h$ is determined by the nucleation of only one kink pair ($L$ is the segment length). Thus, the average velocity $V_0$ of a short dislocation is proportional to its length: $V_0 = hJL$. The second mode is inherent to long segments on which multiple nucleation of pairs has time to occur. The modes dividing boundary $L_0$ is determined by the length at which the average kink nucleation time $t = 1/JL_0$ is compared to the average kink travel time $L_0/v_k$ till its annihilation with an antikink from the neighbouring pair, so that $L_0 = (v_k/J)^{1/2}$. For $L > L_0$, the dependence of the dislocation velocity on its length saturates at the level of $V_d = hL_0 = h(v_kJ)^{1/2}$ and the dependence of velocity on length is absent for $L > L_0$. In fact, this model is reasonably general and exactly the same model describes the motion of steps on the growing crystal surface, where the jogs in the shape of steps play the role of kinks. Correspondence to the model of polynuclear growth (PNG) is illustrated in Fig 1. Below, we give references to studies based on these models without distinction in their particular embodiment.

For the length-independent mode, the kink lifetime $t_0 = (v_k/J)^{1/2}$ is the only value with a time dimension that could be composed of the parameters $J$ and $v_k$. It would be natural to assume that this time completely characterizes the dislocation displacement kinetics. However, an increase in the dislocation displacement variance observed in experiments with Ge [8], which continues at times $t >> t_0$, compels one to assume the presence of another relaxation time, which considerably exceeds $t_0$. A possible solution of this paradox is proposed below.

3. Competition between stochastic and deterministic constituents of the dislocation dynamics

Due to the stochastic nature of the kink-pair nucleation various dislocation portions move with different delays so that the dislocation profile acquires a randomly cut shape. The driven motion of kinks and antikinks with steady opposite velocities and their mutual annihilation, on the contrary, results in smoothing the profile. The competition of these two constituents of the process of dislocation displacement represents the main content of the phenomenon, and there are contradictory opinions in publications about the predominance of one or another factor: whether or not the profile width is finite or increases infinitely with the dislocation length (see e.g. [9-15]). The first point of view is based on the exact solution obtained by Kolmogorov for the problem concerned with a single-layer coating of the space by growing new-phase nuclei [16]. Generalizations on multilayer coatings using the recurrent formulas relating the coatings of consecutive layers result in the conclusion that the deterministic motion and the annihilation of kinks cause a finite width and a relative smoothness of the profile of the new-phase boundary (the dislocation displacement profile in the case under consideration) [10-12].

Another point of view consists in the assumption of the dominance of the stochastic component of the process, making it possible to consider kinks and anti-kinks as a "gas of quasiparticles" [13-15], the fluctuations in which grow with the system size. Both approaches result in very similar values for the velocity $V_d$ of motion of the line as a whole: $V_d = \sqrt{2} h(J^0)^{1/2}$ in the first case, and $V_d = \sqrt{2} h(J^0)^{1/2}$ in the second case ($e = 2.718...$ is Euler's number). A more substantial qualitative difference of the second approach is that it results in the conclusion about growing width and roughness of the profile of a steadily moving dislocation with an increase in its size. Hence, the relaxation time to the steady mode also depends on the total dislocation length $L$ in this case, and is longer than microscopic one, $t_0$.

4. Statistical description of the moving dislocation shape

A dislocation is an extended object having a large number of fluctuating degrees of freedom, its motion is a complex process of nonequilibrium statistical physics. Numerous studies, both theoretical and experimental (see
[17] and references in them), are devoted to similar processes with the participation of vortices in superconductors, steps on crystal surfaces, polymers, and interphase or domain boundaries in spaces of various dimensions. For one-dimensional systems, alongside with numerical calculations, the use of analytical methods is sometimes feasible. In this context, significant progress has been recently achieved in developing these methods due to the efforts of the community of mathematicians and physicists (see, for example, [18-21], for review [22]). This progress revealing a deep connection between seemingly different problems in mathematics and physics makes it possible to refine the theory of the kink mechanism and its comparison to experimental data.

The presence of mutually unambiguous correspondence of the kink mechanism of the dislocation motion to that for the one-dimensional variant of the crystal growth makes it possible to use the nontrivial results obtained there. We mention those that may be useful for experimental study of the dislocation dynamics. First of all, it is the scaling description of the root-mean-square width \( w = \langle (l(x,t) - \bar{l}(t))^2 \rangle^{1/2} \) of the moving dislocation profile \( l(x,t) \) is the dislocation displacement at point \( x, \bar{l} = V_d t \) is the average one along the dislocation line). Quantitatively, it is expressed in the fact that, at times exceeding a certain microscopic value (in our case, \( t_0 \)), i.e., in the mesoscopic scale, \( w \) is described by the following relation between the dimensionless values \( w' = w/h, L' = L/L_0, t' = t/t_0 \):

\[
W' = L'^{\alpha}f(t'/L'^{\beta}z).
\]  

(1)

The function \( f(x) \) has the following general properties. At small values of the argument, \( f(x) \sim x^\beta \), so that the profile width increases with time according to the power law \( w' \sim t'^\beta \), where \( \beta = \alpha/\beta \), at times \( t' < L'z \), i.e., in the transitional mode. At large argument values, i.e., in the saturation mode, \( f(x) \sim \text{const} \), so that the profile width comes to a steady value of \( w' \sim L'^\alpha \) at \( t' > L'z \). For the exponents, the values \( \alpha = 1/2 \) and \( \beta = 3/2 \) were obtained. The same exponents were obtained also for the solution to Kardar-Parisi-Zhang equation with disorder of white-noise-type [17].

Scaling relation (1) and the theoretically predicted values of exponents \( \alpha \) and \( \beta \) repeatedly confirmed by numerical simulation, including that applicable to dislocations [15], and their belonging to the so-called Kardar-Parisi-Zhang universality class has been reasonably convincingly established. Relatively recently, a new impressive breakthrough took place in the theoretical study of the model. The correspondence between the model under consideration and the properties of certain ensembles of random matrices [18-22] was revealed. This made it possible to use the known distributions of eigenvalues of random matrices for description of statistical properties of the profile of one-dimensional growing surfaces so that, as was already noted, it can be extended also to the dislocation dynamics. Due to this, it is possible to analyze more completely the statistical characteristics of the dislocation shape for various configurations and initial conditions. For example, starting from a flat state \( l(x, t = 0) = 0 \), the time evolution is calculated for not only the root-mean-square width \( w \), but also for the total probability of

![Fig. 1. Scheme of the crystal polynuclear growth (on the left) and the dislocation displacement profile as an fragment of random realization of its shape on an arbitrary scale (on the right). The long arrow indicates the nucleation place of new kink pair, and short arrows show the directions of motion of kinks and antikinks.](image-url)
displacement fluctuations at an arbitrary point (because of the statistical uniformity, it is possible to take \(x = 0\) as this point), which is expressed by the formula

\[
P[(l(0,t)-V_d t)/h \leq s(t/t_0)^{1/3}] = F_1(s^{2/3}).
\]  

(2)

Here, \(V_d = h(2Jv_k)^{1/2}\), \(P\) designates the probability of fulfilling the condition described by the argument in square brackets, and \(F_1(z)\) is the Tracy-Widom distribution for the Gaussian orthogonal ensemble of random matrices. The functions \(F_1(z)\) and \(F_1' = dF(z)/dz\) are tabulated in [23].

The displacement distribution density relating to the experimental histograms of dislocation displacements is obtained by differentiating formula (2):

\[
\rho(l(t)/h) = h dP/dl = (2^{2/3} / (t/t_0)^{1/3}) F_1' \left( 2^{1/3} (l-V_d t)/ (h(t/t_0)^{1/3}) \right).
\]  

(3)

The calculation of the root-mean-square profile width yields the value

\[
w = 0.8 h(t/t_0)^{1/3}, \quad t \gg t_0.
\]  

(4)

5. What is accessible to experimental observation?

The overwhelming number of experimental investigations of the dynamics of individual dislocations is focused on the measurements of their average displacement depending on the load application time. Such data enable to find the most important dynamic characteristic, the velocity \(V_d\) of motion of dislocation as a whole, and study its dependence on various parameters: stress, temperature, etc. However, it is difficult to make a choice in favor of some of the mentioned two approaches to the description of the dislocation profile from measuring its velocity only. Therefore, from the point of view of studying the role of the stochastic motion component, the experimental investigation of other profoundly fluctuating quantities may be more convenient. In fact, when studying the dislocation dynamics by the selective-etching method, a similar value (the displacement of the dislocation end emerging on the crystal surface) is measured [4,9]. With reservations for the distortions introduced by the surface effect, nevertheless, it is possible to assume that the statistical properties of the dislocation tip displacements in

![Fig. 2. Time evolution of the distribution of an ensemble of dislocations over length of displacements. Curves 1-4 correspond to the points in time \(t/t_0 = 2, 6, 10,\) and 15, respectively. At inset experimental data for Ge [8] at stress 12 MPa and temperature 450°C are shown for qualitative comparison (on the left). On the right the merging of that data after rescaling \(z = (l-V_d t)/h\) on common curve is shown, which illustrates the self-similar character of the dislocation profile evolution. Symbols mark different durations of stress imposing: \(t = 50\) s (×); 100 s (○); 150 s (●); 300 s (Δ).]
ensemble reflect the dislocation profile after a suitable surface treatment and can be described by the mentioned theory or its variants referring to the half-space [20].

Fig 2 in its left part illustrates the self-similar displacement evolution following from formula (3) at which the dislocation profile is displaced and widened with time. On the right part of Fig 2 experimental data for 60° dislocations in Ge [8] are shown rescaled similarly to Eq. 3, however, with the exponent chosen for the best possible merging of the curves, which turns out to be $\beta \approx 0.5$. One may conclude that self-similarity approximately fulfills, however, the value of exponent is larger than predicted by the ordinary PNG model.

To date, there are only few investigations of displacement distributions measured from the displacements of the dislocation etching pits on the surface of Ge and Si semiconductor crystals before and after applying a load (for example, [8, 24]); therefore, it is untimely to speak about somewhat complete comparison of the theory with experiment. Nevertheless, some facts should be noted [25]. First, the root-mean-square displacement of a point of emerging of a dislocation on the surface $w = \sqrt{\langle (l(t) - \bar{l})^2 \rangle}$ for the displacement lengths used in experiments with Ge as large as 500 $\mu$m varied in the mesoscopic interval of ~2–25 $\mu$m, which are relatively accessible to measurements. Second, it was obtained in [8] that the root-mean-square displacement $w$ continues to grow appreciably with time at displacement much larger than the lattice period. It points to a long duration of the process of dislocation shape relaxation, which can reflect an increase in the relaxation time with the dislocation length $t_r \sim t_0(L/L_0)^{\nu}$ predicted in the theory, so that the non-stationary mode should be observed in the extended time interval up to $t \sim t_0$. In the opinion of the authors of [8], the profile width increases with time as $w \sim t^{1/2}$, which somewhat differs from the dependence $w \sim t^{1/3}$ for the unsteady mode predicted by the theory for the perfect crystals. The cause of the distinction may be, for example, the presence of defects in samples. It was predicted in [26] and confirmed in [27] that impurities or other point defects can qualitatively change the kink propagation mode to the so-called anomalous one characterizing by the non-linear drift. This may change the universality class of the model and values of exponents, as it is known for the random matrices eigenvalue distributions [28]. Additional randomness introduced by fluctuations in defect density creating slowly decreasing spectrum of delay times for kinks (heavy tails) should increase the roughness of the dislocation profile and the value of the exponent $\beta$. The possible influence of defects can also be a reason for a slower decrease in tails of displacement distributions measured in [8], which can be seen in Fig 2, as compared with those prescribed by the ordinary PNG model. Unfortunately, the number of points on the experimental curves available now is insufficient for the reliable assertions. Therefore, it is extremely desirable to increase the statistical array of the corresponding experimental data.

6. Conclusion

The regularities of dislocation motion in the crystalline relief under load are the subject of discussion by researchers. Mapping the model describing this process onto the exactly solved problem of the distribution of eigenvalues of random matrices clarifies this discussion in the favor of the mesoscopically large roughness of the moving dislocation shape. The adaptation of results of the mathematical studies yields the distribution function for the fluctuations of the dynamic dislocation shape in the explicit form for perfect crystals. It is possible to hope that the achieved significant progress in the theoretical description of statistical properties of these fluctuations will stimulate deeper experimental investigation of dislocation dynamics.

Due to the increase in the relaxation time of the dislocation shape with its size, many statistical characteristics of the dislocation at its sufficient length appreciably exceeds the microscopic values and can be studied at the mesoscopic level. The experimental data available at present reveal the self-similar evolution of these values. First of all, this concerns the profile of moving dislocation, whose major parameter is its root-mean-square width. The measurement of exponents describing the relaxation kinetics provides a tool to distinguish between models describing the kink dynamics. The observed deviations from the predictions of the ordinary PNG model are of interest in themselves for the study of interaction of dislocations with other defects and the control of the real structure of crystals. In particular, they may be evidence of the anomalous mode of kink propagation in germanium crystals.
References

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