Anomalous Dislocation Kink Drift in Germanium

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The evolution of kink pairs on dislocations in Ge single crystals under two-level intermittent loading has been studied in order to reveal modes of one-dimensional transport in a random environment. Experimental evidence has been obtained for the anomalous nonlinear kink drift predicted earlier by theory. [S0031-9007(97)03034-2]

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The possibility of the anomalous modes of the particle's motion in the random medium has attracted researchers' attention and has been studied closely during past years (for a review see [1,2]). It was shown that at some critical driving force value F_c the drastic change should be observed in the dependence of the particle displacement on time. With driving force $F > F_c$ the motion should occur with usual linear drift $x = vt$ and

$$v = (D/kT)(F - F_c). \quad (1)$$

With $F < F_c$ the sublinear dependence of the path length x on time t should be observed with the drift in the field of random forces

$$x \sim t^{\delta}(\delta < 1). \quad (2)$$

Here D is the particle diffusivity, k is Boltzmann constant, and T is the temperature. We give below the derivation of an expression for the critical force F_c for the dislocation interacting with point defects.

The transition to the anomalous drift mode first declared in [3] was studied theoretically in many works and appeared with different names: quasilocalization [4,5], transition to the creep phase [6] or to the heterogeneous dynamics [7], and motion in the field of random forces [8]. In accordance with the theory predictions the systems with different physical nature should demonstrate the universal behavior, Eq. (2). To exemplify let us point out the dispersive transport in the dopant semiconductors [9], the motion of the kinks along the dislocation line or of the domain boundaries in two-dimensional phases [3]. For more examples see reviews in Refs. [1,2]. The experimental evidences of these regularities, however, are either absent or rather indirect [5,6].

The chaotic adsorption of the impurities or other point defects on dislocations makes them a suitable object for the study of the one-dimensional transport in random fields. Because of development of the experimental technique for the investigation of the individual dislocation mobility in semiconducting crystals under two-level intermittent loading (TLIL), the possibility has appeared recently to study more in depth the modes of movement of the dislocation kinks along a dislocation line [10].

Dislocation kinks are the direct consequence of the translational symmetry of crystal lattice determining the periodic dependence of the energy of a dislocation on its position in the glide plane, i.e., Peierls potential relief (Fig. 1). With stresses low enough and nonzero temperatures the dislocation overcomes the Peierls barrier by generation of soliton-type nonlinear excitations and their further evolution into the kink pairs. The nascent kink pairs, growing as a result of fluctuations to a collapse-stable configuration, get expanded by means of a drift motion until annihilation takes place with antikinks in the neighboring pairs [11], giving rise to the microscopic mechanism of the dislocation motion.

The TLIL technique is based on the loading of a sample containing individual dislocations by a sequence of load pulses with the resolved shear stress amplitude σ_i, which results in driving force $F = \sigma_i ab$ acting on kinks. Here a is the kink height, i.e., the period of the Peierls relief, and b is the magnitude of the Burgers vector of the dislocation. The duration of an individual pulse t_i is comparable with a mean time of the dislocation displacement by one lattice parameter under conditions of the steady state motion $t_a = a/V_{\mathrm{st}}$, where V_{st} is a mean dislocation velocity under conventional static loading with $\sigma_{\mathrm{st}} = \sigma_i$. The pulses are separated by "pauses" with the duration t_p when either the stress is not applied at all ($\sigma_p = 0$) or small enough stress $\sigma_p \ll \sigma_i$ of opposite sign with respect to σ_i is applied.

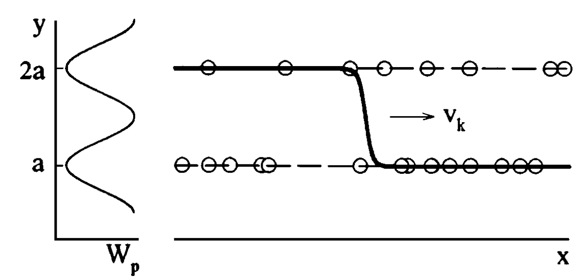

FIG. 1. The sketch of the dislocation kink. $W_P(y)$ shows the Peierls relief, the circles represent randomly distributed point defects.

During the pulse stress action, in addition to thermodynamically equilibrium kinks, extra kink pairs form and spread along the dislocation line. As the pulse separation goes on they become unstable and collapse to the formation centers under the action of the external stress applied as well as the forces caused by the mutual attraction of kinks and the interaction of the dislocation and kink with point defects. In accordance with the Hirth and Lothe theory [11] the dislocation velocity V is proportional to the kink velocity v_k,

$$V = anv_k \, . \tag{3}$$

With small external stresses the density of kinks n is close to thermodynamically equilibrium value n_0. When the directed drift motion of kinks prevails over the chaotic diffusion, we can estimate the average kink velocity during the cycle of TLIL with $(x_i + x_p)/(t_i + t_p)$, where x_i and x_p are the kink displacements during the pulse loading and pause, respectively. We receive for the loading duration $\sum (t_i + t_p)$ the dislocation displacement under TLIL $l = V \sum (t_i + t_p) = an_0(x_i + x_p)/(t_i + t_p) \sum (t_i + t_p)$. The dislocation displacement under static loading $l_{\mathrm{st}} = Vt_{\mathrm{st}} = an_0 v_k t_{\mathrm{st}}$. Assuming that kink velocity under pulse loading $x_i/t_i = v_k$ and taking the active loading duration $\sum t_i = t_{\mathrm{st}}$ we receive

$$l/l_{\mathrm{st}} = 1 + x_p/x_i \, . \tag{4}$$

Equation (4) relates immediately the microscopic kink displacements and experimentally observable macroscopic dislocation path lengths. So TLIL presents a tool allowing one to study experimentally different modes of the kink motion.

The influence of point defects on the dislocation mobility is considered usually as the interaction of a dislocation kink with separate obstacles [12,13]. The additional barriers change the stress dependence of the dislocation velocity but do not modify the linear nature of the kink drift. However, this approach could describe experimental data only if dislocation kinks do not collide on the dislocation line [12]. Later experiments show that kink collision case takes place [14]. The alternative approach [3] deals with the interaction of the whole dislocation with numerous point defects and predicts the anomalous mode of the kink drift, Eq. (2).

This Letter presents the results of experimental study with TLIL of the modes of kink motion along the dislocation lines in Ge single crystals. The data obtained are compared with the regularities predicted by theories [3,12].

Let us consider the model of a dislocation kink motion including the interaction of the dislocation with manifold point defects. The potential of a kink under drift is determined by the work of driving force $-Fx$. Here x is the kink displacement, $F = \sigma ab$, σ is resolved shear stress. The presence of randomly distributed point defects leads to the addition of the random component $uN(x)$ that describes the change in energy of the dislocation-point defect interaction with the kink motion. Here u is the variation of the binding energy of a dislocation to a point defect with the displacement for the distance a, $N(x)$ is the difference in number of point defects in the first and the second Peierls valleys. So the potential $U(x)$ for the kink motion has the form [3,5] $U(x) = -Fx + uN(x)$.

The anomaly in the kink mobility results from the influence of fluctuations in point defects distribution being a collective effect. To understand qualitatively the radical change in the kink mobility with point defect concentration increase, let us calculate, following Ref. [3], average time delay $\langle \tau \rangle$ of the kink at the barriers composed by random pileups of point defects. The time needed to overcome a barrier is given by the expression [15] $\tau \sim \int \exp[U(x)/kT]\,dx$. Then $\langle \tau \rangle \sim \int \langle \exp(uN(x)/kT) \rangle \exp(-Fx/kT)\,dx$. With independent defect distribution over the crystal lattice sites with concentrations c_1 and c_2 in the first and the second potential valleys (Fig. 1) we receive

$$\begin{aligned}\left\langle \exp\!\left(\frac{uN(x)}{kT}\right)\right\rangle &= \left\langle \prod_{i=1}^{x/a} \exp\!\left(\frac{un_i}{kT}\right)\right\rangle \\ &= \Big\{1 + (c_1 + c_2 - 2c_1c_2) \\ &\quad \times \left[\cosh\!\left(\frac{u}{kT}\right) - 1\right] \\ &\quad + (c_1 - c_2)\sinh\!\left(\frac{u}{kT}\right)\Big\}^{x/a} . \end{aligned} \tag{5}$$

Here n_i are the occupation numbers of crystal lattices sites i with defects $n_i = 1$ with the probability $c_1(1 - c_2)$, $n_i = -1$ with the probability $(1 - c_1)c_2$, and $n_i = 0$ with the probability $(1 - c_1)(1 - c_2) + c_1c_2$. It follows from Eq. (5) that $\langle \tau \rangle \sim 1/(F - F_c)$ with $F_c = (kT/a)\ln\{1 + (c_1 + c_2 - 2c_1c_2)[\cosh(u/kT) - 1] + (c_1 - c_2)\sinh(u/kT)\}$. With concentrations of point defects being small enough the expression for the critical force F_c simplifies to $F_c = (kT/a)\{c_1[\exp(u/kT) - 1] + c_2[\exp(-u/kT) - 1]\}$. With $u < kT$ this expression transforms into $F_c \simeq F_0 + F_s$, with $F_s = u(c_1 - c_2)/a = \sigma_s ab$, $F_0 = u^2(c_1 + c_2)/2kTa = \sigma_0 ab$. The divergence of average time of climbing over an obstacle means the existence of the threshold in the dependence of the velocity of kink motion on the driving force, Eq. (1). The derivation of Eq. (1) has been made more comprehensively in Refs. [2,8].

In fact, with $F < F_c$ the motion of kinks does not stop completely but is characterized with qualitatively different regularities, Eq. (2); so they say nothing about the localization of kinks in the random potential with $F \rightarrow F_c$ but about quasilocalization mode [4,5] or creep phase [2] only. In this mode the kink motion is not described any longer in terms of velocity, and the attribute of linearity of kink displacement on time is violated. At first sight the linearity looks as the self-evident and follows from (at least statistical) space homogeneity. More detail analysis shows, however, that with certain conditions (the degree of inhomogeneity being large enough, expressed in the form $F_c > F$) the statistical homogeneity can be violated, and with the space scale increase the larger fluctuations become a factor. As a consequence the time of the displacement is determined mostly by the probability to overcome the strongest obstacle taking place on the length, rather than many "typical" ones, and the linear drift changes to the nonlinear one of Eq. (2) type. Let us represent it in more explicit form,

$$x = x_0(t/t_0)^{\delta}, \delta = F/F_0 \leq 1, x_0 \simeq kT/F_0, t_0 \simeq x_0^2/D\,. \quad (6)$$

The investigated samples were rectangular rods with edge orientations $[1\bar{1}0]$, $[11\bar{2}]$, $[111]$, and dimensions $35 \times 4 \times 0.8$ mm. They were cut from dislocation-free ingots of an n-type Ge single crystal grown by the Czochralski method and doped with antimony until a resistivity 0.4 Ω m was reached. To introduce individual dislocations stress concentrators were produced on (111) faces by a diamond indenter. Dislocation half-loops generated under a subsequent loading were revealed by selective etching. For more details see Ref. [16].

The samples with individual dislocations were loaded with four-point bending around the $[11\bar{2}]$ axis by a sequence of pulses driven from a function generator with required pulse ratio through an electromagnetic force transducer. The pause stress, σ_p, was produced with permanent subloading using a six-point loading jig similar to that described in [17]. As the pulse continues the load is applied to the pair of internal supports and exceeds the permanent subloading applied to the outermost supports. During the pulse separation the subloading action remains only.

To study the characteristics of the kink migration the average glide distances of 60° dislocations were measured as a function of pulse separation $l(t_p)$ for fixed durations of the load pulses t_i. The active loading duration $\sum t_i =$ 7200 s. The width of the leading edge of the load pulses was held constant ($t_f = 4$ ms). The temperature was measured with a thermocouple placed next to the sample and was maintained constant and equal to $T = 583 \pm 1$ K.

The measurements of the dislocation velocity in Ge under conventional loading [18,19] have revealed the sharp decrease in the dislocation mobility with stresses approaching some low threshold. The similar behavior was observed in our crystals (Fig. 2). We found that dislocation velocity near threshold can be described satisfactorily with Eq. (3) with v_k being determined from Eq. (1) with $F_c = \sigma_c ab$ (see inset of Fig. 2).

More information about characteristics of the kink motion under stresses below the threshold, allowing one to test the hypothesis, could be received in TLIL experiments presented in this paper. Figure 3 shows

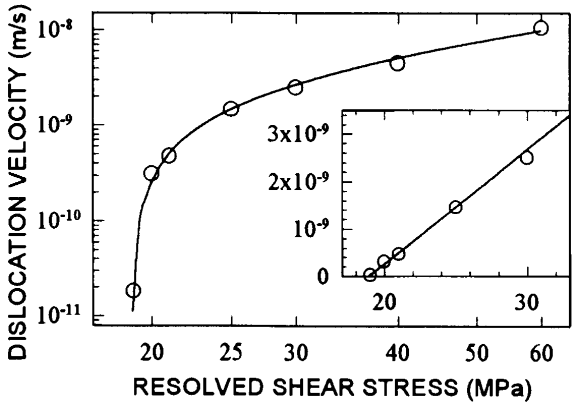

FIG. 2. The stress dependence of average 60° dislocations velocity. The inset shows the data replotted with linear axis to demonstrate the validity of the approximation used. Solid lines represent the results of fitting using Eqs. (1) and (3).

how the plots of mean dislocation glide distances on the relative pulse separation change with the shear stress in pauses increase. The data have been obtained with a fixed pulse stress amplitude ($\sigma_i = +30$ MPa). One can see that the dislocation glide distances decrease is nonlinear, especially for small σ_p values. It should be noted that prediction of theories [11–13] that kink displacement x_p in Eq. (4) depends linearly on pulse separation t_p is inconsistent with the results obtained.

Now let us compare the experimental data with the theory considering the nonlinear kink drift during the pulse separation. We suppose that kink pair expansion occurs under shear stress being high enough and standard linear drift takes place $x_i = v_i t_i$ with kink velocity renormalized by dislocation-point defects interaction, Eq. (1), with $F = \sigma ab$ and $F_c = \sigma_c ab$ consequently. The values of σ_c were estimated with the fit of the stress dependence of dislocation velocity (solid line in Fig. 2). The path length

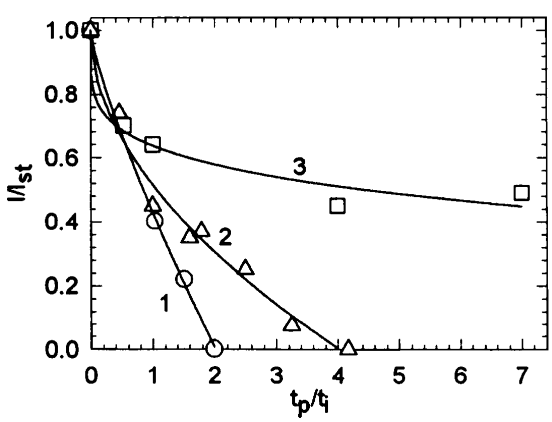

FIG. 3. The normalized dislocation displacement vs relative pulse separation: $\sigma_p = -8$ MPa, $t_i = 45$ ms (1); $\sigma_p = -4$ MPa, $t_i = 48$ ms (2); $\sigma_p = 0$, $t_i = 30$ ms (3). Solid lines are curve fits with Eq. (7).

during the pause x_p is determined with Eq. (6) with x_0 and t_0 being fitting parameters.

Substituting the expressions for x_i and x_p into Eq. (4) we reduce it to the form

$$\frac{l}{l_{\mathrm{st}}} = 1 - K\left(\frac{t_p}{t_i}\right)^{\delta}, \tag{7}$$

with $\delta = (\sigma_p + \sigma_s)/\sigma_0$, $K = (t_0/t_i)^{1-\delta}\sigma_0/(\sigma_i - \sigma_s - \sigma_0)$. Solid lines in Fig. 3 depict the results of fitting of experimental data with Eq. (7). One can see satisfactory agreement of the theory with experiment.

To check the validity of the model the results of several TLIL experiments have been plotted in coordinates δ vs $(\sigma_p + \sigma_s)$ (Fig. 4). In accordance with Eq. (7) the dependence should be linear with the slope $1/\sigma_0$. One can see good agreement between theory and experimental data.

The second fitting parameter t_0 allows one to estimate the kink diffusivity with Eq. (6) and the kink migration enthalpy W_m with expression [11] $W_m = kT \ln(2\nu_D b^2/D)$, where ν_D is the Debye frequency. All calculated values are in the range $W_m = 1 \pm 0.1$ eV, those are in reasonable agreement with the ones obtained by other methods [14,20].

Using parameters obtained, one may check the validity of the drift approach used. Say for the curve (3) in Fig. 3 the displacement of a kink by the drift is $(x_i)_{\mathrm{dr}} = v_i t_i \simeq 9.6$ nm $\simeq 25b$ and the one by the diffusion is $(x_i)_{\mathrm{dif}} \sim (Dt_i)^{1/2} \simeq 7$ nm $\simeq 18b < (x_i)_{\mathrm{dr}}$ (fitting parameters are $\sigma_c = 18.92$ MPa and $W_m = 1.01$ eV). Mean kink free path is then $X \simeq 100b$, so the linear density of defects $c_1 \gg 10^{-2}$. Taking $c_1 = 10^{-1}$ we receive the volume concentration along the dislocation core $\sim 10^{19}$ cm^{-3}. This value could be achieved due to gathering of point defects by moving dislocation. The theory is based on a rather general assumption of short-range point defects-dislocation interaction, so we do not consider the details of the dislocation core structure, dislocation splitting, etc.

The simple model, Eqs. (4) and (7), connects the experimental data on dislocation displacements under intermittent loading with the values of kink displacements governed by the pulse and pause duration values. This provides a promising technique for the investigation of different modes of the kink dynamics at the most elemental level possible. The parameters' values obtained allow one to characterize the dislocation point defect atmosphere state. The comparison of data obtained for Ge crystals with the theory based on assumption of nonlinear kink drift the pulse separation shows their satisfactory agreement. Hence theoretical knowledge of existence in the medium with chaotic distribution of point defects of anomalous modes of the kink motion gets it s experimental corroboration.

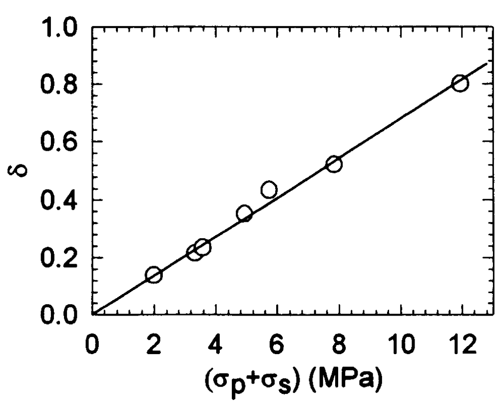

FIG. 4. Stress dependence of the parameter δ.

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