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Mobility of Dislocations in Germanium*

V. CELLI, M. KABLER, T. NINOMIYA
AND R. THOMSON
University of Illinois, Urbana, Illinois, U.S.A.

Experimental curves obtained by Kabler can be best plotted as $v=v_0\exp(-E/kT-\tau_0/\tau)$. In order to explain this law, we suppose that kinks are nucleated on segments of the line between pinning points. At the pinning points, the kinks are momentarily stopped until a fluctuation of sufficient size is available. If the segment is short or the stress low, the activiation barrier for kink collapse is less than the barrier for forward motion beyond the pinning point, and the segment cannot supply successful kinks to the line. If the segment is sufficiently long, successful kinks can be created. Two ranges of velocity are obtained; the first valid in the kink collision range and the second when the ends of the dislocation represent the kink sinks.

Introduction

Experiments on the mobility of dislocations in germanium have been perfomed by Chaudhuri, Patel and Rubin[1], and by Kabler[2]. Kabler measured the velocities of individual isolated dislocations, while Chaudhuri *et al.* measured the dislocations at the head of slip planes produced by the scratch process. The primary motivation in studying the dislocation motion in the semiconductors is that one expects in these crystals that the main effect limiting the velocity is the high Peierls energy[3]. In further checking on this point, Kabler has etched in the active slip planes of dislocations and found etch lines of the dislocations lying in nearly crystallographic directions, with sharp corners where the dislocation loops turn from screw orientation to 60°. This evidence on the moving dislocations in germanium corroborates the earlier decoration pictures of Dash[4]. The strongly polygonal shape of the dislocations in these crystals can only be explained in terms of a high Peierls energy.

Chaudhuri *et al.* and Kabler find the activation energy for the dislocation motion to be 1.6 eV. Kabler, who can distinguish screw dislocations from the 60° type, finds 1.5 eV for the 60° and 1.6 eV for the screw. Chaudhuri *et al.* have reported their results on the stress dependence of the velocity in terms of a power law, $v\alpha(\tau)^n$. The exponent n varys between about 1.5 and 2 depending upon the temperature. Kabler, however, finds that his data more nearly conform to a law of the form

$$v=v_0e^{-E_k/kT}e^{-\tau_0/\tau}\ . \qquad (1)$$

The activation energy is E_k, τ is the stress, T is the temperature, τ_0 is a constant which depends upon temperature. In this work, we shall describe a model of dislocation kinks which predicts a law of the form (1). In the limited space of this preprint, we shall outline the physical assumptions of the theory in fairly complete form and indicate more sketchily the results of the comparison with experiment.

A Kink Model

A dislocation lying initially in a straight crystallographic direction along a given Peierls valley moves to the next valley by the nucleation and growth of a local pair of kinks in the line. We have attempted to explain the stress dependence of the experiments in terms of the stress dependence of the kink activation energy, but on no reasonable model have we been successful in explaining the exponential law observed. We, therefore, propose that the stress dependence of the velocity is due to the interaction between the expanding kinks with pinning points on the line caused probably by impurities. We suppose that these pinning points are distributed at random on the dislocation.

If a kink pair is created upon a particular segment of the line, then the energy of the pair as a function of its separation is sketched in Fig. 1. An energy E_k must be supplied sufficient to create the kink pair, but once formed, as the kinks separate, they gain energy at the rate τabl from the external stress, τ. The Burgers vector is b, a is the

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distance between parallel Peierls valleys, and the kink separation is l.

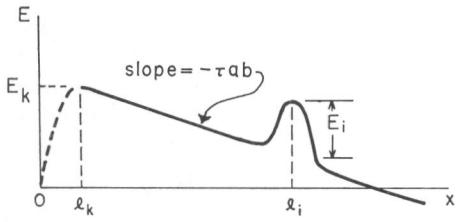

Fig. 1. The energy of a kink pair as a function of its separation. E_k is the kink pair formation energy and l is the kink separation. The pinning point is shown as an additional energy barrier of height E_i.

After nucleation, the kink pair expands under the stress until it comes against the pinning points at l_i, where a barrier to further expansion exists. While held up at the barrier, they then test both the pinning point barrier for further expansion and test the barrier over which they have just come against collapse. If (see Fig. 1)

$$E_i < \tau a b l_i \,, \tag{2}$$

the pinning barrier is lower than the barrier for collapse, and the kinks continue to expand.

Physically, this model states that there are some segments of the line between pinning points where (2) is not satisfied, which do not contribute successful kinks to the general motion of the line, and that only those longer segments where (2) is satisfied are capable of creating successful kinks. As the stress is increased, a larger fraction of the line becomes activated.

The quantity of interest is the number of segments with free length greater than the critical length and the result is given by a radioactive decay formula. If one begins with a large number of kinks nucleated on different segments, as these kinks expand, the number which meet barriers during an increment of expansion, dl, is given by $df = -f(l)\cdot dl/\bar{l}$. The function, $f(l)$, is the number of kinks which have not yet collided with the first barrier after reaching length l. In this expression, the barriers are assumed randomly placed on the dislocation. Thus, the normalized fraction of free segments of length l or greater between pinning points is

$$f(l) = e^{-l/\bar{l}} \,,$$

where $\bar{l}$ is the average length between pinning points. From this it follows that the density of segments of length l per unit length of line is

$$\rho(l) = \frac{1}{\bar{l}^2} e^{-l/\bar{l}} \,. \tag{3}$$

The total velocity of the dislocation is given by the product of the density of successful kinks on the line with the velocity of a successful kink.

$$v = n v_k b \tag{4}$$

n is the density of single kinks per cm of line, and v_k is the kink velocity. We assume that the kink velocity is determined by the rate of jumping the barriers, so

$$v_k = \bar{l}\nu_{i0} e^{-E_i/kT} \,. \tag{5}$$

ν_{i0} is the basic "kink frequency" on the dislocation.

On this model the kink density is determined by the balance between the nucleation rate of successful kinks and the rate of disappearance of the kinks either by (Case I) collision with other kinks or (Case II) at sinks at the end of the line. The creation rate per lattice site of kinks must be equal to the destruction rate. In the two cases, this condition becomes respectively

$$\begin{aligned} &\text{I:}\quad n^2 v_k = \nu_k \int_{l_c}^{\infty} \rho(l)\,dl, \quad l_c = E_i/\tau b a; \\ &\qquad n = \{\nu_k e^{-l_c/\bar{l}}/\bar{l} v_k\}^{1/2} \\ &\text{II:}\quad \frac{n v_k}{L} = \nu_k \int_{l_c}^{\infty} \rho(l)\,dl; \\ &\qquad n = \frac{L}{\bar{l}} \frac{\nu_k}{v_k} e^{-l_c/\bar{l}} \,. \end{aligned} \tag{6}$$

L is the total length of line between sinks in case II. ν_k is the frequency of kink nucleation which in the simplest theory is

$$\nu_k = \nu_{0k} e^{-E_k/kT} \,. \tag{7}$$

Finally, the total dislocation velocity becomes

$$\begin{aligned} &\text{I:}\quad v = v_0 \exp\{-((E_k + E_i/2kT + E_i/2\tau b^2 \bar{l})\}; \\ &\qquad v_0 = b\sqrt{\nu_{0k}\nu_{i0}} \\ &\text{II:}\quad v = v_0 \exp\{-(E_k/kT + E_i/\tau b^2 \bar{l})\}; \\ &\qquad v_0 = \frac{bL}{\bar{l}} \nu_{0k} \,. \end{aligned} \tag{8}$$

This formula is of the form sought.

There are three ways in which this simple formula is modified by a more strict theory of the kink nucleation problem. a) The kink formation energy is a function of stress. An analysis of a simple model of the kink system

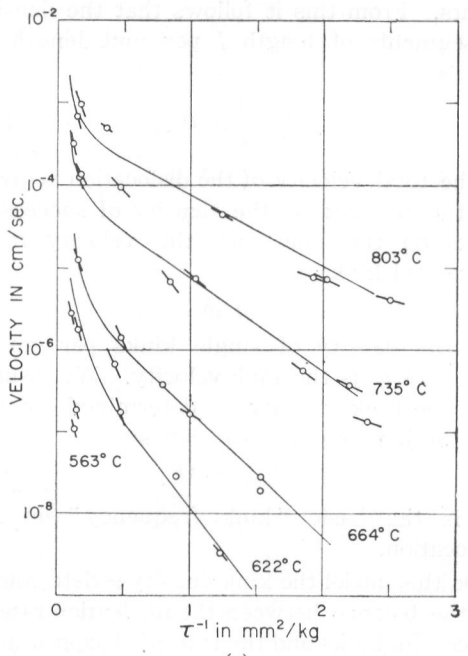

Fig. 2. Velocity of dislocations in Ge as a function of stress. (a) 60° dislocation (b) Screw dislocations. (Unpublished data of Kabler)

suggests that at high stresses, the velocity should become greater than predicted in (8). b) At high stresses, the impurities can be pushed along under the stress by a kink, and in addition, the kink frequency, ν_{0i}, should increase. These two effects also increase the velocity above (8), but their effect is not so strong as a). c) The kink collision and collapse problem can be treated in a much more sophisticated manner and leads to essentially the same result as (8). d) The statistics of the nucleation of kinks can be extended with the use of the theory of absolute reaction rates, but again, the simple results of (8) are not changed in important ways.

Detailed comparison with the experimental data given in Fig. 2 does not allow one to distinguish clearly between cases I and II. Parameters appropriate to the two cases are

	Case I	Case II
$\bar{l}$	Approx. 50 b	Approx. 50 b
E_i	$0.8\,\text{eV} \leq E_i \leq 1.6\,\text{eV}$	$E_i \leq 0.8\,\text{eV}$
E_k	$0.8\,\text{eV} \leq E_k \leq 1.2\,\text{eV}$	1.5—1.6 eV

The nature of the pinning points remains unknown. Either jogs or impurities could be the cause. In the case of the 60° dislocations, there is a shift in the value of $\bar{l}$ with temperature in such a way as to suggest that $\bar{l}$ is governed by an activation energy of 0.25 eV. One is thus tempted to suggest that oxygen impurities in the lattice are picked up by the moving dislocation and carried with it in something approaching equilibrium quantities. This possibility needs further experimental study.

References

1 A. R. Chaudhuri, J. R. Patel and L. G. Rubin: J. Appl. Phys., to be published.

2 M. Kabler: Unpublished data.

3 See calculation of Peierls energy in Ge and Si: V. Celli; J. Phys. Chem. Solids **19** (1961) 100.

4 W. C. Dash: *Dislocations and Mechanical Properties of Crystals*, (Wiley, New York, 1957), p. 62.

DISCUSSION

Amelinckx, S.: 1) It is not clear to me which model was assumed for the dislocations in germanium. Would your results be sensitive to the exact model? 2) I would also like to make a comment. We have evidence from electron microscopic observations* that dislocations in silicon are visibly dissociated (equilibrium distance$\simeq$100 Å). There

is good reason to believe, that although the equilibrium separation is smaller in germanium it is nevertheless present. I suppose that the mechanism for the movement of kinks in dissociated dislocations should be different from that for kinks in undissociated ones.

* E. Aerts, P. Delavignette, R. Siems and S. Amelinckx: To be published in J. Appl. Phys.

Thomson, R.: 1) The model as presented is not particularly sensitive to details of the core structure. We simply assume i) that the dislocation motion is limited by the Peierls energy and ii) that the kinks interact with some sort of inhomogeneity on the dislocations (jogs or impurities), but are free to move between them. The parameters in the theory are then expressed as the nucleation energy to overcome the Peierls energy and the interaction strength between the kinks and the inhomogeneities. We have, of course, gone beyond this simple almost phenomenological framework and calculated the parameters on the basis of detailed models. Such detailed calculations will be sensitive to the particular model. 2) If the dislocations are split, then the jogs on 60° dislocations will have a barrier for motion. The barrier will correspond to punching an extra atom along the stair rod between the two jogs on the partials.

Suzuki, T.: 1) Such a kind of calculation you did seems to be applicable to other substances, too. Have you tried to apply to such a problem as the low temperature relaxation peak in metals and non-metals? 2) Have you got an information of the Peierls stress for germanium by applying your theory to your experiment?

Thomson, R.: 1) We have not *really* tried to apply this work to other materials. LiF shows the same type of law, but an estimate of the parameters in the law from the experiments of Gilman and Johnston does not lead to very realistic values. In addition, the shape of the loops in LiF is not crystallographic, and we are reluctant to claim that the dislocations in that case are limited by the Peierls force. However, I am certainly inclined to agree that there are a number of other situations where these ideas should be applicable besides the case of germanium. In particular, the work of Hasiguti reported in this conference on the low temperature peaks is very closely related to our own. 2) One can estimate the Peierls stress by adopting a more detailed model of the kink such as Seeger's string model, and the calculated Peierls energy from this estimate using the experimental value for the kink nucleation energy is in agreement with an earlier estimate (0.1 eV per atom plane) of the Peierls energy in germanium by Celli.