STATISTICS OF KINK FORMATION ON DISSOCIATED DISLOCATIONS

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Résumé.- En se fondant sur le concept de double décrochement, on a développé un modèle prédisant la vitesse des dislocations en fonction de la contrainte et de la température. Ce modèle rend compte de la dissociation des dislocations dans les cristaux semiconducteurs et de l'existence de constrictions (comme obstacles au mouvement latéral des doubles crans). On le compare à des mesures de $v(\tau)$ dans le Ge, Si et GaAs.

Abstract.- A model for the dislocation velocity depending on stress and temperature is developed based on the concept of the double kink mechanism. It takes into account the dissociation of dislocations in semiconductor crystals and the existence of constrictions (as obstacles for the lateral kink motion). It is compared with $v(\tau)$-measurements in Ge, Si and GaAs.

1. Introduction.- There is now good experimental evidence that dislocations in many semiconductor materials /1/ are dissociated and are likely to move in the dissociated state /2/. A systematic weak-beam TEM investigation on deformed germanium crystals additionally showed that the stacking fault ribbon between the partial dislocations is interrupted by constrictions at a mean (temperature dependent) distance $\ell \simeq 0.1 - 0.3\ \mu m$ /3/. In the following a model for the dislocation velocity is developed which takes into account the dissociation of dislocations and the constrictions.

2. Double kink nucleation rates.- Because of the covalent bond structure of semiconductor crystals one can assume a Peierls potential to exist for the partial dislocations. A dislocation can move by nucleating double kinks on each partial. The nucleation rate (per unit length) at which kink pairs are created on a dislocation segment may be given by /4/.

$$J = J_o\ e^{-E/KT}(1+ \frac{\tau_1}{\tau})e^{-\tau_1/\tau} \qquad (1)$$

if one takes into account the existence of a periodic obstacle potential (E_d) along the dislocation line. ($\tau_1 = E_d/ab_p\ell$, b_p the partial Burgersvector, a=period of the Peierls potential, ℓ mean distance of obstacles). The nucleation energy E of a kink pair on a partial has shown to be stress dependent according to /5/.

$$E_u(\tau) = E_{DK}^u - a^* (\tau-\tau_c)^{1/2} \qquad (2)$$

with $\tau_c = \mu ab_p\beta/4\pi d^2$, d equilibrium distance of the moving partials, μ shear modulus, β orientation factor, E_{DK}^u self energy of the kink pair, and $a^* = E_{DK}/\tau_p{}^{1/2}$, where τ_p is the Peierls stress for the partial. The elastic interaction of the two partials reduces the external stress τ acting on the single kinks by τ_c. From equation (2) one can conclude that the nucleation of a stable double kink is only possible if $\tau > \tau_c$. It has been proposed, however, that for stresses $\tau < \tau_c$ the nucleation of a kink pair becomes possible if a second kink pair on the other partial is built up simultaneously. Then one has to supply the energy of the correlatedly nucleated double kinks :

$$E_c(\tau) = E_{DK}^c - 2a^*\tau^{1/2} \qquad (3)$$

Inserting equations (2) and (3) into (1) obtain the double kink nucleation rates in the limiting cases $\tau > \tau_c$ and $\tau < \tau_c$.

3. Statistical treatment of the dislocation velocity.- During the stationary motion of a straight dissociated dislocation segment of length L both partials remain straight on average and move with the same velocity. Therefore one can resolve the motion into identical steps of distance a. If we start the time t = 0 when one step has just been finished the probability P(t) that during the time interval (0,t) the dislocation has moved one elementary step is equal to the probability that a kink pair has been created (in the direction of motion) at an arbitrary point of a partial (and on the other as well because of the same velocity). Then the velocity v of the dislocation is given by

$$v = a \Big/ \int_0^\infty t\ \frac{\delta P}{\delta t}\ dt \qquad (4)$$

Calculating the probability P(t) that a kink pair appears at a certain point on a partial (for simplicity at the center) one has to consider that a second kink pair on the other partial already exists and the nucleation probability in face of this kink pair is enhanced (see figure 1, region I). The mean length $\bar{s}(t)$ of a kink pair created with the probability P is given by

$$\bar{s} = 2v_K\left(t-\int_0^t t\,\frac{\delta P}{\delta t}\,dt \Big/ \int_0^t \frac{\delta P}{\delta t}\,dt\right) \qquad (5)$$

with v_K = kink migration velocity.

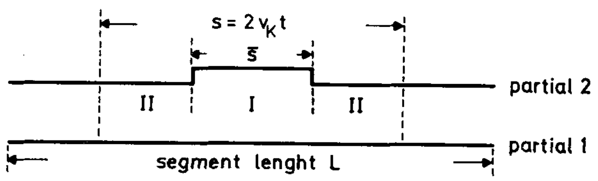

Fig. 1 : Dissociated dislocation segment containing a kink pair on one partial.

To derive simple equations we first restrict ourselves to the limiting cases $\tau < \tau_c$ and $\tau > \tau_c$. P(t) may be derived from the following equations.

$$\frac{\delta P}{\delta t} = J_u\, s\, [1-P] \qquad \tau > \tau_c \qquad (6)$$

$$\frac{\delta P}{\delta t} = J_c\, \bar{s}\, [1-P] \qquad \tau < \tau_c \qquad (7)$$

At high stresses the double kink nucleation on one partial is not affected by the presence of kink pairs on the other, whereas at low stresses the nucleation is only possible with the help of a second of length $\bar{s}$. Furthermore the equations include that the double kinks are nucleated before an expanding kink pair would have reached the segment ends (that means $2L^2J/v_K \gg 1$). The solution of equation (6) has been given elsewhere /5/; equation (7) can be solved numerically. Inserting P(t) into equation (4) yields

$$v = \frac{2}{\sqrt{\pi}}\, a\, (v_K J_u)^{1/2} \qquad \tau > \tau_c \qquad (8)$$

$$v = \frac{2}{0.75}\, a\, (v_K J_c)^{1/2} \qquad \tau < \tau_c \qquad (9)$$

In the stress range $\tau \approx \tau_c$ both the calculation of the nucleation rate and the probability P becomes very complicated. Therefore an interpolation formula may be tried /5/

$$v = 2a\, [v_K(J_u+J_c)]^{1/2} \qquad (10)$$

which approximately contains equations (8) and (9) as limiting cases. The final equation for the dislocation velocity is obtained if one inserts J_c and J_u and the earlier derived equation for the kink migration velocity v_K /4/ ($\nu_o \approx 10^{10}\,s^{-1}$)

$$v_K = \nu_o \ell_o e^{-(E_d+\varepsilon)/KT} \qquad (11)$$

Here it is assumed that the mean distance of obstacles the kinks have to overcome is temperature dependent according to $\ell = \ell_o e^{-\varepsilon/KT}$ (11a).

4. Comparison with experimental results.- It is possible to fit equation (10) to velocity measurements in Ge, Si and GaAs /5/. A typical result is given in figures 2a,b. 5 free parameters were used : $E^u_{DK} + E_d$, $E^c_{DK} - E^u_{DK}$, ε, ν_o and $\tau_1^o = E_d/ab_p\ell_o$.

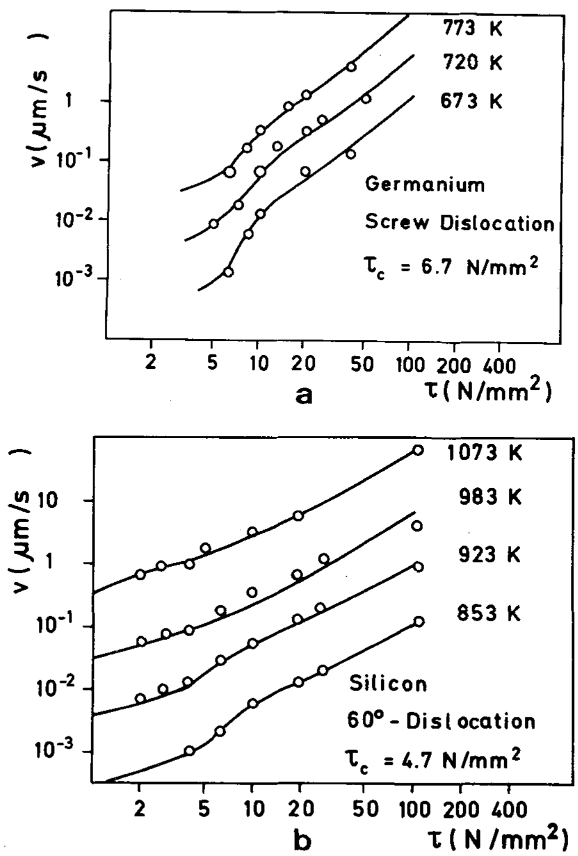

Fig. 2 : Simultaneously fitted v (τ) - curves to dislocation velocity measurements in germanium (a) and silicon (b).

The equation was fitted simultaneously for all temperatures to $v(\tau)$-measurements. τ_c was calculated from measured dissociation widths d of dislocations. Values of some derived parameters are given in table I. The mean distance of obstacles ℓ (at 0.6 $T_{melting}$) $\simeq$ 0.2 - 10 µm agrees within the error limits with the experimentally observed density of constrictions in deformed Ge /3/ : $\ell \approx 0.1 - 0.3$ µm. Additionally a temperature dependence of ℓ was observed according to equation (11a). E_d could not be determined separately from the fit, but is expected to be high (> 1eV) because of the large values of $D^u_{DK} + E_d$. The increase of the nucleation energy $E^c_{DK} - E^u_{DK}$ at low stresses is rather small which is not really understood. The prefactor $\nu_o = J_o b_p$ is of the order of $10^9\ s^{-1}$ as expected. At high stresses equation (10) may be approximated by the well established equation /6/

$$v = A\tau^{m} e^{-Q/KT} \tag{12}$$

where Q is given by

$$Q = \frac{1}{2} (E^{u}_{DK} + E_{d} + \varepsilon)/KT \tag{13}$$

which demonstrates well the influence of the obstacles on the dislocation velocity.

Table I : E^{u}_{DK}, E^{c}_{DK} double kink nucleation energy (at high and low stresses, respectively), E_d obstacle potential, ε binding energy of the obstacles to dislocations, ν_0 frequency factor, ℓ mean distance of obstacles, τ_c calculated critical stress, d dissociation width. The E^{c}_{DK}-E^{u}_{DK} values are recalculated and differ from those mentioned in /5/.

	Ge(60°)	Ge(0°)	Si(60°)	Si(0°)	GaAs(α)	GaAs(β)	
$E^{u}_{DK} + E_{D}$	2.5	2.4	3.5	3.5	1.8	2.3	eV
$E^{c}_{DK} - E^{u}_{DK}$	0.25	0.2	0.3	0.3	0.1	0.15	eV
ε	0.6	0.6	0.9	0.8	0.1	0.2	eV
ν_o	$10^{9.6}$	$10^{8.8}$	$10^{9.6}$	$10^{9.5}$	$10^{8.7}$	$10^{8.4}$	s^{-1}
$\ell\,(0.6T_M)$	0.2-1.3	0.3-20	0.5-40	0.4-40	0.7-20	1.8-16	μm
τ_c	4.3	6.7	4.7	5.3	4.2	3.7	N/mm^2
d	45	29	64	42	-	-	Å

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