Comment on "Electronic effects on dislocation velocities in heavily doped silicon" by J. R. Patel, L. R. Testardi, and P. E. Freeland

W. Schröter, R. Labusch, and P. Haasen
Institut für Metallphysik, Universität Göttingen, Göttingen, Germany
(Received 2 July 1976)

The influence of doping on the dislocation velocity in Si and Ge has been attributed to an effect of the line charge of the dislocation on the creation or motion of double kinks. A phenomenological theory of Patel *et al.* for this effect is criticized. It is pointed out that a microscopic theory by Haasen explains all the known facts.

I. INTRODUCTION

In a recent paper Patel, Testardi, and Freeland[1] (PTF) report on measurements of the dislocation velocity in silicon as a function of dopant concentration. They analyze their results in terms of a model for localized electron states at dislocations and by an assumption for the influence of the line charge on the velocity of the dislocation. They come to conclusions, which strictly contradict our own findings. We shall present evidence here that the assumptions underlying their model are basically unacceptable.

The influence of doping N_c on the dislocation velocity v in Si and Ge has been ascribed by both Patel *et al.*[1-3] and by us[4,5] to the influence of the line charge Q of the dislocation on the creation or motion of double kinks. The problem of evaluating $v(Q)$ on the basis of this mechanism is tackled in two steps: (i) A calculation of the line charge Q of the dislocation as a function of temperature T and dopant concentration N_c. (ii) A calculation of the rate of formation or of the movement of kinks as a function of Q. The two approaches to this problem available now, that of Patel *et al.*[1-3] and our own model[4,5] proceed however quite differently.

With regard to the first step, PTF treat dislocation acceptor and donor states separately by statistical mechanics assuming that the line charge Q of the dislocation is smeared out homogeneously over the region of the screening cloud surrounding the dislocation. We on the other hand used a relation between the Fermi level E_F and the line charge Q, extrapolated to high temperatures, whose validity has been established for lower temperatures by a number of authors.[6,7]

With regard to the second step, Patel *et al.*[1-3] introduce an *a priori* assumption for $v(Q)$, while our own calculation is based upon a mechanistic model of one of us[4,5] which describes the influence of the line charge on the rate of formation of double kinks.

PTF derive from a fit of their experimental data to the result of their calculation the density and energetical position of the localized states at dislocations. In our model the density, the type and the energy position of dislocation states are derived from independent measurements at low T. The dependence of the neutral dislocation level on temperature is not known and therefore its position with respect to the energy bands at the high temperatures, at which the velocity measurements are done, is a free parameter of the model. At present we have no possibility to analyze the experimental data of PTF in terms of our model because the localized states at screw dislocations, the dislocation type investigated by those authors, have not been studied by electrical or optical methods so far in Si. It is therefore hardly meaningful if PTF compare their screw dislocation level E_b with the one we have found electrically for 60° dislocation.

In Secs. II and III we compare in detail the different approaches of the two steps mentioned above.

II. OCCUPATION STATISTICS FOR DISLOCATIONS

The influence of dislocations on the electrical and optical properties of semiconductors, i.e., on carrier density, carrier mobility, lifetime, photoconductivity, optical absorption, luminescence, etc., has been studied mainly at lower temperatures, between 4 and 300 K in Ge and up to 400 K in Si.[6-12]

We have analyzed these results in terms of a statistical concept which may be summarized in the following equations (for p-type material):

$$E_F = E_0 + E_e + E_s \cdots , \tag{1}$$

$$E_e = (e^2 f / 2\pi\epsilon b)(\ln \lambda_0 / r_0 - \tfrac{1}{2}) , \tag{2}$$

$$E_s = T\frac{\partial S}{\partial f} = \begin{cases} kT \ln[f/(1-f)], & \text{empty band} , \\ 0 , & \text{half-filled band} , \\ kT \ln[(1-f)/-f], & \text{full band} . \end{cases} \tag{3}$$

e is the elementary charge; ϵ the dielectric constant. E_F in the Boltzman approximation is given by $E_F = kT \ln(N_v/p)$ (k is the Boltzmann constant, N_v is the effective density-of-states of the valence band, p is the density of free holes). E_0 is an energy parameter which characterizes the position of the neutral dislocation level within the band gap. $1/b$ is the number of states per unit length of the dislocation, λ_D is the Debye screening length, r_0 is the radius of the wave function of the dislocation states, f is the fraction of dislocation states which are occupied by an additional electron ($f>0$) or hole ($f<0$). $E_e = \partial E_{el}/\partial f$ where E_{el} is the energy of the electrostatic interaction between all charges at the dislocation, between the line charge and the screening cloud, and between the charges of the screening cloud. The charges at the dislocation form with respect to the neutral state ($f=0$) the line charge $Q = ef/b$.

S is the configurational part of the entropy for the electrons at the dislocation. It should be noted that for small deviations in f from zero the difference in E_s between a half-filled and an empty or full band is significant.[7]

The electrostatic shift E_e has been calculated in different approximations by solving Poisson's equation with the line charge of the dislocation as the source term of the field and the redistribution of free charge carriers or of the ionized impurities in the local field as the response term.[10]

The type and energetical position of the dislocation states have been derived from the analysis of Hall-effect, mobility, lifetime, and photoconductivity data at low T in terms of the model described above.[6-11] A consistent interpretation of all these data has been given during the last years in terms of a one-dimensional, half-filled band for the neutral 60° dislocation in Ge($E_0 = 0.09$ eV) and Si($E_0 = 0.3$ eV) and of an empty and a full band, separated by an energy gap, for neutral screw dislocations in Ge.[12]

The question whether the description by a row of point charges or by a line charge is more appropriate for the dislocation has been decided recently in favor of the line charge.[9] Equations (1)–(3) in fact give a rather simplified description of this more complicated problem. We mention a few complications. As far as the occupation statistics is concerned the dislocation presents a set of states, whose distribution and position on the energy scale is dependent on its occupation. Our approach is applicable to the case that the range of the electrostatic potential, i.e., the Debye screening length λ_D is large compared to the half width of the eigenfunction of the dislocation states, i.e., r_0. For $r_0 \ll \lambda_D$ the dislocation states in fact maintain their distribution as a function of f and are rigidly shifted by $-eV(0)$ on the energy scale, where $V(r)$ is the potential of the line charge and its screening cloud. The condition $r_0 \ll \lambda_D$ limits the validity of our approach to doping concentrations below 10^{19} cm^{-3}. This also limits an analysis of the results of Patel *et al.* by our model.

In their treatment of the occupation statistics for the dislocation PTF assume that the structure of the set of states at the dislocation remains rigid up to doping concentrations of 5×10^{19} cm^{-3}. The electrostatic energy shift E_e is calculated in the following way: (a) The dislocation states are assumed to be homogeneously distributed over a cylinder of the radius λ_D around the dislocation. Their occupation as a function of T and N_c is derived from the neutrality condition within the cylinder. The density of states A_0 associated with the dislocation is then $A_0 = 1/\pi b \lambda_D^2$ and dependent on temperature and doping concentration. The electrostatic shift E_e as well as the carrier density thus are constant within the cylinder but change discontinuously at its surface. The authors furthermore make the following assumptions concerning the dislocation states: (b) In n-type Si only acceptor states exist while in p-type Si only donor states at the dislocation change their occupation.

Our main objections against this way of treating the occupation statistics for dislocations are the following:

(a) The method of calculating E_e seems to us permissible only, if the dislocation charge consists of a row of point charges and if the distance between those charges b/f is larger or at least comparable with the Debye radius: $b/f > \lambda_D$. Under this condition E_e remains rather small because the charged sites along the dislocation are well screened among each other. But these conditions do not appear to us to be realistic, because electrical data at low temperatures show that E_e as the difference between the Fermi level E_f and the position E_0 of the neutral dislocation (and E_s) does not remain small, when E_f runs all over the band gap.

(b) According to Fig. 10 of the PTF paper the Fermi level inside the dislocation cylinder takes on different values in n- and p-type material in the limit of low-doping concentrations. Apparently the authors believe that in intrinsic Si the position of the Fermi level inside the dislocation cylinder is determined only by the dislocation acceptor level in one case and only by the dislocation donor level in the other, although it is not clear which case is supposed to be which in the intrinsic material.

This inconsistency arises because the authors

do separate analysis for n- and p-type Si as if the dislocation states in the two materials had nothing to do with each other while actually it is of course the same dislocation with the same set of eigenstates in both materials and the difference can only be in the occupation of those states. There seems to be no way to reconcile their analysis with basic facts of semiconductors physics. The existence of an acceptorlike and a donorlike level (or, as we believe, one-dimensional band) at screw dislocations is not unlikely by analogy with the results on screw dislocations in Ge,[12] but obviously there can be only one Fermi level in intrinsic material and its position must be above the full levels (donors) and below the empty level (acceptors).

We therefore conclude that the physical basis of the PTF analysis is not sound and that the coincidence of their calculated curves in Figs. 7–9 with some of their experimental data is fortuitous.

III. DYNAMICAL BEHAVIOR OF DISLOCATIONS IN DOPED SEMICONDUCTORS

The results of measurements of the dislocation velocities in intrinsic Ge and Si have been described by the relation[13]

$$v(\tau, T) = f(\tau) e^{-U/k_B T} ,$$

with τ the applied shear stress.

It has been proposed that the formation and motion of double kinks are the relevant processes which determine the velocity of dislocations. Because of the difficulties in calculating pre exponential factors for the process it was not possible till now to derive an unambiguous proof for this model by comparison with the experimental results.

Recently, one of us has pointed out[4] that the electrostatic self energy of a system of charges on a straight line is lowered by any deviation from the straight line. A calculation has shown that the difference ΔU in the electrostatic part of the self energy between a straight dislocation and a dislocation with a double kink in the saddle point configuration is proportional to the square of the line charge, i.e., to Q^2. It has been shown that this effect can roughly account for the experimentally established variation of the activation energy U with doping.[4,5]

PTF have proposed a direct proportionality between the dislocation velocity v and the line charge Q, i.e., $v \sim Q$, without specifying a mechanism which would yield such a relation. Actually they assume in their paper a proportionality to the absolute value of Q, $v \sim |Q|$. This function has a singularity at $Q = 0$, where $\partial v/\partial Q$ is a step function and it also yields $v \to 0$ for $Q \to 0$. It seems impossible that the relation could be valid for small values of Q. This is a crucial point because Patel *et al.* normalize all their results to the values in the intrinsic material which according to their model means small occupation ratios f. So the validity range of the $v \sim Q$ assumption for small Q would directly affect all their conclusions drawn from the comparison with experimental results.

[1] J. R. Patel, L. R. Testardi, and P. E. Freeland, Phys. Rev. B 13, 3548 (1976).

[2] J. R. Patel and A. R. Chaudhuri, Phys. Rev. 143, 601 (1966).

[3] H. L. Frisch and J. R. Patel, Phys. Rev. Lett. 18, 784 (1967).

[4] P. Haasen, Phys. Status Solidi 28, 145 (1975).

[5] W. Schröter and P. Haasen, Proceedings of the Conference, Hohegeiss, 1975 (unpublished).

[6] W. Schröter, Phys. Status Solidi 21, 211 (1967).

[7] R. Labusch and W. Schröter, in *Dislocations, Collective Treatise*, edited by F. N. R. Nabarro (North-Holland, Amsterdam, 1976); W. Schröter and R. Labusch, in *Lattice Defects in Semiconductors* (Institute of Physics, London, 1974), Series No. 23, p. 56.

[8] R. Labusch and R. Schettler, Phys. Status Solidi A 9, 455 (1972).

[9] E. Scheibe, diploma thesis (Göttingen, 1976) (unpublished); F. Düster, thesis (Göttingen, 1976) (unpublished).

[10] W. Schröter and R. Labusch, Phys. Status Solidi 36, 359 (1969).

[11] D. Mergel, diploma thesis (Göttingen, 1975) (unpublished).

[12] R. Wagner, Phys. Status Solidi A 24, 575 (1974); R. Wagner and P. Haasen, in *Lattice Defects in Semiconductors* (Institute of Physics, London, 1974) Series No. 23, p. 387.

[13] H. Alexander and P. Haasen, Solid State Phys. 22, 27 (1968).