Carrier interactions with dislocations in germanium and silicon

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The anisotropy of the resistance of n-Ge with dislocation is measured in the microwave band. It is concluded that the influence of the dislocations on the resistance is determined by the detour effect and that the dislocation occupation coefficient is a nonmonotonic function of the temperature.

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Introduction of dislocations into the crystals n-Ge,¹ p-Ge,² and Si^{3,4} leads to a noticeable increase of the resistance and to the appearance of anisotropy of the electric conductivity (i.e., to a difference in the resistance of the sample in the directions along and across the dislocations). It is proposed that the dislocations change the resistance for two reasons. First, scattering of the carriers by the dislocations can decrease the mean free path. Second, the sample resistance increases when the dislocations are introduced on account of the detour effect.¹ The gist of this effect is the following: the dislocations in Ge and Si are surrounded by dielectric Read cylinders and the charges must detour around these cylinders when they move from contact to contact. Bending the current lines is equivalent to increasing the length, meaning also the resistance of the sample. The detour effect becomes noticeable when the average distance between the dislocations is comparable with the radius of the Read cylinder.

It is clear that there exists a critical dislocation density $N_D^{\rm er}$ at which no current will flow at all from contact to contact. At dislocation densities N_D smaller than but close to $N_D^{\rm er}$ the sample resistance should depend very strongly on N_D , and the anisotropy of the electric conductivity can be exceedingly high. (Similar phenomena are well known in the physics of disordered media: they are described by percolation theory.⁵)

It is of interest to clarify the relative role of these two mechanisms whereby the dislocations influence the resistance of Ge or Si. We have therefore investigated the anisotropy of the electric conductivity of n-Ge with dislocations in the microwave band (frequency $f \approx 10^{10}$ Hz). The choice of the frequency band is determined by the following considerations. If the role of the dislocations reduces to a decrease of the mean free path of the carriers, then the anisotropy of the resistance in the microwave band should be close to the anisotropy of the dc resistance.¹ On the other hand, if the contribution of the dislocations to the resistance is determined by the detour effect, then the resistance in the microwave band can remain isotropic (in contrast to the dc resistance), since the influence of the detour effect in the microwave band should be weaker than at direct current.

This is easiest to verify by considering a particular case wherein the dislocations, settling in the glide plane, form a thin dielectric layer. Such a layer increases strongly the dc resistance in a direction perpendicular to the layer, and consequently leads to very large electric anisotropy. At the same time, in the microwave band the sample resistance may not decrease at all, since the action of the layer is similar to that of a capacitor connected resistor in series with a resistor in an ac circuit. Consequently there may be no anisotropy of the resistance in the microwave band.

We have measured in the microwave band the resistance and its anisotropy of *n*-Ge samples with dislocations. The dislocation density was chosen such that the average distance between dislocations was comparable with the radius of the Read cylinder. The same condition was satisfied in studies by others.¹⁻⁴ The results of the measurements are shown in Figs. 1 and 2 (the experimental procedure is described in Ref. 6). In the region of temperatures T below 6 K, the conductivity is due to carrier motion along the dislocations, and the conductivity anisotropy is determined by the anisotropy of the dislocation structure. No conductivity of this type was observed so far in direct current.

The dislocation conductivity was investigated in detail in Refs. 6-8. We are presently interested in another region, T > 6 K. In this region the concentration of the electrons excited into the conduction band from the chemical donors becomes large enough to introduce a



FIG. 1. Temperature dependence of the resistivity (in relative units) of samples with dislocations in the microwave band for samples with different dislocation densities N_D and different degrees of doping N_g : \Box correspond to $N_D=0$, $N_g=10^{13}$ cm⁻³; $\bigcirc -N_D=2.7 \cdot 10^6$ cm⁻², $N_g=10^{13}$ cm⁻³; $\bigtriangleup -N_D=3.5 \cdot 10^6$ cm⁻², $N_g=2 \cdot 10^{13}$ cm⁻³; $\bigtriangledown -N_D=5 \cdot 10^6$ cm⁻², $N_g=10^{13}$ cm⁻³. ρ_0 is the resistivity of the sample \Box at T=20 K.



FIG. 2. Temperature dependence of the anisotropy of the conductivity in the microwave band. K is the ratio of the conductivities of the sample for cases when the electric microwave field is parallel and perpendicular to the dislocations. The characteristics of the samples are the same as in Fig. 1.

noticeable (at our sensitivity) contribution to the conductivity. With increasing number of free electrons, the resistance of the samples decreases (Fig. 1). The anisotropy coefficient K decreases simultaneously (Fig. 2). At such large T that the contribution of the band electrons to the conductivity dominates over the contribution of the electrons moving along the dislocation cores, the value of K is close to unity.

We can thus conclude that the contribution of the dislocations to the mean free path is small enough (otherwise we would have K > 1, just as in dc measurements¹) and their influence on the resistance is due to the detour effect. It is of interest in this connection to discuss the results of Refs. 3–5, where the strongest influence of the dislocations on the electric conductivity was noted. It was observed³⁻⁵ that in a definite interval of T the dislocations lead to a very drastic increase (up to four orders of magnitude) in the mobility in a direction transverse to the dislocations (μ_{\perp}). This interval lies near 16 K in p-Ge,² and near 100 K in $n-Si.^{3,4}$

The minimum value of μ_{\perp} depends extremely strongly on N_D . Thus, Osip'yan and Shevchenko² observed a change of μ_{\perp} of almost four orders of magnitude when N_D changed from 4×10^6 to 10^7 cm⁻², while in the study of Milevskii and Zolotukhin³ an increase of N_D by 10%(from 2.25×10^8 to 2.5×10^8 cm⁻¹) led to a decrease of μ_{\perp} by one order of magnitude. The electric anisotropy $\mu_{\parallel}/\mu_{\perp}$ greatly exceeds the structural anisotropy. Thus, it follows from the data of Osip'yan and Shevchenko² that at T = 16 K the values of $\mu_{\parallel}/\mu_{\perp}$ for samples with $N_D = 4 \times 10^6$, 6×10^6 , and 10^7 cm⁻² are respectively 3, 10, and 1000.

All these facts provide, in our opinion, most convincing evidence that in the experiments of Refs. 2-4 we are dealing with the detour effect at N_D close to N_D^{cr} , so that the strong dependence of μ_{\perp} on N_D and the large values of $\mu_{\parallel}/\mu_{\perp}$ can be attributed to proximity to the percolation threshold. There remains, however, one seeming contradiction. The point is that the detour effect should lead to a monotonic temperature dependence of μ_{\perp} , if it is assumed (following Read⁹) that the linear density of the charge q trapped by the dislocation is a monotonic function of T. According to Read,⁹ q (meaning also the radius of the cylinder r) decreases with increasing T, and consequently the influence of the dislocations on the electric conductivity should decrease with increasing T. The experiments²⁻⁴ show, however, that the influence of the dislocations increase sharply in a certain temperature interval.

It seems to us that all the experimental results must inevitably refute Read's conclusion⁹ that q(T) is a monotonic function. (More accurately, one should refute the simple model of the dislocation energy spectrum on which Read's theory is based.⁹) The proposed q(T) dependence is shown in Fig. 3. According to this dependence the radii of the Read cylinders increase with increasing T in a certain interval of T, the conditions for the percolation of the current become worse, and the plot of μ_{\perp} acquires a minimum, as was in fact observed.²⁻⁴ It is clear that the resistance of the sample depends just as strongly on q as on N_D , since the total volume of the Read cylinders is proportional to the product $N_p q$. In Refs. 3 and 4 they measured the concentration of the carriers in the band (meaning also q), and no significant change of q was observed in the investigated interval of T. From our point of view, however, under the corresponding conditions (near the percolation threshold) even an insignificant change of q (within the limits of the experimental error) can lead to very large changes in the electric conductivity. We note also that the measured²⁻⁴ value of μ should be regarded not as a microscopic characteristic but as a quantity that characterizes the dislocation structure of the sample as a whole.

Thus, the results of our study can be formulated in the following manner:

1. The influence of the dislocations on the electric conductivity under conditions when Read cylinders exist is determined by the detour effect.

2. The filling coefficient of the dislocation is a nonmonotonic function of T, as is evidenced by the complicated energy structure of the dislocations.

In the discussion Refs. 2-3 we based ourselves on the Shockley-Read theory of the electric activity of dislocations. There exists, however, also another point of view, according to which a dislocation interacting with



FIG. 3. Proposed temperature dependence of the linear density of the charge trapped by the dislocation. The arrows indicate the temperature interval in which the function q(T) increases.

impurity centers transforms them into electrically active complexes. Milevskii¹⁰ has indicated that if the binding energy of the electron at the center exceeds the migration energy of the center, then electrically active complexes can remain in the glide planes. The existence of such complexes was observed experimentally in Ref. 11. These experiments were made on Si crystals with high concentration of oxygen (and possibly of other electrically inactive impurities). Therefore the concentration of the active centers in the glide planes was so high, that two-dimensional potential barriers were produced in them. The conductivity of such crystals in a direction perpendicular to the glide planes was much less than the conductivity in directions parallel to the glide planes. It was assumed in Ref. 11 that this fact can be attributed to detouring of the carriers around the dielectric regions produced in the glide regions (private communication from E.B. Yakimov). In our relatively pure crystals these effects could not take place. The conclusions of our paper do not depend on the nature of the electric activity of the dislocations. No matter what produces the dielectric cylinders, it can be asserted (in our opinion) that these cylinders affect the resistance of the sample because of the detour effect, and that the radii of the cylinders should depend nonmonotonically on T.

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Self-localized excitations in the Peierls-Fröhlich state

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We show that stationary excited states of a one-dimensional Peierls dielectric are amplitude solitons. They originate as the result of self-trapping of an electron which is initially excited across the optical gap $2\Delta_0$. The energy of the soliton $W_x = (2/\pi)\Delta_0$, its charge $e_x = 0$, and its spin s = 1/2. The gap parameter has the form $\Delta(x) = \Delta_0 \tanh(\Delta_0 x/v_F)$. The soliton carries a singly occupied $v_0 = 1$ localized state with an energy in the center of the forbidden band $E_0 = 0$. For systems with a commensurability 1:2 the multiplicity of occupation may be arbitrary, $v_0 = 0, 1, 2$, and the soliton can have a charge $e_x = -e, 0, e$. We show that inclusion of electron-electron interactions conserves the property $e_x = 0$. A small local charge occurs as the result of phonon dispersion in the vicinity of $2p_F$. Interaction between the chains leads to a smoothing of the jump in the phase of the function $\Delta(x)$ at distances $l \sim v_F/T_c \gg v_F/\Delta_0$ (T_c is the three-dimensional ordering temperature). A charge $\sim e$ is localized in that region. An effective coupling between the chains or a commensurability of the order of more than two causes an attraction between solitons with a force $\sim v_F/l^2$ at distances $\leq l$. The presence of solitons produces spin resonance effects, absorption, or luminescence at a frequency Δ_0 , and a broadening of the fundamental absorption edge $2\Delta_0$.

1. INTRODUCTION

1. It is well known that the quasi-one-dimensional gas of non-interacting electrons on a system of deformed chains at zero temperature T is in a Peierls-Fröhlich ground state (see the reviews in Refs. 1 to 3). It is characterized by a static deformation of the lattice $\varphi(x)$ and a charge density wave (CDW) q(x) of the form

$q(x) \circ \varphi(x) = \varphi_0 \cos (2p_F x + \chi),$

where x is the coordinate along the chain, p_F the Fermi momentum for the electrons in the metallic phase, and χ the CDW phase.

The electrons occupy states with negative energies $E_{\mathbf{k}} = -\varepsilon_{\mathbf{k}}$, where