## FIFTH ALL-UNION CONFERENCE ON THE THEORY OF SEMICONDUCTORS

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Usp. Fiz. Nauk 81, 557-566 (November, 1963)

THE Fifth All-Union Conference on the Theory of Semiconductors was held from October 29 to November 3, 1962 in Baku; it was convened by the Commission on Semiconductors of the U.S.S.R. Academy of Sciences in conjunction with the Academy of Sciences of the Azerbaĭdzhan S.S.R. and the S. M. Kirov State University of Azerbaĭdzhan. Over 250 participants were present, representing scientific establishments in 23 cities in the Soviet Union: Moscow, Leningrad, Kiev, Baku, Vilnius, Tartu, Kishinev, Tbilisi, Tashkent, Khar'kov, Kazan', Tomsk, Sverdlovsk, Odessa, Chernovtsy, etc. The Organizing Committee selected 37 out of 96 papers submitted, and the selected papers were presented at five general sessions and two evening seminars of restricted membership.

The majority of the papers dealt with problems of the band structure of semiconductors, theory of galvanomagnetic and thermomagnetic effects, various resonance effects, low-mobility semiconductors, and optical properties of crystals. The participants of the Conference heard with great interest the review papers of <u>S. I. Pekar and L. V. Keldysh</u> (at the first session) and of <u>V. E. Khartsiev</u> (at a seminar) on the International Conference on the Physics of Semiconductors held in Exeter (England).

The general impression of the Exeter Conference was that experimental studies of semiconductors in the Soviet Union lag considerably behind those carried out abroad, particularly in the U.S.A. There is also a lag in some aspects of the theory, for example, in bandstructure calculations.

### 1. BAND THEORY OF SEMICONDUCTORS

The largest number of papers dealt with this problem. V. L. Bonch-Bruevich, I. P. Zvyagin and A. G. <u>Mironov</u> (Moscow State University) reported in their paper "On the theory of heavily doped semiconductors" a determination of the density of states  $\rho(\omega)$  in the region of the bottom of the conduction band of a semiconductor containing a large amount of randomly distributed impurity. The total potential of the impurity was assumed to be a slowly varying function. Electron interaction was allowed for by means of well-known expansions and the quantity  $\lambda = (na_0^3)^{-1/3}$  was used as the small parameter (n is the impurity concentration and  $a_0$  is the screening radius). At energies higher than the edge of the conduction band,  $\omega = 0$ ,  $\rho(\omega)$  was found to vary as  $\omega^{1/2}$ ; for  $\omega \approx 0$  the density varied linearly and approached zero for  $\omega < 0$  as

 $\exp - \left| \frac{\omega_0}{\omega} \right| \ln \left| \frac{\omega}{\omega_0} \right|$ . The level density below the bottom of the conduction band was found to depend considerably on the nature of the distribution of the impurity and was calculated without allowing for correlation in the distribution.

The same problem was solved using similar methods by L. D. Keldysh (Physics Institute, Academy of Sciences, U.S.S.R.) in the paper "Energy spectrum of heavily doped semiconductors." The small parameter was this time the quantity  $\alpha = na_B^3$ , where  $a_B$  is the radius of the ground state of an electron in the crystal in the Coulomb field of the impurity. When  $lpha \ll 1$  a discrete negative level  $\epsilon = \epsilon_0$  and a band with the density  $\rho \sim \sqrt{\epsilon}$  is obtained for  $\epsilon > 0$ . On increase of  $\alpha$  an impurity band with diffuse edges appears (as the result of disorder in the impurity distribution), which then merges with the conduction band. When  $\alpha \gg 1$  the Coulomb potential of the impurity should be replaced by a screened potential, and, because of strong scattering of low-energy electrons, it is necessary to sum all the diagrams since the momentum is not even approximately a quantum number. The density of local levels for  $\epsilon \sim \epsilon_0$  varies as

 $\left| \frac{\epsilon_0}{\epsilon - \epsilon_0} \right| \ln \left| \frac{\epsilon - \epsilon_0}{\epsilon_0} \right|, \text{ and below the bottom of the band it decreases as exp} - (\epsilon/\Delta)^2, \text{ which is due to the Gaussian nature of the distribution of fluctuations in the impurity concentration. The quantity <math>\Delta$  is proportional to  $\epsilon_0 \alpha^{5/13}$ . In reply to a question from M. Ya. Azbel', Keldysh stated that it is permissible to neglect correlations in the impurity distribution even for high impurity concentrations, since the quantity aB is much greater than the atomic dimensions. The reason for the difference between the results of Keldysh and Bonch-Bruevich for the form of  $\rho(\omega)$  for levels below the bottom of the conduction band, obtained under the same assumptions, is not clear and requires a careful check of the calculations in both papers.

In a joint paper "On the problem of investigating the electron energy spectrum in a crystal" <u>V. A.</u> <u>Chaldyshev, N. V. Kudryavtseva and G. F. Karavaev</u> (Physico-technical Institute, Tomsk) described a general method for a qualitative study based on the symmetry properties of a crystal, and giving an approximate dispersion law for the whole band using approximating functions with free parameters, found by comparison with experiment. The dispersion law was investigated at symmetry points in crystals of  $Th_3P_4$ type and throughout the band in diamond and sphalerite-type crystals. K. D. Tovstyuk, D. E. Germus, and M. V. Tarnavskaya (Chernovtsy State University) in "Investigation of the dispersion laws for carriers in semiconducting crystals of  $Oh^5$ ,  $Oh^6$ and  $D_{2h}^{15}$  type" also investigated the dispersion laws in the region of symmetry points of the crystals specified; they used group theory without employing any properties of actual crystals.

K. B. Tolpygo (IPAN Institute of Semiconductors, Academy of Sciences, Kiev) in "Treatment of the motion of a carrier in a crystal as a many-electron problem" proposed a method for calculating the band structure of a semiconductor when the motion of an excess electron (hole) from site to site may be assumed to be slow compared with the frequency of motion around a nucleus. This makes it possible to allow approximately for the correlation in the motion of all the electrons in the crystal during the motion of the excess charge in the form of polarization reversal of all the atoms. The contribution of this correlation to the dispersion law E(k) is estimated. Tolpygo gave the results of calculations, by this method, of the electron and hole bands in NaCl and KCl and hole bands in Ge with allowance for spin-orbit interaction. The method, in the form presented, was found to be inapplicable to electron bands in Ge because the forbidden band is narrow. In a discussion, M. I. Kaganov expressed doubt about its usefulness and the possibility of calculating band structure with any accuracy. In his opinion, which was shared by Bonch-Bruevich, a theoretical development of the methods for experimental studies of the band structure is more desirable.

The paper of <u>E. I. Cheglokov</u> (Siberian Physicotechnical Institute, Tomsk), "Structure of the valence bands in crystals of hexagonal selenium and tellurium," dealt with the possible generalization of Hartree-Fock equations by dropping the assumption of the duality of occupation of space orbitals by electrons. On allowing for spin-orbit interaction an even richer system of valence bands is obtained for Se and Te crystals, which accounts for the features of polarized infrared absorption by transitions within the bands. Several participants in the discussion remarked that the physical considerations connected with the wave function of the crystal selected by the author are not sufficiently clear.

The papers of <u>V. A. Khartsiev</u> (Physico-technical Institute, Leningrad), "Optical properties and structure of the energy bands of some semiconducting compounds," and of <u>I. B. Levinson</u> (Institute of Physics and Mathematics, Vilnius), "Chemical binding and structure of energy bands in cuprous oxide" were characteristic in that they used not only the symmetry properties but also the related crystallochemical properties in band analysis. In the former paper group-theoretical considerations are compared with

calculations by the OPW method and the localized orbit method, as well as with experimental data on optical properties. This makes it possible to draw a number of conclusions: semiconductors of SnS type have minima at the points  $\Gamma$  and V; four pairs of nondegenerate levels, between which two dipole transitions are possible, exist at the point  $\Gamma$ . At the point V the levels are doubly degenerate (without allowance for spin). In the semiconductors CdSb and ZnSb the valence band maximum is at the point  $\Gamma$  (two types of hole are possible), and conduction band minima lie at the points  $\Gamma$  and R. In CdSnAs<sub>2</sub> compounds there is a toroidal energy surface in the valence band. I. B. Levinson investigated in detail the crystal chemistry of cuprous oxide and showed that the ionic and covalent contributions to the chemical binding are approximately equal. Certain considerations, based on a quantum-chemical analysis of binding, showed that the 3d-electrons of copper do not participate in the formation of chemical bonds and the valence band. The symmetry and positions of the bands were considered in the limiting cases of purely covalent and purely ionic binding. It was then shown that the ionic models of Elliot and Zhilich have a number of inconsistencies. From the limiting cases conclusions were drawn about the symmetry and positions of the bands in the actual intermediate case. Comparison of these conclusions with recent experimental data made it possible to solve the problem of the participation of atomic states in the formation of energy bands.

A. B. Almazov (Institute of General and Inorganic Chemistry, Moscow) in "Theta expansions of dispersion laws for quasi-particles in crystals" suggested expanding the dependences E(k) not as Fourier series, as it is done automatically in the strong-coupling approximation, but as theta-function series. Then even one term of the series allows for an infinite number of coordination spheres. Theta expansions are particularly convenient in application to dispersion formulas for phonons.

## 2. INTERACTIONS OF SEMICONDUCTORS WITH ELECTROMAGNETIC RADIATION

The majority of papers on this subject dealt with the theory of the fundamental and impurity absorption of visible and infrared light. In three papers the absorption of microwaves in the presence of a magnetic field (resonance effect) was considered, and one was concerned with the theory of reflection and transmission of light through a crystal surface in the presence of surface excitons. In this latter paper—"Influence of surface excitons on the optical properties of crystals" (S. I. Pekar, Institute for Semiconductors, Academy of Sciences, Kiev)—the limiting case was considered when the imaginary part  $\kappa$  of the wave vector of the exciton, normal to the surface, is much smaller than the reciprocal of the lattice constant. The exciton states then make an additional contribution to the volume current produced by the electromagnetic wave, and the field near the surface is given by the superposition of plane waves with real and complex wave vectors with equal (real) tangential components. The presence of surface waves changes the form of the boundary conditions for volume waves and leads to a generalization of Fresnel's formulas. This change is found to be important even at frequencies other than those corresponding to the formation of surface excitons, and near resonance a narrow total-reflection line appears. The theory predicts that the transmitted light is elliptically polarized in the absence of absorption. In a discussion F. G. Bass, M. I. Kaganov and others expressed doubts about the existence of surface excitons macroscopically extended in the direction at right angles to the surface. In their opinion it is preferable to formulate a new boundary condition which allows for the presence of surface excitons. Pekar stressed that this is possible only if  $\kappa$  is much greater than the wave vector of the additional light wave.

The paper of L. É. Gurevich and I. P. Ipatova (Physico-technical Institute, Leningrad), "On the theory of the resonance absorption linewidth in ionic crystals," dealt with the theory of infrared absorption. The line width  $\Gamma$ , due to anharmonicity, was calculated by the method of Green's temperature functions using the diagram technique of Abrikosov et al. In the high-temperature limit the cubic anharmonic terms lead to a proportionality of  $\Gamma$  and T, while terms of fourth order lead to the dependence  $\Gamma \sim T^2$ . Since in the latter case the number of phonon combinations, for which the energy sum is  $\hbar\omega$ , is much greater, the contributions of third and fourthorder terms may be comparable. Experiment gives the dependence  $\Gamma \sim T^{\alpha}$  where  $1 < \alpha < 2$ . Answering a question of Yu. E. Perlin, I. P. Ipatova stressed that the application to this problem of the Wigner-Weisskopf method, which allows only for the decay but not for the re-establishment of the initial state, gives the incorrect result  $\Gamma \sim T^3$ .

The main problem in the theory of absorption and luminescence of impurity centers dealt with in the papers presented was the derivation of the correct intensity and band shape at various temperatures. Here, as a rule, the adiabatic approximation was used in considering the fast (electron) and slow (phonon) subsystems, and one can introduce an adiabatic potential, usually of parabolic form, which differs for the ground and excited states of the lighter subsystem. This difference, with simultaneous allowance for the quantum indeterminacy of the oscillator coordinates, is responsible for the band broadening. The main difficulty is to allow for the change in the curvature of the potential, i.e., of the frequencies of phonons, during a phototransition.

The paper of <u>K. K. Rebane, R. A. Praém</u>, A. P. Purga, O. N. Sil'd and V. V. Khizhnyakov (Institute of

Physics and Astronomy, Tartu), "Some problems of the participation of lattice vibrations in electron and intranuclear transitions in crystal-forming particles," deals with the study of the influence of local and crvstal vibrations (LV and CV) on the electron and nuclear spectra. High-temperature experiments on luminescence and absorption of impurity centers give relatively little information on an impurity center. More promising are quasi-linear spectra observed at low temperatures (for example, the Shpol'skii effect and spectra of rare-earth ions in ionic crystals; Mössbauer effect). Transitions involving a change in the number of CV quanta give rise to a continuous background; transitions in which only the number of LV quanta changes, and the vibrational state of CV remains completely unaltered, give rise to separate lines on a background of continuous bands. In the case of moderate Stokes losses a number of lines appear. which are related to LV only. Similarly in the Mössbauer effect (in a non-ideal crystal) there may appear, apart from the resonance line, lines which are connected with LV excitation and which, in principle, may exceed the main line in integral intensity. In reply to Yu. E. Perlin, V. A. Moskalenko and others, K. K. Rebane explained that the effect of frequency change on excitation was allowed for and that it is small in the Shpol'skii effect. The difference between the half-widths of absorption and luminescence lines is not necessarily related to the presence of LV. It may also appear in the absence of LV in a center of small radius due to a change of elastic constants. Moreover, a considerable contribution may come from the multiplicity of excited electron levels and from the anharmonicity of the vibrations. A more detailed description of the results on the theory of the Mössbauer effect was given in the paper of V. V. Khizhnyakov (Institute of Physics and Astronomy, Tartu) "Some calculations on the processes of resonance absorption and emission of  $\gamma$ -quanta by nuclei in a crystal."

The paper of <u>S. V. Tyablikov, V. A. Moskalenko</u> and <u>M. E. Polistrant</u> (Mathematics Institute, Academy of Sciences, Moscow; Institute of Physics and Mathematics, Kishinev), "On the theory of optical bands in crystals," dealt with similar problems. The method of quantum Green's functions was used, which makes it possible to allow for the displacement of the oscillators from their equilibrium positions as well as for effects related to the change of the lattice vibration frequencies during an electron transition. The temperature dependence was found for the shift  $\Delta \nu$  of the absorption band maximum of an F-center, due to the frequency effect. Allowance for the change of the frequency also leads to an additional broadening of the band (at high temperatures we have  $\Delta \nu \sim T$ ).

<u>N. N. Kristofel'</u> and <u>G. S. Zavt</u> (Institute of Physics and Astronomy, Tartu) in "The Condon approximation and optical properties of impurity centers" used group theory to discuss effects related to deviations from

the Condon approximation (CA) in the theory of impurity centers. If one of the states is fully symmetric, then a forbidden dipole transition to a state of symmetry  $\Gamma_{\beta}$  becomes allowed by vibrations of that symmetry  $\Gamma_{\mu}$ , which is contained in  $\Gamma_{\beta} \times \Gamma_{1u}$ , and the polarization of the transition is the same as the polarization of the allowed transitions  $\Gamma_{\beta} \rightarrow \Gamma_{\mu}$ . Radiationless transitions, caused by the nonadiabaticity operator, are discussed in a similar way. It is shown, moreover, that if the CA is disturbed by a vibration which is active in the Jahn-Teller effect, then the Jahn-Teller splitting may appear in the absorption spectrum as well. This occurs if  $\Gamma_{\beta} \times \Gamma_{iu}$  and  $[\Gamma_{\beta}]^2$  contain one non-identical irreducible representation of the vibrations of the quasi-molecule. In the discussion V. A. Moskalenko remarked that the anharmonicity of the vibrations leads, in the quadratic approximation for the displacements of the normal coordinates  $y_{\mu}$  from their equilibrium positions  $y^0_{\mu}$ , to an additional effect on the frequency. It was also mentioned that in problems concerning this type of deviation from the Condon principle, the nonadiabaticity and the Jahn-Teller effect should be considered simultaneously.

Hitherto, in work on the resonance absorption of microwaves in a magnetic field it has been usual to consider separately the absorption related to the orbital motion of electrons (cyclotron resonance - CR) and the absorption related to the change in the spin state (paramagnetic resonance - PR). In fact these effects are closely related due to the spin-orbit interaction and we have the so-called combined resonance (COR).

G. L. Bir, E. Butikov and G. E. Pikus (Institute for Semiconductors, Academy of Sciences, Leningrad) in "Paramagnetic and combined resonance of acceptor centers in undeformed and deformed crystals of p-germanium type," dealt with the influence of deformation on the resonance effect. In an undeformed crystal in the absence of external fields the ground state of an acceptor center is quadruply degenerate, as with the valence band for k = 0. On deformation by an amount  $\epsilon$  this state is split into two levels with energies  $\pm \Delta_{\epsilon}$ . Transitions are possible between these deformation levels when alternating electric or magnetic fields are applied. In a constant magnetic field H each of the deformation levels splits into two spin levels, but the splitting is different in the two cases. The observed PR is due to transitions between the lower levels. The dependence of the g-factor on the direction of the deformation  $\epsilon$  was calculated, as well as corrections to this factor proportional to  $\epsilon$ and appearing in the second order of the perturbation theory. Comparison with experiment makes it possible to find the g-factors for various acceptors as well as the sign of deformation potential constants for bound holes. In an undeformed crystal the resonance linewidth is determined by the interaction with acoustical

vibrations. Transitions between the spin levels are allowed in the first approximation and an estimate of the relaxation time  $\tau_0$  shows that  $\tau_0 \approx 10^{-8} - 10^{-9}$ sec. In a deformed crystal these transitions are, in the first approximation, forbidden and the relaxation time  $\tau_1$  is found to be greater than  $\tau_0$  by a factor of  $(\Delta_{\epsilon}/\hbar \omega_0)^2$ , with the exception of the case when **E** and **H** are directed along the principal axis (100) or (111). In the latter case the relaxation is due to transitions between the deformation levels and not the spin levels. The corresponding relaxation time then includes a multiplier  $\exp(\Delta_{\epsilon}/kT)$  and is strongly temperaturedependent, as found experimentally.

G. A. Baranidze, B. E. Gurgenishvili, M. G. Pkhakadze, Z. K. Saranidze, G. R. Khutsishvili and O. D. Cheishvili (Institute of Physics, Academy of Sciences, Tbilisi) in the paper "On the quantum theory of cyclotron resonance in a degenerate band," considered CR in the valence band of germanium, in the spherical symmetry approximation of Luttinger's Hamiltonian. Energy levels were calculated and average values found of the projection of the spin moment  $S_Z$  along the magnetic field direction for each of the levels. The levels consisted of four groups: a<sup>+</sup>, b<sup>+</sup> (for light holes) and  $a^-$ ,  $b^-$  (for heavy holes). The usual CR is related to transitions within one of those groups. In addition to the transitions  $a^+ - a^-$  and  $b^+ - b^-$ , found by Goodman for the case when the alternating electric field is  $E \perp H$ , they indicated the possibility of the transitions  $a^{\pm}-b^{\pm}$  and  $a^{\pm}-b^{\mp}$  in the case  $E \parallel H$ , which are possible even when  $k_z = 0$ . For the lower levels the probabilities of these additional transitions are of the same order as the probabilities of the main transitions  $a^{\pm}-a^{\pm}$  and  $b^{\pm}-b^{\pm}$ . In the latter transitions Sz changes and therefore they are not really CR but COR. In the discussion G. E. Pikus remarked that the longitudinal resonance is strongly broadened because of the  $k_z$  spread.

The work of É. I. Rashba and V. I. Sheka (Institute for Semiconductors, Kiev), on "Combined resonance at local centers of large radius," dealt with COR in crystals without an inversion center. Resonance at centers of large radius could reasonably be expected because it was predicted for band carriers and the state of such a center has a packet of band states. The effective matrix element of absorption is estimated as  $\langle x \rangle \sim (\delta / E) (\beta H / E) R_0$ , where  $R_0$  is the radius of the state. The ratio  $\delta/E$  is the ratio of the spin-orbit splitting  $\delta(k)$  for  $\delta \sim R_0^{-1}$  to the ionization energy of the center; it appears because the COR is caused by the spin-orbit interaction. The second ratio appears because the energy in a magnetic field  $\beta$ H mixes the components of the Kramers doublet and allows transitions between them. This estimate refers to the case of the orbital state 1s and the spin state s = 1/2. For s = 3/2 we can have the transitions +3/2 - 1/2 and -3/2 - 1/2 without the small multiplier  $\beta$  H/E. Therefore, to intensify COR it is

necessary to select substances with strong spin-orbit interaction and centers with large spins.

#### 3. PHOTOCONDUCTIVITY

Two papers, of the total of three on photoconductivity, were methodological in nature, their aim being to obtain formulas for non-steady-state photoconductivity which would permit determination of several semiconductor parameters by comparison with experiment. É. I. Adirovich and E. M. Kuznetsova (Physico-technical Institute, Tashkent), in "Influence of local levels on relaxation processes in homogeneous semiconductors and in p-n junctions," solved the general problem of finding the variation with time of the density of free electrons and holes, and of those captured by various centers, in the linear approximation. In general, the relaxation time does not coincide with the recombination lifetime. In the limiting cases the Guro and Shockley-Read formulas were obtained. I. A. Mirtskhulava, R. I. Chikovani and A. L. Shkol'nik (Tbilisi State University), in "Investigation of the parameters of local centers by the study of the kinetics of induced photoconductivity," investigated the variation of photocurrent with time when electrons are liberated from local levels by light of suitable frequency and are then displaced to other levels. The theory predicts that the photocurrent should pass through a maximum and then decrease to zero or to a steady value. Comparison of the theory with experiment was carried out for CdS single crystals, for which some local-center parameters were estimated.

The work of M. I. Kaganov and I. M. Lifshitz (Physico-technical Institute, Khar'kov) on "Photoeffect without a threshold in metals of graphite type" attracted the greatest interest; it dealt with the frequency dependence of the optical absorption coefficient and photoconductivity of substances whose energy surfaces intersect at a singular point, for example, two cones with a common vertex or two surfaces in contact. The limiting case  $\omega \tau \gg 1$  was considered, where  $\tau$ is the relaxation time for an electron gas which gives the lower limit of the frequency. The conductivity at the lowest frequencies is proportional to  $\omega^3$  and to  $\omega^2$  at higher frequencies, without any important temperature dependence. The threshold absorption was also discussed. Depending on the position of the singular point  $p_0$  with respect to the Fermi surface the relationships  $\sigma \sim (\omega - \omega_0)^{3/2}$  and  $\sigma \sim (\omega - \omega_0)$ , were obtained where  $\omega_0$  is the threshold frequency.

## 4. THEORY OF RADIATIONLESS TRANSITIONS

Two papers on this subject dealt with the problems of luminescence and photoconductivity, stimulated by a field. In the former case a radiationless transition from the excited to the ground state reduced the luminescence yield. However, the absolute value of the probability of a transition is found to be many orders of magnitude greater than the value calculated theoretically. V. A. Kovarskii and É. P. Sinyavskii (Institute of Physics and Mathematics, Kishinev), in "Resonance effect in the theory of radiationless transitions," showed that the agreement is considerably improved by allowing for the fact that at the point where the adiabatic potential curves approach, the electron wave functions are considerably different from the corresponding minima of the potentials. For photoconductivity in strong fields, as shown by Yu. E. Perlin and A. G. Cheban (Kishinev State University) in their paper "On the theory of local state decay in an electric field," the tunnel effect plays an important role in transitions of the local center from the excited to the ground state. Their calculations allow for the change in the potential energy of an electron in the field of a defect because of the inertial polarization of the lattice. In relatively weak fields the liberated electron goes into a polaron state, and in stronger fields it goes into a band state. Comparison with experiment indicates the important role of thermal ionization even at low temperatures, because the energy of ionization from the excited state is small and it is reduced further by the field. In the discussion L. É. Gurevich and L. V. Keldysh suggested that the concept of auto-ionization is not sufficiently clear because the presence of an external field cannot destroy the interaction of the electron with the inertial polarization.

#### 5. TRANSPORT IN THE CASE OF LOW MOBILITY

Great interest was shown in the papers on the transport theory of semiconductors with low mobility. The most detailed papers on this subject were "Theory of transport phenomena in semiconductors with low mobility" by M. I. Klinger (Institute for Semiconductors, Academy of Sciences, Leningrad) and "Transport theory of semiconductors with low mobility" by I. G. Lang, Yu. A. Firsov (Institute for Semiconductors, Academy of Sciences, Leningrad) and <u>L. A. Éfros</u> (Physico-technical Institute, Leningrad).

Lang, Firsov and Efros have developed a method for dealing with transport phenomena by interpreting the general formula of Kubo in the case of strong coupling between electrons and polarized vibrations of the lattice. At low temperatures (below the Debye temperature) the conductivity is of the normal type with nonlocalized small-radius polarons acting as carriers. Above the Debye temperature the mechanism of carrier motion is intrinsically related to the manyphonon processes, even after renormalization and liberation of a polaron. This mechanism may be described as follows. An electron is localized at a lattice site in the form of a polaron for a time  $\Delta t$  and then moves to another site. This transition does not take place by a tunnel leakage through a barrier because the time for such a process  $\, t_p \gg \Delta t \, . \,$  The transition

is the classical transfer over a barrier in a time  $t_0 \ll \Delta t$ . Thus we have infrequent but fast electron transitions from site to site; the nature of the motion depends on the comparative values of  $t_0$ ,  $\Delta t$  and the time for the establishment of polarization of the lattice  $1/\omega_0$ , where  $\omega_0$  is the frequency of longitudinal polarized phonons. Since, on the one hand,  $t_0 \ll 1/\omega_0$ , the polarization is unable to follow the electron during the time of its transition and therefore in transferring to a new site the electron leaves the polarization corresponding to the old site. But, on the other hand,  $\Delta t \gg 1/\omega_0$ , therefore during the stay of the electron at the new site, the polarization will change in accordance with the new position of the electron. For such a mechanism the temperature dependence of the mobility has an exponential "activated" nature  $u \sim \exp(-E_a/kT)$ , where the activation energy  $E_a$ is less than the polaron binding energy  $E_p$ ; therefore this dependence is not connected with the polaron dis-

is less than the polaron binding energy  $E_p$ ; therefore this dependence is not connected with the polaron dissociation and increase of the number of free carriers in the conduction band.

In Klinger's paper a theory of transport coefficients was developed, based on the general expressions of Kubo and the resolvent method of Van Hove. Carriers are small-radius polarons generated as the result of the strong electron-phonon interaction. At low temperatures  $T < T_0$  (T<sub>0</sub> is of the order of the Debye temperature) a polaron-type carrier is described by a band state and transport is due to scattering between such band states. At high temperatures  $T > T_0$  there is a different transport mechanism, involving transitions of a localized polaron between cells. The criterion of this mechanism is  $\eta = \Delta/\Gamma$ , the ratio of the two energy parameters describing the localized state of the polaron. Here  $\Delta$  is the width of the polaron band, i.e.,  $1/\Delta$  is the time taken by a localized packet to spread out for a given number of phonons;  $\Gamma$  is the width of such a state, so in other words  $1/\Gamma$  is the lifetime for a transition of a localized state to the next cell accompanied by a phonon redistribution. When  $T > T_0$  we have  $\Delta \ll \Gamma$  and the localized packet executes several transitions between cells and then decays by spreading. Effects which are odd with respect to the magnetic field, like the Hall effect, are then governed by the phase-correlated parts of such transitions. In that sense the process of transport does not reduce completely to normal diffusion, in which there is no phase correlation. When the temperature is reduced the ratio  $\eta$  increases and the "wave" contribution to the process becomes greater than the "diffusion" contribution. When  $T < T_0$  we have  $\Delta \gg \Gamma$  and in the lowest approximation for  $\Gamma/\Delta$ we obtain the usual transport equation. Another criterion of the theory is  $\zeta = \Gamma \omega_{\rm D} \ll 1$ , where  $\omega_{\rm D}$  is the characteristic frequency of phonons. This criterion means that the equilibrium deformation of the lattice, corresponding to a given localization of a carrier, may be established during the lifetime of

the localized carrier. When  $T > T_0$  the theory yields an activation type of temperature dependence for the drift and Hall mobilities; the activation energies are, in general, different but of the same order of magnitude.

In the discussion of these two papers it was remarked that although the work in both cases was based on similar physical ideas and the final conclusions were very similar, the details of the temperature dependences and criteria of the theories were different and the reasons for this were not clear. The problem of low mobility was also dealt with by E. L. Nagaev (Institute for Current Sources, Moscow) in "Energy spectrum and mobility of small-radius polarons"; this author deduced the transport equation for polarons. This equation was solved for the case when the scattering potential depends only on the electron coordinates. This gives, at high temperatures, a mobility rising exponentially with temperature, the activation energy being of the order of the formation energy of a polaron.

# 6. GALVANOMAGNETIC AND THERMOMAGNETIC EFFECTS

The paper of M. Ya. Azbel' (Physico-technical Institute, Khar'kov), "Theory of galvanomagnetic effects in semiconductors of finite size," attracted considerable attention. The author predicted a complex dependence of the resistivity of a conductor of sufficiently small thickness on the direction and magnitude of a magnetic field. Azbel' stressed the essential difference between the roles of scattering in conduction with and without a magnetic field. In the former case we have  $\sigma = 0$  for an infinite free path *l*. In a strong magnetic field  $\sigma(H) = \sigma(0) (r/l)^2 \sim r^2/l$ , where r is the orbit radius. If scattering by the surface plays the principal role, then  $\sigma(H) \sim \sigma(0) (r/l)$ , since the moment of collision with the surface is uniquely determined for a given initial state of the electron motion and the path travelled at right angles to the magnetic field is represented by the quantity r instead of l. As a result the total conductivity of the sample for volume and surface scattering is proportional to  $\sigma(0) [(r/l)(l/d) + (r/l)^2]$ , and for a small thickness of the sample d, when d  $\ll l^2/r$  the current flows mainly near the surface. In an oblique magnetic field the current density exhibits strong oscillations as one moves away from the surface and it even changes sign. The theory makes it possible to compare with experiment the quantities r, l and the form of the Fermi surface.

<u>A. I. Ansel'm</u> (Institute for Semiconductors, Academy of Sciences, Leningrad) and <u>B. M. Askerov</u> (Physics Institute, Academy of Sciences, Baku), in "Longitudinal thermomagnetic effects in a strong magnetic field," considered the effects of changes of the thermo-emf and the electronic part of the thermal conductivity in a quantizing magnetic field, parallel to an electric field, for a temperature gradient in a semiconductor with simple band structure. It is known that these effects vanish for such semiconductors in the quasiclassical approximation when the transport equation is used and it is assumed that the relaxation and chemical potential are independent of the magnetic field. Since the magnetic field does not affect the motion of an electron along the field, the transport equation method may be retained but the assumptions about the relaxation and chemical potential must be dropped. In calculating the thermo-emf the authors considered scattering on acoustical phonons and ionized impurities. For acoustical phonons in the quantum limit  $\tau \sim \epsilon_{\rm Z}^{1/2}$ , while without a field  $\tau \sim (\bar{\epsilon})^{1/2}$ . In the case of impurity scattering  $\tau \sim \epsilon_z^{3/2}$  (with or without the field). Calculations showed that the change of the thermo-emf in a magnetic field is a considerable fraction of the thermo-emf without a field.

The theory of galvanomagnetic effects in the relaxation-time approximation was also dealt with by R. G. Arkhipov, V. V. Kechin, A. I. Likhter and Yu. A. Pospelov (Institute of High-pressure Physics, Moscow), in "Influence of pressure on the electron spectrum of graphite"; here the model of Slonchevskii and Weiss was considered. Since the carriers occupy a narrow region near the Brillouin zone edges, the relaxation time was assumed to depend only on the component of the momentum along the edge. This dependence was found from experiment at atmospheric pressure. Moreover, a comparison was made between such combinations of expressions for galvanomagnetic effects which are independent of the relaxation time but depend only on the electron-spectrum parameters. Experimental studies at various pressures make it possible to establish the pressure dependence of the electron parameters.

In an interesting paper "On the theory of thermomagnetic effects in quantizing magnetic fields," <u>Yu. N. Obraztsov</u> (Institute for Semiconductors, Academy of Sciences, Leningrad) considered the problem of determining flows in the phenomenological theory. He showed that to determine correctly the microscopic flows of charge and energy it is necessary to allow for surface currents, equivalent to magnetization. This leads to the introduction of terms with the curl of magnetization into the well-known expressions.

<u>E. P. Pokatilov</u> (Kishinev State University), in "Magnetoresistance of semiconductors with a loop of extrema," solved the transport equation to deduce expressions for the current in the cases of strong degeneracy and no degeneracy of electrons in a semiconductor in which the energy minima in a band lie on a closed curve (known as a loop of extrema). Formulas for the magnetoresistance were deduced and analyzed.

Somewhat outside this group was the paper of  $\underline{Yu}$ . <u>P. Irkhin and Sh. Sh. Abel'skii</u> (Institute of Metal Physics, Sverdlovsk), "On the theory of the spontaneous Hall effect in ferromagnetic semiconductors". In this paper the density matrix method was used to obtain the transport equation, allowing for electron scattering on phonons up to the second order. In contrast to the impurity case, corrections to the electron velocity, due to the change in the scattering potential under the influence of spin-orbit interaction, were absent in scattering on phonons. Therefore, only the field part of the transport equation in the second approximation contains a term linear in spinorbit interaction. This leads to the dependence  $R_S \sim \rho^2$  (where  $\rho$  is the electrical resistivity) for the spontaneous Hall coefficient.

E. A. Turov and V. G. Shavrov (Institute of Metal Physics, Sverdlovsk), in the paper "On the phenomenological theory of galvanomagnetic effects in antiferromagnetic semiconductors," considered galvanomagnetic phenomena in antiferromagnetic crystals with various magnetic and crystallographic symmetries. The resistivity tensor  $\rho_{\alpha\beta}$  was considered as a function of a magnetic field H, total sublattice field M = M<sub>1</sub> + M<sub>2</sub> and the direction of antiferromagnetic ordering L = M<sub>1</sub> - M<sub>2</sub>. The nature of the expansion of  $\rho_{\alpha\beta}$  as a series in terms of H, M, and L is governed by the symmetry and determines the nature of possible effects. The presence of antiferromagnetic structure leads to several special effects.

#### 7. NONLINEAR PHENOMENA AND GENERATION

The behavior of electrons in a semiconductor in a strong electric field was considered in several papers. In this case nonlinear effects appear and situations frequently occur in which the system is unstable and capable of generation.

A typical paper of this type was that of V. L. Gurevich (Institute for Semiconductors, Leningrad) on "Avalanche generation of optical phonons in semiconductors." In dielectrics the damping  $\gamma_L$  of optical phonons (excitons) is related to the anharmonicity and defects. In semiconductors there is an additional damping  $\gamma_e$ , due to the interaction with conduction electrons, and therefore the total damping is  $\gamma = \gamma_L + \gamma_e$ . In a strong electric field  $\gamma_e$  may become negative, i.e. electrons take the energy from the field and transfer it to the lattice. This occurs if the phonon phase velocity is less than the electron drift velocity. If, moreover, it is found that  $|\gamma_{\rm e}| > \gamma_{\rm L}$ , then avalanche generation of optical phonons will occur. Such generation should lead to the appearance of infrared radiation over a narrow range of frequencies near the limiting phonon frequency, although the emergence of such radiation from the crystal is likely to be difficult. In reply to a question by Moizhes, Gurevich pointed out that although acoustical phonons are generated earlier than optical ones, generation of the latter may still be observed. For this purpose it is necessary to increase the electric field rapidly so

that at the moment of generation of optical phonons the acoustical phonons have not yet had chance to multiply. In reply to a question by Sh. M. Kogan, Gurevich said that in his theory vibrations are generated which are stabilized by nonlinearity and not the vibrations which depend on the dimensions of the sample.

L. É. Gurevich and I. V. Ioffe (Physico-technical Institute, Leningrad), in "The theory of current instability in semiconductors," proposed a theory of the self-excitation of oscillations in a semiconductor to which almost parallel electric and magnetic fields are applied. This theory is based on the use of an expression for the current in the presence of fields, and a density gradient, as well as the Poisson and continuity equations. After linearization of these equations with respect to the deviations of the field E(x, t) and density n(x, t) from the steady-state values E(x) and n(x), two solutions are obtained, one of which corresponds to low-frequency oscillations whose amplitude increases with time. Qualitatively this effect is related to the fact that when the density fluctuates diffusion tends to reduce the density gradient and the Hall field tends to increase it. The paper gave rise to many questions on the criteria of instability, actual dependences, and qualitative explanations of the phenomenon. M. Ya. Azbel' spoke of the important role of scattering on the surface which should be allowed for in the case of strong magnetic fields.

R. F. Kazarinov and V. G. Skobov (Physico-technical Institute, Leningrad), in the paper "On the theory of nonlinear galvanomagnetic effects in semiconductors," investigated the electrical conductivity of ionic semiconductors in strong crossed electric and magnetic fields. At low temperatures the relaxation of electron momentum is due to scattering on ionized impurities and the energy relaxation is due to piezoelectric phonons or the weak dispersion of optical phonons. For a small current j Ohm's law is valid for the dependence of E<sub>i</sub> (projection of E on j) on j and the resistance is proportional to the frequencies of collisions with impurities  $v_i$ . For large j the electron gas is heated and  $\gamma_i$  decreases, which leads to a reduction of magnetoresistance with increase of j. In this region we have the descending part of the currentvoltage characteristic. For still larger j the electrons become so hot that  $v_i$  becomes smaller than the frequency of collisions with optical phonons  $\nu_0$ . Since  $\nu_0$  is independent of the electron energy, the magnetoresistance ceases to depend on j and again Ohm's law applies, but with the resistance proportional to  $\nu_0$  and not to  $\nu_i$ .

Considering similar problems in the paper "On the theory of hot electrons," <u>Sh. M. Kogan</u> (Institute of Radio and Electronics, Moscow) used a semi-phenomenological approach based on the concept of the electron temperature T being higher than the lattice temperature  $T_0$ . The power p(T) transferred by elec-

trons to the lattice was calculated in terms of the correlation function of the electron density at various points of space and time. The calculations were carried out for the acoustical and piezoelectric interactions with and without a magnetic field. Temperature dependences of the transferred power p(T) and conductivity  $\sigma(T)$  were used to plot the current-voltage characteristics of the semiconductor. The case of a nondegenerate electron gas, when  $\sigma \sim T^{3/2}$ , and scattering is due to the piezopotential, was of interest. Then at high electron temperatures  $p \sim T^{1/2}$ , so that when  $T > 2T_0$ , a negative differential conductivity  $\sigma_d$  is obtained. For very high T, other mechanisms start to play a part (deformation potential, optical phonons), which again gives  $\sigma_d > 0$ . As a result of this, the current-voltage characteristic is S-shaped.

V. A. Chuenkov and Ch'en K'o-ming (Physics Institute, Academy of Sciences, Moscow), in the paper "On the variation of breakdown with time," generalized the theory of one of the authors to the non-steadystate case. They considered both impact and thermal ionization of impurity centers, based on the solution of the transport equation for electrons in strong electric and magnetic fields. The state when the number of ionizations exceeded the number of recombinations was regarded as the beginning of breakdown. The temperature dependence of the critical field  $E_{C}$  was established: it had a maximum at a certain temperature  $T_c$ . When  $T < T_c$  the electrical breakdown predominates but when T  $\geq$  T<sub>c</sub> we have mixed thermal and electrical breakdown. In strong magnetic fields when  $\omega \tau \gg 1$  ( $\omega$  is the Larmor frequency, and  $\tau$  is the time to traverse the mean free path),  $E_C$  increases linearly with H. The process of thermal breakdown was studied as a function of time using square pulses the duration of which was either much longer or much shorter than the time necessary for heat transfer in the semiconductor. In the discussion Yu. E. Perlin pointed out the important role of the Frenkel effect which reduces the breakdown field. The authors of the paper estimated that the effective lowering of the barrier  $\alpha \sqrt{E_c}$  at breakdown fields is small. However, this result depends strongly on the proposed model of an impurity center.

## 8. WORK ON THE THERMODYNAMICS OF CRYSTALS

Three papers on this subject dealt with the thermal and magnetic properties of semiconductors. <u>A. E.</u> <u>Marinchuk and V. A. Moskalenko</u> (Institute of Physics and Mathematics, Kishinev), in the paper "On the thermodynamics of the crystal lattice," described a method of calculating the thermodynamic potential of a crystal allowing for anharmonic terms of third and fourth orders. The method is based on the use of Green's temperature functions and a diagram technique. The authors used the variation principle which made it possible to carry out this calculation approximately.

In his paper "Theory of the anisotropy of indirect exchange in the many-electron model," Yu. M. Seidov (Physics Institute, Academy of Sciences, Baku) carried out an approximate diagonalization of the Hamiltonian of a crystal, allowing for the spin-orbit interaction by the Bogolyubov-Tyablikov method. As the expansion parameter  $\epsilon$  the author used the ratio of the overlap of  $\psi$ -functions of magnetic ions to the overlap of nonmagnetic crystal CuCl<sub>2</sub>·2H<sub>2</sub>O. The energy spectrum of the crystal has a gap and consists of four branches, similar to the acoustical and optical vibrations, corresponding to the different spin orientations.

K. B. Vlasov and A. I. Mitseka (Institute of Metal Physics, Sverdlovsk), in the paper "On the thermodynamic theory of substances in which ferromagnetism and antiferromagnetism may coexist," investigated the mechanism of unidirectional (exchange) anisotropy and obtained conditions under which it may appear. The behavior of ferromagnets and antiferromagnets was considered in those cases when unidirectional anisotropy is absent.

The collective properties of an exciton gas were dealt with in the paper "Energy spectrum and thermohydrodynamics of excitons," by V. A. Moskalenko and A. N. Bobrysheva (Institute of Physics and Mathematics, Kishinev). If the exciton density is very high, the mutual interaction between excitons plays the dominant role. On reaching the temperature of Bose condensation, a phase transition of the second kind occurs and the specific heat discontinuity is of the same order as the specific heat itself. Elementary excitations of the system of almost completely condensed excitons and phonons possess a complex energy spectrum E(k); there are "acoustic excitons" for which  $E(k) \sim k$  at low momenta. Criteria were obtained for the applicability of the theory which impose restrictions on the density and nature of interaction between excitons.

Z. I. Uritskiĭ (Kazan') considered a new mechanism of phonon scattering in dielectrics by the formation of virtual electron-hole pairs which are annihilated to form two phonons. At low temperatures, this process may govern the thermal conductivity in dielectrics, giving a temperature dependence different from that due to the process connected with anharmonicity. Estimates were carried out for acoustical phonons. Some special features were noted for the interaction with the electron-hole vacuum compared with the electron-positron system in quantum electrodynamics (Furry's theorem was not satisfied).

In a resolution passed at the end of the Conference, it was agreed that "... The Conference deems it desirable to continue and develop work in the following directions:

1. Theory of transport processes and investigation of instability phenomena in semiconductors.

2. Investigation of the energy band structure in crystals.

3. Investigation of properties of non-ideal crystals.

4. Investigation of the behaviour of "hot" electrons in semiconductors.

5. Development of the theory of carrier recombination in semiconductors and the theory of radiationless transitions.

6. Theory of resonance phenomena in semiconductors.

7. Investigation of irradiation effects in solids.

8. Investigation of optical phenomena in semiconductors.

9. Theory of various semiconducting devices.

The Conference draws attention to the lag in the experimental work on the physics of semiconductors. This leads to the situation that many theoretical ideas, developed first in the Soviet Union, are realized experimentally abroad (cyclotron resonance in metals, combined resonance, cyclotron resonance in deformed semiconductors, indirect transitions in tunnel diodes, etc.). Moreover, theoretical work appears which lacks contact with experiment and is of little methodological importance.

In spite of the difficulties in organizing all-Union conferences on the theory of semiconductors (due to the continuing rise in the number of participants), it is desirable to continue holding such conferences at the rate of one every two years. The Conference recommends that the Sixth All-Union Conference on the Theory of Semiconductors should take place in Kishinev at the end of September, 1964. The Conference is of the opinion that the agenda of the present meeting was greatly overloaded with papers, and, therefore, the Organizing Committee of the Sixth Conference should take the following steps: 1) use the rapporteur system so that one person presents a critical review paper on the work on a certain subject; 2) reduce the number of papers at a session, allowing more time for each paper.

The Conference is of the opinion that in addition to the all-Union conferences on the theory of semiconductors, the following should be widely held: 1) meetings of small groups of theoreticians working on a definite subject; 2) schools for improving the qualifications of theoreticians; 3) schools for improving the qualifications of experimentalists, employing theoreticians to present lectures and papers."

Translated by A. Tybulewicz