

$x=0$ and $x=l$, the variation of J is

$$\delta J = -B \int_0^l \frac{d^2 q_2}{dx^2} \delta q_2 dx + Qh \int_0^l \left[\left(\frac{dq_1}{dx} + q_2 \right) \delta q_2 - \left(\frac{d^2 q_1}{dx^2} + \frac{dq_2}{dx} \right) \delta q_1 \right] dx. \quad (7.9)$$

If a force f is applied to the surface of the plate per unit area in the z -direction, the virtual work of this force is

$$\int_0^l f \delta w dx = \int_0^l f \delta q_1 dx. \quad (7.10)$$

Applying Eq. (6.10) of the previous section, the variations (7.9) and (7.10) must be equal. The expressions multiplying δq_1 in (7.9) and (7.10) must be equal and

that multiplying δq_2 in (7.9) must vanish. We derive the differential equations:

$$B \frac{d^2 q_2}{dx^2} = Qh \left(\frac{dq_1}{dx} + q_2 \right), \quad Qh \left(\frac{d^2 q_1}{dx^2} + \frac{dq_2}{dx} \right) = -f. \quad (7.11)$$

Eliminating q_2 , we find

$$\frac{d^4 q_1}{dx^4} = \frac{f}{B} - \frac{1}{Qh} \frac{d^2 f}{dx^2}. \quad (7.12)$$

The first term on the right-hand side corresponds to a bending deflection while the second term corresponds to a shearing deformation. We must remember that the differential equation (7.12) is also an operational equation in the time variable since B and Q are time operators. It is therefore also an integro-differential equation.

Thermal Ionization and Capture of Electrons Trapped in Semiconductors*

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(Received October 27, 1954)

The use of Coulombic wave functions rather than plane waves for the free electron states is found to increase the calculated rate of capture of electrons by a factor of about 200 at liquid helium temperatures. Results calculated for shallow traps in Ge and Si are now found to be consistent with the upper limit set on the photoconductive lifetime by the experiment of Burstein, Overly, and Davisson. The Born-Oppenheimer and Hartree approximations used in our calculations were found to yield identical results at low temperatures in these materials.

THE thermal ionization of an electron from a trapped state into the conduction band has previously been calculated using plane (or Bloch) waves for the final state.¹⁻⁴ Such a procedure neglects the effect of Coulomb attraction on the final state which should be represented by a Coulomb wave function. It is well known that the correct wave function has a density at the origin higher than the plane wave by the Sommerfeld factor $y/[1 - \exp(-y)]$ with $y = 2\pi/(ka)$, where k is the propagation constant of the final state and a is the effective Bohr radius of the electron in the crystal. It is important to note that during ionization the major contribution to the total transition probability comes from final states with $ka \ll 1$, so that

the correction factor is always large. At room temperature the factor is about 50, at He temperature it is about 200. On capture, only electrons with $ka \ll 1$ have large capture cross sections. And in any case, only electrons of thermal velocities are present, which at most temperatures of interest have $ka < 1$.

We have made a calculation of the ionization and capture probabilities in Si and Ge using Coulombic wave functions. The calculation was done both in the Hartree and the Born-Oppenheimer approximation. Results were applied to the case where the highest phonon energy is larger than the ionization energy, i.e., one-phonon processes are possible. Then both approximations yield the same result if multiphonon processes are unimportant, i.e., at low temperatures. The Hartree approximation in first order gives one-phonon processes only at any temperature, while the Born-Oppenheimer approximation gives many-phonon processes at higher temperatures. This result is independent of the particular mechanism considered for the interaction as long as one restricts oneself to an interaction potential that is linear in the displacements of the atoms from their equilibrium positions. We considered two types of

* Supported in part by the U. S. Air Force, through the Office of Scientific Research of the Air Research and Development Command and in part by the Office of Naval Research. A preliminary report of these results was presented on March 19, 1954 to the Detroit meeting of the American Physical Society, Phys. Rev. **94**, 1419(A) (1954).

¹ Goodman, Lawson, and Schiff, Phys. Rev. **71**, 191 (1947).

² Paul J. Leurgans, thesis, University of Illinois, 1952 (unpublished).

³ R. Kubo, Phys. Rev. **86**, 929 (1952).

⁴ L. Tewordt, Z. Physik **137**, 604 (1954).

interaction of the electron with the lattice, the Bardeen-Shockley⁵ deformation potential and the interaction used by Goodman, Lawson, and Schiff¹ which depends exclusively on the motion of the impurity atom. Without committing ourselves as yet to a particular mechanism, we consider an interaction potential of the form

$$V = N^{-1} B_t(\mathbf{r}, \boldsymbol{\tau}) q_t(\boldsymbol{\tau}), \quad (1)$$

where $q_t(\boldsymbol{\tau})$ is the amplitude of the mode of propagation vector $\boldsymbol{\tau}$ and of type t . Denoting the matrix element of $B_t(\mathbf{r}, \boldsymbol{\tau})$ between the final and initial unperturbed electronic states (a for initial state, \mathbf{k} for free state with propagation vector \mathbf{k}) by $B_t(\boldsymbol{\tau})_{ka}$ and with a corresponding notation for the matrix elements between like states, we obtain⁶ for the transition probabilities to state \mathbf{k} and from state \mathbf{k} :

$$W_{ka} = \hbar^{-2} \int \exp[iE_{ka}t/\hbar + f(t)] \{h(t) + [g(t)]^2\} dt, \\ W_{ak} = \hbar^{-2} \int \exp[-iE_{ka}t/\hbar + f(t)] \{h(t) + [g(t)]^2\} dt, \\ f(t) = \langle \Phi(t, \omega) (B_{kk} - B_{aa}) / (2\hbar M \omega^3) \rangle, \quad (2) \\ h(t) = \langle [\Phi(t, \omega) + (2\bar{n} + 1)] (\hbar\omega / 2M) \\ \times [\hbar B_{ka} / (E_k - E_a)]^2 \rangle, \\ g(t) = \langle \Phi(t, \omega) \hbar B_{ka} (B_{kk} - B_{aa}) [2M\omega (E_k - E_a)]^{-1} \rangle, \\ \Phi(t, \omega) = (\bar{n} + 1) \exp(i\omega t) + \bar{n} \exp(-i\omega t) - (2\bar{n} + 1).$$

Here the angular braces $\langle \rangle$ denote an average over the modes of one type and a summation over all types. The indices $\boldsymbol{\tau}$ and t have been suppressed in B , \bar{n} = mean quantum number and ω , the frequency of the mode in question. M is the mass of one Ge atom. E_k and E_a are the unperturbed final and initial electronic energies and E_{ka} is their difference plus the energy change due to the shift of the equilibrium positions of the atoms. To obtain the ionization probability W_{ion} we have to integrate W_{ka} over all final free electron states, while for the capture probability W_{cap} we take the average of W_{ak} over the thermally distributed \mathbf{k} -states of the electron. If the exponential containing $f(t)$ is expanded the integration over t can be performed immediately, giving rise to delta functions. At low temperatures in Ge and Si, only the first term in this expansion, representing one-phonon processes, is important.⁷ If, in the neighborhood of $k=0$, the matrix element $|B_t(\boldsymbol{\tau})_{ka}|^2$ is proportional to k^λ , we obtain at low temperatures:

$$W_{ion} = FN\Omega^2 A(T) \exp(-I/k_0 T) / (64\pi^5 M I), \quad (3) \\ W_{cap} = F\Omega / (8\pi^2 M I),$$

⁵ J. Bardeen and W. Shockley, Phys. Rev. **80**, 72 (1950).

⁶ For the methods used consult M. Lax, J. Chem. Phys. **20**, 1752 (1952). For a review of the literature see M. Lax, *The Influence of Lattice Vibrations on Electronic Transitions in Solids*, Proceedings of the Nov. 1954 Atlantic City Conference on Photoconductivity (John Wiley and Sons, Inc., New York, 1955).

⁷ The same conclusion was obtained by Y. Yafet for transitions between bound states (private communication).

where

$$F = \sum_t \int \gamma_{\lambda t} |B_t(\boldsymbol{\tau})_{ka}|^2 \delta[I/\hbar - \omega_t(\boldsymbol{\tau})] d\boldsymbol{\tau}, \\ A(T) = \int \exp[-E(\mathbf{k})/k_0 T] d\mathbf{k}, \\ \bar{k}^\lambda = A(T)^{-1} \int k^\lambda \exp[-E(\mathbf{k})/k_0 T] d\mathbf{k}, \\ \gamma_\lambda = \bar{k}^\lambda / \langle \bar{k} \rangle^\lambda.$$

Here Ω is the volume of the unit cell and I the ionization energy. If the mechanism causing the transition is the deformation potential, the B are given by

$$B_t(\mathbf{r}, \boldsymbol{\tau}) = (i/\sqrt{2}) E_1 (e_t(\boldsymbol{\tau}) \cdot \boldsymbol{\tau}) \exp(i\boldsymbol{\tau} \cdot \mathbf{r}), \quad (4)$$

where the $e_t(\boldsymbol{\tau})$ are unit polarization vectors. It is adequate to use a Debye spectrum (longitudinal speed of sound = v) in the present calculation. To get an order of magnitude result it is probably adequate to use a scalar effective mass m^* . For the deformation potential interaction, we thus obtain⁸

$$W_{ion} = 32\Omega E_1^2 (\pi a^4 M I v)^{-1} (\tau_0 a)^{-4} 2m^* a^2 \hbar^{-2} k_0 T \\ \times \exp(-I/k_0 T), \quad (5)$$

$$W_{cap} = 256\pi^{\frac{1}{2}} \Omega E_1^2 (V a M I v)^{-1} (\tau_0 a)^{-4} \\ \times (2m^* a^2 \hbar^{-2} k_0 T)^{-\frac{1}{2}}, \quad (6)$$

where a is the effective Bohr radius = Bohr radius times dielectric constant times ratio of electronic to effective mass; τ_0 is the propagation constant of those modes for which $\hbar\omega(\tau_0) = I$, and V is the volume of the crystal. These equations apply if $k_0 T \ll I$ and $k_0 T \ll (k_0 \theta - I)$, where $k_0 \theta$ is the Debye energy.

For n -type silicon, using as ionization energy $I \simeq 0.04$ eV and an interaction constant $E_1 = 15$ eV,⁹ we obtain

$$V W_{cap} \simeq (40/T)^{\frac{1}{2}} \times 10^{-8} \text{ cm}^3/\text{sec}.$$

If we assume 10^{15} minority carriers (acceptors) per cm^3 to be present and have one donor and one acceptor level only, the lifetime of free electrons at 4°K is of order 3×10^{-8} sec. This is consistent with experiments on the photoconductive lifetime by Burstein, Oberly, and Davisson¹⁰ who find an upper limit to the lifetime of 10^{-4} sec. If one uses the interaction of Goodman, Lawson, and Schiff,¹ the value for the capture probability at 4°K is smaller by a factor of about 17.

⁸ Details of the above calculations will be submitted to this journal shortly.

⁹ This value for the interaction constant is obtained by using the formula (see reference 5):

$$\mu = \frac{4(2\pi)^{\frac{1}{2}} e \hbar^4 M v^2}{3\Omega (m^*)^{\frac{5}{2}} (k_0 T)^{\frac{1}{2}} E_1^2}$$

taking $\mu = 1200 \text{ cm}^2/\text{volt-sec}$ [M. B. Prince, Phys. Rev. **93**, 1204 (1954)], and letting $(m^*)^{-\frac{5}{2}} = (m_1 m_2 m_3)^{-\frac{1}{2}} \times \frac{1}{2} [(1/m_1) + (1/m_2) + (1/m_3)]$ with $m_1 = m_2 = 0.19m$; $m_3 = 0.98m$.

¹⁰ Burstein, Oberly, and Davisson, Phys. Rev. **89**, 331 (1953).