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# Thermal Ionization of Trapped Electrons

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The rate of thermal ionization of an electron trapped on an impurity atom is treated on a quantum mechanical basis. From the standpoint of an adiabatic approximation, the multiphonon transitions are attributed to the dependence of the atomic vibrations on the electronic states. Approximate formulas based on an Einstein model are derived for the total ionization rate by using a generating function which is intimately related to density matrices. It is shown that the rate can be expressed as $256(m/M)\omega(\rho/2)^{\epsilon_0/\hbar\omega-1}$ $\exp(-\epsilon_0/kT)$ for low temperatures, where $m$ is the mass of electron, $M$ that of the atom, $\omega$ the frequency of atomic vibration, $\epsilon_0$ the energy of ionization, and $\rho$ is the fractional difference of the frequencies of atomic vibrations in the trapped and the ionized states, which can be of the order 0.1. For high temperatures we can expect a similar formula to that given by the activated states theory. Generally, we have reasons to expect much greater rates than those given by Goodman, Lawson, and Schiff.

## INTRODUCTION

IN semiconductors and luminescent materials, electron traps play important roles in various electronic processes. The trapped electrons can be thrown up into free states by absorbing the energy of incident light, of impacting particles, or of the vibration of surrounding atoms; and conversely, a conduction electron can be trapped at a trapping center, radiating part of its energy as a photon or phonons. Quantum-mechanical theories of such elementary reaction processes are needed for thorough studies of solid-state electronics.

In this article, we confine ourselves to the study of the third process mentioned above, that is, the thermal ionization of trapped electrons. To clarify the nature of this process, one has to consider the interrelation of the electronic and vibrational states of the crystal in more detail than in the usual cases, such as in the theory of electronic conduction, because, in contrast to the latter process, thermal ionization is essentially a multiphonon process.

Twenty years ago, in his theory of the dissipation of light energy absorbed in insulating crystals, Frenkel[1] pointed out that slight differences between the modes of lattice vibrations in the electronically excited states and those in the ground state are responsible for the multiphonon emission which takes place when the electron goes back to the normal state. Möglich and Rompe,[2] on the other hand, insisted that the higher terms in the expansion of the interaction potential between the electron and the lattice give the probabilities of multiphonon jumps. Their theory was used by Riehl[3] for an explanation of luminescent phenomena. Mathematical difficulties, however, forced them to forego a quantitative treatment and to content themselves with a qualitative discussion.

More recently Goodman, Lawson, and Schiff[4] presented a simple theory of the thermal ionization process in semiconductors along similar lines to that of Möglich and Rompe. Their calculation shows that the ionization rate will decrease by the factor $10^{-6}$ as the ionization energy increases by $\hbar\omega$, that is the energy of a phonon. This leads one to a surprisingly small probability for the thermal ionization process of impurity levels.

The writer feels that the latter analysis is inadequate, for reasons to be clarified in the following sections. Hence, he wishes to present another theory concerned with the same problem, based on the idea of Frenkel, but differing from it in some essential points. Owing to mathematical difficulties, we also do not give any detailed treatment of actual crystals but confine ourselves to a discussion of a simplified model. Our result, however, shows that we can expect much larger probabilities for the multiphonon jumps. This conclusion will be important for the understanding, for instance, of semiconductor rectifiers. Moreover, the theory presented here will be interesting as an example of a purely quantum mechanical treatment of the reaction rate problem. The use of density matrices for such problems proves to be very helpful.

## I. COUPLING BETWEEN THE LATTICE AND THE ELECTRON

Generally speaking, the Hamiltonian of a polyatomic system is of the form

$$H=H_R+H_r+V, \tag{1}$$

where $H_R$ is the sum of the kinetic energy terms of the nuclei and their interaction potentials, $H_r$ the similar expression for the electron system, and $V$ the interaction energy between the nuclei and the electrons. As is well known, we can seek the eigenstates of the Hamiltonian along the lines of the adiabatic potential method. Considering the coordinates $\mathbf{R}$ of the nuclei as fixed, the eigenvalue equation,

$$[H_r+V(\mathbf{r},\mathbf{R})]\varphi_l(\mathbf{r},\mathbf{R})=E_l'(\mathbf{R})\varphi_l(\mathbf{r},\mathbf{R}), \tag{2}$$

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[1] J. Frenkel, Phys. Rev. **37**, 17 and 1276 (1931); Physik. Z. Sowjetunion **9**, 158 (1936).

[2] F. Möglich and R. W. Rompe, Z. Physik **115**, 707 (1940).

[3] N. Riehl, *Physik und technische Anwendungen der Lumineszenz* (Verlag. J. Springer, Berlin, 1941).

[4] Goodman, Lawson, and Schiff, Phys. Rev. **71**, 191 (1947).

gives the adiabatic potential $E_l'(\mathbf{R})$ for the $l$th electronic state. Then in this electronic state the motion of the nuclear system is determined by

$$[H_R+E_l'(\mathbf{R})]\zeta_{lv}(\mathbf{R})=E_{lv}\zeta_{lv}(\mathbf{R}). \tag{3}$$

Thus a quantum state of the whole system is specified by the quantum numbers $l$ and $v$, and the wave function takes the form

$$\Psi_{lv}(\mathbf{r},\,\mathbf{R})=\varphi_l(\mathbf{r},\,\mathbf{R})\zeta_{lv}(\mathbf{R}). \tag{4}$$

As shown by Born and Oppenheimer,[5] this wave function is a good approximation for stationary states. Wigner and Pelzer[6] have also shown that the adiabatic method is justified for some chemical reactions under certain conditions.

It is clear, however, that we must look for the perturbation causing the transition between different electronic states just in the approximate nature of the wave functions given by Eq. (4) if we are interested in such processes as thermal excitation. In fact, we can write

$$\begin{aligned}H\Psi_{lv}(\mathbf{r},\,\mathbf{R})&=[H_R+E_l'(\mathbf{R})]\zeta_{lv}(\mathbf{R})\varphi_l(\mathbf{r},\,\mathbf{R})\\&=E_{lv}\Psi_{lv}+H'\Psi_{lv},\end{aligned}$$

where

$$H'\Psi_{lv}\equiv H_R\zeta_{lv}\varphi_l-\varphi_l H_R\zeta_{lv}, \tag{5}$$

does not vanish because of the differentiation operators in $H_R$. Thus we are forced to seek a solution of the form

$$\Psi=\sum a_{lv}(t)\Psi_{lv}(\mathbf{r},\,\mathbf{R}). \tag{6}$$

Inserting $\Psi$ into the time dependent wave equation, we obtain the equation,

$$i\hbar\dot{a}_{lv}=\sum_{l'v'}(lv|H|l'v')a_{l'v'}, \tag{7}$$

where the relation,

$$(lv|H|l'v')=E_{lv}\delta_{lv,\,l'v'}+(lv|H'|l'v'), \tag{8}$$

holds because of the orthogonality relations

$$\int\varphi_l^*(\mathbf{r},\,\mathbf{R})\varphi_{l'}(\mathbf{r},\,\mathbf{R})d\mathbf{r}=\delta_{ll'},$$

$$\int\zeta_{lv}^*(\mathbf{R})\zeta_{lv'}(\mathbf{R})d\mathbf{R}=\delta_{vv'},$$

which follow from Eqs. (2) and (3).

From a physical point of view the eigenstates described by Eq. (4) must be considered as "good." Nevertheless it is important to recognize that they are not stationary in the exact sense, and that the whole system oscillates to and fro among various good quantum states of almost the same energy. This should be interpreted as the transition from one electronic state to another, accompanied by a transition in the quantum states of the nuclear motion.[7]

The ordinary time-dependent perturbation method gives at once the transition probability from the initial $(l,\,v)$ to a final $(l'v')$ state as

$$w(lv\rightarrow l'v')=(2\pi/\hbar)|(lv|H'|l'v')|^2\rho_f, \tag{9}$$

where $\rho_f$ is the state density of the final state, and the $(l'v')$ must satisfy the law of conservation of energy,

$$E_{l'v'}=E_{lv}. \tag{10}$$

In the ionization case, the final state is that in which an electron is set free. Hence, $\rho_f$ is approximated by

$$\rho_f=4\pi\Omega m^*hk/h^3, \tag{11}$$

where $\Omega$ is the volume of the space under consideration, $m^*$ the effective mass of the free electron, and $\mathbf{k}$ its wave number.

The idea outlined above can be widely applied to other problems, but at present we confine ourselves to a treatment of a simplified model similar to that discussed by Goodman, Lawson, and Schiff.[4]

## II. A SIMPLIFIED MODEL OF TRAPPED ELECTRONS

Suppose that a substitutional impurity atom creates a trapping center, where an electron can be trapped with a localized wave function $\varphi_0$. Strictly speaking, $\varphi_0$ is a function of the configuration of all the atoms in the crystal. However, to clarify the nature of our problem and to get a simple approximation, we assume there that only the instantaneous positions of the impurity atom affects the wave function $\varphi_0$ strongly and that the dependence of $\varphi_0$ upon the motion of other atoms can be neglected. Thus, the wave function $\varphi_0$ is regarded as a function of $\mathbf{r}$ and $\mathbf{R}$, which are the coordinates of the trapped electron and of the impurity atom, respectively. Moreover, we introduce another simplification by using an Einstein model for the vibrational motion of the atoms. In a more rigorous theory this model should be replaced by the Debye model.

With such a simplified model, it is clear that the difference of the modes of vibration, that is the difference of the vibrational frequencies of the central atom in the ground and the excited electronic states, is the cause of the multiphonon jump in the process of thermal ionization.

The Hamiltonian of the simplified model will be

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[5] M. Born and F. Oppenheimer, Ann. Physik **84**, 457 (1927).

[6] H. Pelzer and E. Wigner, Z. physik Chem. **B15**, 445 (1932).

[7] This point of view has also been adopted by K. Huang and A. Rhys [Proc. Roy. Soc. (London) **A204**, 406 (1950)], who have discussed the light absorption and nonradiative transition of *F*-centers. Assuming a continuum model of a crystal they have treated the vibrational motion of the nuclei as lattice waves, which is, in principle, more rigorous than the Einstein model assumed in the present paper, and they gave the probabilities of nonradiative transitions in terms of the difference of the equilibrium positions of the lattice atoms between different electronic states. The author was not aware of their work when he prepared the present paper, and he wishes to leave detailed discussion to a later paper.

written as

$$H=-(\hbar^2/2M)\Delta_R+U_0(\mathbf{R})-(\hbar^2/2m)\Delta_r+V'(\mathbf{r})+V(\mathbf{R}-\mathbf{r}), \quad (12)$$

where $M$ is the mass of the impurity atom, and $U_0(\mathbf{R})$ its interaction with the surrounding crystal atoms. $V(\mathbf{R}-\mathbf{r})$ and $V'(\mathbf{r})$ mean the Hartree fields of the electron associated with the central atom and the neighboring atoms, respectively. Although in fact $V'(\mathbf{r})$ depends on the configuration of the surrounding atoms, we have not taken this into consideration in our present simplified model.

Goodman, Lawson, and Schiff have assumed that

$$V(\mathbf{R}-\mathbf{r})=Ze^2/|\mathbf{R}-\mathbf{r}|,$$

and that $\mathbf{R}$ can be expressed as

$$\mathbf{R}=\mathbf{R}_0+\delta\mathbf{R}=\mathbf{R}_0+\textstyle\sum_j \mathbf{a}_j \exp[i(\omega_j t-\mathbf{k}_j\mathbf{R}_0)].$$

Thus, expanding $V$ in a power series of $\delta\mathbf{R}$, they obtained the probability of the multiphonon jumps from the higher terms of the expansion. It is essentially at this point that the author feels their treatment is inadequate, since the electronic state of the trapped electron should follow adiabatically the changes in $\mathbf{R}$. It is clear that any periodic displacement of the nucleus of a hydrogen atom cannot cause the ionization of its electron, unless the frequency is very high. It is true that the adiabatic approximation breaks down if the electronic energy of the excited state is very near to the ground state, in our case, for example, if the ionization energy is very small. In such cases, both theories, that of Goodman, Lawson, and Schiff and that of the writer, will give a large probability just for $w\sim\omega$, which shows that the trapped state has no real meaning. But for other cases the two theories give definitely different pictures. It should also be noticed that the situation is different for the scattering of metal electrons by lattice waves. In this case the Bloch waves of electrons remain a good approximation even for a deformed lattice, and the excitation of a few electrons has no effect on the modes of the lattice vibrations, so that the ordinary conduction theory is justifiable from a physical point of view. However, in our case, so long as we consider the wave function of the trapped electron to be localized around the impurity atom, we have to admit that the ionization definitely changes the binding of the impurity to its neighbors.

From the standpoint adopted in Sec. 1, we take

$$H'\zeta_{lv}\varphi_l\equiv-(\hbar^2/2M)(\Delta_R\zeta_{lv}\varphi_l-\varphi_l\Delta_R\zeta_{lv}), \quad (13)$$

for the reasons explained above. For our simplified model, $\varphi_0$ is a function of $(\mathbf{r}-\mathbf{R})$, so that we may write

$$\nabla_R\varphi_0=-\nabla_r\varphi_0.$$

Hence Eq. (13) is of the form

$$H'\zeta_{0v}\varphi_0=-(1/M)(\mathbf{P}\zeta_{0v}\cdot\mathbf{p}\varphi_0-\tfrac{1}{2}\zeta_{0v}\mathbf{p}^2\varphi_0), \quad (14)$$

where $\mathbf{P}$ is the momentum operator of the central atom and $\mathbf{p}$ that of the electron. Thus the matrix element in Eq. (9) is given by

$$(0v|H'|kv')=-\frac{1}{M}\int d\mathbf{R}\zeta_{kv'}{}^*\mathbf{P}\zeta_{0v}\int d\mathbf{r}\varphi_k{}^*\mathbf{p}\varphi_0+\frac{1}{2M}\int d\mathbf{R}\zeta_{kv'}{}^*\zeta_{0v}\int d\mathbf{r}\varphi_k{}^*\mathbf{p}^2\varphi_0, \quad (15)$$

where $\zeta_{0v}$ and $\zeta_{kv'}$ are the eigenfunctions of a three-dimensional isotropic harmonic oscillator, with different frequencies for the ground state $\varphi_0$ and the ionized state $\varphi_k$ of the electron.

For simplicity, we further assume the wave functions of the electron to be hydrogenlike,

$$\varphi_0=(a^3/\pi)^{\frac{1}{2}}\exp(-a|\mathbf{r}-\mathbf{R}|), \quad (16)$$

for the trapped ground state, and to be plane waves,

$$\varphi_k=e^{i\mathbf{k}\mathbf{r}}/\Omega^{\frac{1}{2}}, \quad (17)$$

for the free states. Then, we obtain

$$\int\varphi_0\mathbf{p}\varphi_k dr=\hbar\mathbf{k}\left(\frac{a^3}{\Omega\pi}\right)^{\frac{1}{2}}\frac{8\pi a}{(a^2+k^2)^2}e^{i\mathbf{k}\mathbf{R}}. \quad (18)$$

$$\int\varphi_0\mathbf{p}^2\varphi_k dr=-\hbar^2\mathbf{k}^2\left(\frac{a^3}{\Omega\pi}\right)^{\frac{1}{2}}\frac{8\pi a}{(a^2+k^2)^2}e^{i\mathbf{k}\mathbf{R}}. \quad (19)$$

Inserting these in Eq. (15), we may take $\exp(i\mathbf{k}\mathbf{R})\sim 1$, since the higher terms of the expansion of $\exp(i\mathbf{k}\mathbf{R})$ can be neglected because of the localized nature of $\zeta_{0v}$ and $\zeta_{kv'}$.

The vibrational wave functions of the central atom are of the form

$$\zeta_{0v}=\zeta_{0v_1}(X_1)\zeta_{0v_2}(X_2)\zeta_{0v_3}(X_3),$$
$$\zeta_{kv'}=\zeta_{kv_1'}(X_1)\zeta_{kv_2'}(X_2)\zeta_{kv_3'}(X_3),$$

where $X_1$, $X_2$, and $X_3$ are the three orthogonal coordinates of the atom, and $\zeta_{0v_j}$ and $\zeta_{kv_j'}$ are the eigenfunctions of harmonic oscillators in quantum states $v_j$ and $v_j'$ with proper frequencies $\omega$ and $\omega'$, respectively. For brevity, we introduce the following notation:

$$\alpha=M\omega/\hbar, \quad \alpha'=M\omega'/\hbar, \quad (20)$$

$$(v_j|v_j')=\int\zeta_{0v_j}\zeta_{0v_j'}dX_j, \quad (21)$$

$$[v_j|v_j']=(\alpha\alpha')^{-\frac{1}{4}}\left(v_j\left|\frac{\partial}{\partial X_j}\right|v_j'\right)$$
$$=(\alpha\alpha')^{-\frac{1}{4}}\int\zeta_{0v_j}\frac{\partial}{\partial x_j}\zeta_{kv_j'}dX_j, \quad (22)$$

$$\epsilon_0=\hbar^2/2ma^2, \quad \epsilon_k=\hbar^2k^2/2m. \quad (23)$$

With Eqs. (11), (15), (18), and (19) the transition probability (9) becomes, after simple calculations:

$$w(0v\to kv')=\nu_1\frac{\epsilon_0^{5/2}\epsilon_k^{3/2}}{(\epsilon_0+\epsilon_k)^4}\big|[v_1|v_1'](v_2|v_2')(v_3|v_3')\big|^2$$
$$+\nu_2\frac{\epsilon_0^{3/2}\epsilon_k^{5/2}}{(\epsilon_0+\epsilon_k)^4}\big|(v_1|v_1')(v_2|v_2')(v_3|v_3')\big|^2, \quad (24)$$

where,

$$\nu_1=64(m/M)(\omega\omega')^{\frac{1}{2}}, \quad \nu_2=32(m/M)^2(\epsilon_0/\hbar). \quad (25)$$

In Eq. (24), the second term may be neglected for all practical cases, because the ratio $\nu_2/\nu_1$ turns out to be $\frac{1}{2}(m/M)[\epsilon_0/\hbar(\omega\omega')^{\frac{1}{2}}]$, which is only of the order of magnitude $10^{-2}$ if we take $m/M\sim10^{-4}$, and $\epsilon_0\sim1$ ev.

The total rate of the thermal ionization $W_t$ is given by the sum of $w(0v\to kv')$ over all the initial states weighted by their Boltzmann factors, and over all the final states which satisfy the condition of energy conservation (10). Thus, $W_t$ is given by

$$W_t(x_0)=\sum_{v_1}{}'\cdots\sum_{v_3'}{}' w(0v\to kv')e^{-\beta(v_1+v_2+v_3)}(1-e^{-\beta})^3, \quad (26)$$

where the summation follows the conditions

$$(v_1+v_2+v_3+\tfrac{3}{2})-(v_1'+v_2'+v_3'+\tfrac{3}{2})(\omega'/\omega)$$
$$=(\epsilon_0+\epsilon_k)/\hbar\omega\equiv x, \quad (27)$$

and

$$x\geqq x_0\equiv\epsilon_0/\hbar\omega. \quad (28)$$

The total rate $W_t(x_0)$, Eq. (26), may be written as

$$W_t(x_0)=\sum_{x\geqq x_0}W(x), \quad (29)$$

where,

$$W(x)=(1-e^{-\beta})^3\sum_{v_1}{}'\cdots\sum_{v_3'}{}' w(0v\to kv')e^{-\beta(v_1+v_2+v_3)}, \quad (30)$$

the summation being taken over all integral values of $v_1\cdots v_3'$ that satisfy the condition (27) for a fixed value of $x$. In these expressions $\beta$ means, of course,

$$\beta=\hbar\omega/kT. \quad (31)$$

## III. EVALUATION OF THE RATE OF THERMAL IONIZATION

In this section, we seek closed expressions for $W(x)$ and $W_t(x_0)$. For this purpose, as shown below, it is most convenient to use Slater sums or density matrices.

Define a function $F(x)$ by

$$F(x)=(1-e^{-\beta})^3\sum_{v_1}{}'\cdots$$
$$\times\sum_{v_3'}{}'\big|[v_1|v_1'](v_2|v_2')(v_3|v_3')\big|^2e^{-\beta(v_1+v_2+v_3)}, \quad (32)$$

in which the summation has the same meaning as in Eq. (30). $W(x)$ is then given by,

$$W(x)=\nu_1x_0^{5/2}(x-x_0)^{3/2}x^{-4}F(x), \quad (33)$$

as seen from Eq. (24).

To calculate the function $F(x)$, we introduce here its generating function $Z(\lambda)$ defined by,

$$Z(\lambda)=\sum_x F(x)e^{-\lambda x}, \quad (34)$$

which can be transformed as follows: By the condition (27)

$$Z(\lambda)=\sum_x F(x)\exp[-\lambda(v_1+v_2+v_3+\tfrac{3}{2})$$
$$+\lambda(\omega'/\omega)(v_1'+v_2'+v_3'+\tfrac{3}{2})]$$
$$=\sum_{v_1}\cdots\sum_{v_3'}\big|[v_1|v_1']\big|^2\big|(v_2|v_2')\big|^2\big|(v_3|v_3')\big|^2$$
$$\times\exp\{-(\beta+\lambda)(v_1+v_2+v_3+\tfrac{3}{2})$$
$$+\lambda(\omega'/\omega)(v_1'+v_2'+v_3'+\tfrac{3}{2})+\tfrac{3}{2}\beta\}$$
$$=e^{3\beta/2}\Big[\sum_{v_1}\sum_{v_1'}\big|[v_1|v_1']\big|^2\exp\{-(\beta+\lambda)(v_1+\tfrac{1}{2})$$
$$+\lambda(\omega'/\omega)(v_1'+\tfrac{1}{2})\}\Big]\Big[\sum_{v_2}\sum_{v_2'}\big|(v_2|v_2')\big|^2$$
$$\times\exp\{-(\beta+\lambda)(v_2+\tfrac{1}{2})+\lambda(\omega'/\omega)(v_2'+\tfrac{1}{2})\}\Big]$$
$$\times\Big[\sum_{v_3}\sum_{v_3'}[(v_3|v_3')\big|^2\exp\{-(\beta+\lambda)(v_3+\tfrac{1}{2})$$
$$+\lambda(\omega'/\omega)(v_3'+1)\}\Big]. \quad (35)$$

Using the well-known Slater sum for a harmonic oscillator,

$$\Phi(x|x',\xi)\equiv\sum_{v=0}^{\infty}\zeta_v(x)\zeta_v(x')\exp\{-\xi(v+\tfrac{1}{2})\}$$
$$=(2\pi\sinh\xi)^{-\frac{1}{2}}\exp[-\tfrac{1}{4}(\tanh\tfrac{1}{2}\xi)(x+x')^2$$
$$-\tfrac{1}{4}(\coth\tfrac{1}{2}\xi)(x-x')^2], \quad (36)$$

we can easily derive the following formulas,

$$\sum_v\sum_{v'}\big|(v|v')\big|^2\exp\{-(\beta+\lambda)(v+\tfrac{1}{2})+\lambda(\omega'/\omega)(v'+\tfrac{1}{2})\}$$
$$=(\alpha\alpha')^{\frac{1}{2}}\int\!\!\int_{-\infty}^{\infty}\Phi(\alpha^{\frac{1}{2}}X|\alpha^{\frac{1}{2}}X',\beta+\lambda)$$
$$\times\Phi(\alpha'^{\frac{1}{2}}X|\alpha'^{\frac{1}{2}}X',-(\omega'/\omega)\lambda)dXdX'$$
$$=[2g(\beta,\lambda)]^{-\frac{1}{2}}, \quad (37)$$

and,

$$\sum_v\sum_{v'}\big|[v|v']\big|^2\exp\{-(\beta+\lambda)(v+\tfrac{1}{2})+\lambda(\omega'/\omega)(v'+\tfrac{1}{2})\}$$
$$=\int\!\!\int_{-\infty}^{\infty}\Phi(\alpha^{\frac{1}{2}}X|\alpha^{\frac{1}{2}}X',\beta+\lambda)\frac{\partial}{\partial X}\frac{\partial}{\partial X'}$$
$$\times\Phi(\alpha'^{\frac{1}{2}}X|\alpha'^{\frac{1}{2}}X',-(\omega'/\omega)\lambda)dXdX'$$
$$=2\sqrt{2}\{(1-\rho)^{-\frac{1}{2}}\sinh(\beta+\lambda)-(1-\rho)^{\frac{1}{2}}\sinh\lambda\}$$
$$\times\{g(\beta,\lambda)\}^{-3/2}, \quad (38)$$

with the function $g(\beta, \lambda)$ defined by,

$$g(\beta,\lambda)=\cosh(\beta+\lambda)\cosh(1-\rho)\lambda$$
$$-\tfrac{1}{2}[1-\rho+1/(1-\rho)]\sinh(\beta+\lambda)\sinh(1-\rho)\lambda, \quad (39)$$

and the parameter $\rho$ defined by

$$\omega'/\omega=1-\rho. \quad (40)$$

Inserting Eq. (37) and Eq. (38) into Eq. (35), we then arrive at a closed expression for the generating function $Z(\lambda)$, which is conveniently written as

$$Z(\lambda)=2^{5/2}(\sinh\tfrac{1}{2}\beta)^3 Z_1(\lambda)Z_2(\lambda), \quad (41)$$

where

$$Z_1(\lambda)=2\{(1-\rho)^{-\frac{1}{2}}\sinh(\beta+\lambda)-(1-\rho)^{\frac{1}{2}}\sinh(1-\rho)\lambda\}, \quad (42)$$

$$Z_2(\lambda)=\{g(\beta,\lambda)\}^{-5/2}. \quad (43)$$

The function $F(x)$ in Eq. (32), has finite values only for a discrete set of values of $x$ defined by Eq. (27), and therefore, the series of Eq. (34) is essentially a Dirichlet series. Hence, the step-function defined by,

$$G(x)=\sum_{y\leq x} F(y),$$

is obtained by the well-known inverse formula of the bilateral Laplace-transformation,

$$G(x)=\frac{1}{2\pi i}\int_{-i\infty}^{i\infty} Z(\lambda)e^{\lambda x}\frac{d\lambda}{\lambda}.$$

From this, after a formal differentiation, we obtain

$$F(x)=\frac{1}{2\pi i}\int_{-i\infty}^{i\infty} Z(\lambda)e^{\lambda x}d\lambda, \quad (45)$$

where $F(x)$ is, however, to be interpreted as constructed from an infinite set of delta-functions. By the convolution theorem the inverse transformation, Eq. (45), is given by

$$F(x)=2^{5/2}(\sinh\tfrac{1}{2}\beta)^3\int f_1(x')f_2(x-x')dx', \quad (46)$$

where

$$f_1(x)=\frac{1}{2\pi i}\int_{-i\infty}^{i\infty} Z_1(\lambda)e^{\lambda x}d\lambda$$
$$=(1-\rho)^{-\frac{1}{2}}\{e^{\beta}\delta(x+1)-e^{-\beta}\delta(x-1)\}$$
$$-(1-\rho)^{\frac{1}{2}}\{\delta(x+1-\rho)-\delta(x-1+\rho)\}, \quad (47)$$

and

$$f_2(x)=\frac{1}{2\pi i}\int_{-i\infty}^{i\infty}[g(\beta,\lambda)]^{-5/2}e^{\lambda x}d\lambda. \quad (48)$$

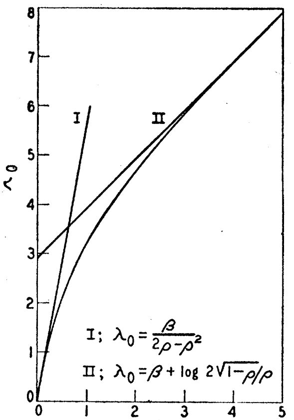

FIG. 1. The function $\lambda_0(\beta)$, which is the real solution of the equation $g(\beta,-\lambda_0)=0$ (see Eq. (49)). The parameter $\rho$ is assumed to be 0.1. Curves I and II are the approximate solutions for high temperatures and low temperatures, respectively.

The function $g(\beta, \lambda)$, Eq. (39), has an infinite set of zero points because of the discrete nature of $F(x)$. On the real axis it has only two zeros, one on the positive side, and the other on the negative side. Since we are interested in the positive values of $x$, only the negative zero is to be considered. It must be noticed here that an exact evaluation of Eq. (45) or Eq. (48) is of little importance for us, because it leads to the series of Eq. (33), where the matrix elements may also be evaluated by direct integrations or by use of generating functions of Hermite polynomials. Such a series, in itself, is not tractable because it cannot be summed to give the desired rate $W_t(x_0)$. In fact, the merit of the method introduced here is that it is a short cut to a convenient approximation. From this standpoint, we evaluate the integral of Eq. (48) in some approximate ways.

The function $g(\beta, \lambda)$ can be transformed to

$$g(\beta,\lambda)=\cosh(\beta+\rho\lambda)-1$$
$$-\frac{\rho^2}{2(1-\rho)}\sinh(\beta+\lambda)\sinh(1-\rho)\lambda$$
$$=\frac{(2-\rho)^2}{4(1-\rho)}\cosh(\beta+\rho\lambda)$$
$$-\frac{\rho^2}{4(1-\rho)}\cosh\{(2-\rho)\lambda+\beta\}. \quad (49)$$

Now we assume $\rho$ to be small, which will be true for most cases of interest. Let the negative zero point be $-\lambda_0$, which is given approximately by

$$\lambda_0\simeq\beta+\log[2(1-\rho)^{\frac{1}{2}}/|\rho|] \quad (50)$$

for large $\beta$, and by

$$\lambda_0\simeq\beta/(2\rho-\rho^2) \quad (51)$$

for small $\beta$ provided that $\rho>0$. Equation (50) remains valid even for $\rho<0$, but Eq. (51) must be replaced by another formula if $\rho<0$. On physical grounds, however, $\rho$ is usually expected to be positive, that is, $\omega'<\omega$. Figure 1 shows the numerical solution $\lambda_0$ of the equation

$$g(\beta,-\lambda_0)=0$$

for $\rho=0.1$. The function $g$ of Eq. (49) can be written as

$$g(\beta,\lambda)=C\left[1-\frac{\cosh\{(2-\rho)\lambda+\beta\}}{\cosh\{(2-\rho)\lambda_0-\beta\}}\right], \quad (52)$$

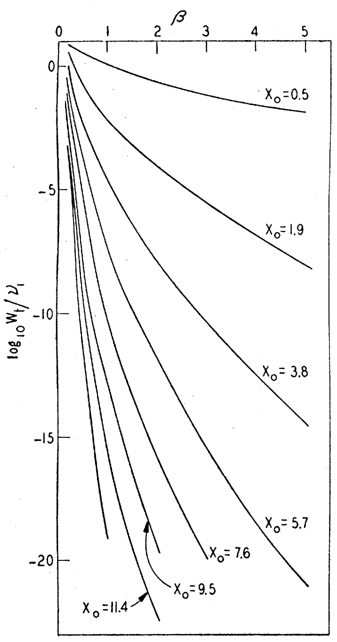

FIG. 2. Thermal ionization rates as functions of $\beta=\hbar\omega/kT$, calculated from Eq. (5.8) for some values of $x_0=\epsilon_0/\hbar\omega$, $\rho$ being assumed to be 0.1.

where

$$C=\frac{(2-\rho)^2}{4(1-\rho)}\cosh(\beta-\rho\lambda_0)-1. \tag{53}$$

If $\lambda_0 \gtrsim 1$, Eq. (52) can be approximated by

$$g(\beta,\lambda)=C[1-e^{-(2-\rho)(\lambda+\lambda_0)}], \tag{54}$$

for the domain $\Re\lambda \lesssim -\lambda_0$. Hence, the integral of Eq. (48) will be given approximately by

$$f_2(x)=Ce^{-\lambda_0 x}\sum_{n=0}^{\infty}(-)^n\binom{-5/2}{n}\delta\{x-(2-\rho)n\}, \tag{55}$$

which is obtained by making the transformation $(2-\rho)(\lambda+\lambda_0)=z$ and expanding $[g(\beta,\lambda)]^{-5/2}$, making use of Eq. (54).

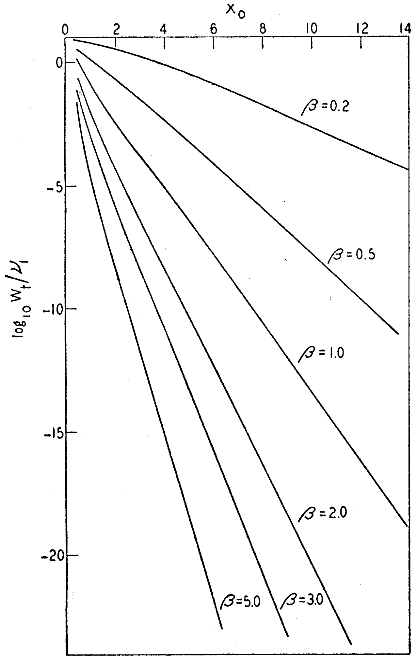

FIG. 3. Calculated rates of thermal ionization as functions of $x_0$ for some given values of $\beta$.

Inserting Eq. (55) into Eq. (46), we get an approximation for $F(x)$, which has positive values at $x=-1$, $1-\rho$, $3-2\rho$, $5-3\rho$, $\cdots$ and negative values at $x=-1+\rho$, $1$, $3-\rho$, $5-2\rho$, $\cdots$. As defined in Eq. (33), however, $F(x)$ must have only positive values. This contradiction arises from our approximation, so it is more reasonable to introduce another approximation of $F(x)$, with the required positive character, by adding the contributions from $x=(2n-1)-n\rho$ and $(2n-1)-(n-1)\rho$ to give $F(x)$ for $x=(2n-1)(1-\frac{1}{2}\rho)$. Thus a reasonable approximation for $F(x)$ will be

$$F(x)=\sum_{n=0}^{\infty}F_n\delta(x-a_n),\quad a_n=(2n-1)(1-\tfrac{1}{2}\rho),$$
$$n=0,1,2\cdots, \tag{56}$$

where

$$F_0=2^{5/2}(\sinh\tfrac{1}{2}\beta)^3C^{-5/2}\{(1-\rho)^{-\frac{1}{2}}e^{\beta}-(1-\rho)^{\frac{1}{2}}\},$$

$$F_n=2^{5/2}(\sinh\tfrac{1}{2}\beta)^3C^{-5/2}(-)^{n-1}\binom{-5/2}{n-1}e^{-\lambda_0(2-\rho)(n-1)}$$
$$\times[\{(1-\rho)^{\frac{1}{2}}-(1-\rho)^{-\frac{1}{2}}e^{-\beta}\}+(1+3/2n)$$
$$\times e^{-\lambda_0(2-\rho)}\{(1-\rho)^{-\frac{1}{2}}e^{\beta}-(1-\rho)^{\frac{1}{2}}\}]. \tag{57}$$

Eq. (56) gives the total rate $W_t(x_0)$ as

$$W_t(x_0)=\int_{x_0}^{\infty}W(x)dx$$
$$=\nu_1\sum_{a_n>x_0}F_n x_0^{5/2}(a_n-x_0)^{3/2}a_n^{-4}, \tag{58}$$

which converges rapidly for $\lambda_0 \gtrsim 1$. According to Eq. (58), $W_t(x_0)$ shows sudden decreases at the points $x_0=a_n$. This detailed behavior is not, however, particularly significant, because it originates from our approximations. The rigorous functions $W_t(x_0)$ will be much more complicated. So, rather arbitrarily, we calculate $W_t(x_0)$ for $x_0=0.5$, $1.9$, $3.8$, $\cdots 2n(1-\frac{1}{2}\rho)\cdots$ and replace $W_t(x_0)$ by a smoothed function. The results are shown in Fig. 2 and Fig. 3.

If $\beta$ is very small, $\lambda_0$ will be also small. In such cases $g(\beta,\lambda)$, Eq. (39), or (49), is approximated by

$$g(\beta,\lambda)=\tfrac{1}{2}\beta^2\{1-(2\rho/\beta)(1-\tfrac{1}{2}\rho)\lambda\}. \tag{59}$$

Thus, the integral of Eq. (48) turns out to be

$$f_2(x)=2^{5/2}\beta^{-5}\lambda_0^{5/2}x^{3/2}e^{-\lambda_0 x}/\Gamma(5/2), \tag{60}$$

where $\lambda_0$ is given by Eq. (51). Then Eqs. (46) and (47) give

$$F(x)=\frac{4}{\beta^2}\frac{\lambda_0^{5/2}}{\Gamma(5/2)}e^{-\lambda_0 x}\Big[(1-\rho)^{-\frac{1}{2}}\times\{(x+1)^{\frac{3}{2}}e^{\beta-\lambda_0}-(x-1)^{\frac{3}{2}}e^{-\beta+\lambda_0}\}+(1-\rho)^{\frac{1}{2}}\{(x-1+\rho)^{\frac{3}{2}}e^{\lambda_0(1-\rho)}-(x+1-\rho)^{\frac{3}{2}}e^{-\lambda_0(1-\rho)}\Big],$$

which, after neglecting $\rho$, is approximated by

$$F(x)=\frac{4}{\beta}\frac{\lambda_0^{5/2}e^{-\lambda_0(x-1)}}{\Gamma(5/2)}\{(x-1)^{\frac{3}{2}}+(x+1)^{\frac{3}{2}}e^{-2\lambda_0}\},\quad(61)$$

where the first term in the bracket should be put equal to zero for $x<1$ and the second term for $x<-1$.

The total rate $W_t(x_0)$ is then found to be

$$W_t(x_0)=\nu_1\int_{x_0}^{\infty}F(x)x_0^{5/2}(x-x_0)^{\frac{3}{2}}x^{-4}dx,\qquad(62)$$

which cannot be evaluated in a simple form. However, if $x_0$ is large, $W_t(x_0)$ is roughly approximated by

$$W_t(x_0)\simeq\nu_1(4/\beta)e^{-\lambda_0 x_0}\{(1-1/x_0)^{\frac{3}{2}}e^{\lambda_0}+(1+1/x_0)^{\frac{3}{2}}e^{-\lambda_0}\},\qquad(63)$$

and if $0<x_0<1$, it is approximated by

$$W_t(x_0)\sim(4\nu_1/\beta)[x_0^{5/2}(1-x_0)^{\frac{3}{2}}+(1+1/x_0)^{\frac{3}{2}}e^{-\lambda_0}].\qquad(64)$$

Equation (63) and Eq. (64) are not good for very small $\lambda_0$; but they should be correct, at least in order of magnitude, if $\lambda_0$ is not too small, that is, except for extremely high temperatures.

## IV. DISCUSSIONS

Our model is too simplified to apply quantitatively to any actual cases. However, it seems to have succeeded in clarifying some important features of the thermal ionization process, so it might be worth while to add some remarks here.

The most remarkable point is the behavior of $\lambda_0$ with changes in $\beta$ [Eqs. (50) and (51)]. As shown in Eqs. (57), (58), (61), (62), etc., $\lambda_0$ has a dominant effect on the rate $W_t$. If $\beta$ is large (and consequently $\lambda_0$ is large), Eq. (58) may be replaced by its first term, which may be simplified to read

$$W_t(x_0)\simeq4\nu_1\left[\frac{\rho}{2(1-\rho)^{\frac{1}{2}}}\right]^{x_0-1}e^{-\beta x_0}\simeq4\nu_1(\rho/2)^{\epsilon_0/\hbar\omega-1}e^{-\epsilon_0/kT},\qquad(65)$$

if we remember that $\beta$ is also large and use the approximation of Eq. (50). For small $\beta$, on the other hand, we can apply Eq. (51) so that the rate [see Eq. (63)] is dominated by the factor

$$W_t(x_0)\propto(4\nu_1/\beta)\exp\{-\beta x_0/(2\rho-\rho^2)\}=\frac{4\nu_1}{\beta}\exp\left\{-\frac{\epsilon_0}{2\rho-\rho^2}\Big/kT\right\}.\qquad(66)$$

Intermediate to these two extremes, $W_t(x_0)$ exhibits of course a more complicated behavior.

The simple results of (65) and (66) can be easily interpreted. Figure 4 shows the energy configuration diagram of our model. The energy factor of (65) is simply the excitation probability from the level $A$ to the level $B$. On the other hand, the entropy factor (or frequency factor) is governed by the square of the matrix element between two quantum states of oscillators with the difference of quantum numbers $x_0$ and with fractional difference $\rho$ of the proper frequencies, and is roughly proportional to $(\frac{1}{2}\rho)^{x_0-1}$.

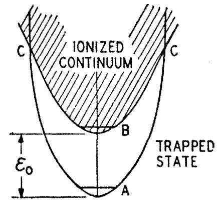

FIG. 4. The simplified model of adiabatic potentials assumed in this theory.

As shown in Fig. 4 the potential curve of our ground state crosses the continuum of ionized states at $C$, because we have assumed $\rho$ to be positive, which means that the curvature of the bottom of the continuum is smaller than that of the ground state. The energy of the intersection $C$ is just equal to

$$\epsilon^*=\frac{\omega^2}{\omega^2-\omega'^2}\epsilon_0=\frac{\epsilon_0}{2\rho-\rho^2}.\qquad(67)$$

Hence the expression (66) can be written as,

$$W_t\propto256(m/M)(kT/\hbar)e^{-\epsilon^*/kT},\qquad(68)$$

which is to be compared with

$$\begin{aligned}W_t&=\kappa(kT/h)e^{-\Delta F^{\ddagger}/kT}\\&=\kappa(kT/h)e^{\Delta S^{\ddagger}/k}e^{-\epsilon^*/kT},\end{aligned}\qquad(69)$$

a formula so well known that it is often considered universal. Equation (68) means that for high temperatures the transition may take place mostly over the activation states; this seems quite reasonable.[8]

However, it must be realized that we should be led to an erroneously small rate of thermal ionization by applying Eq. (68) or Eq. (69) at low temperatures. Actually, in such cases, transitions occur not by surmounting the potential barriers but through a quantum mechanical resonance, something like a tunnel effect.

It must be admitted here that our treatment is not

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[8] This fact can be established in general. A detailed discussion will be given in a later paper.

really satisfactory for the high temperature case. In fact, the simple assumptions of Eq. (16) and Eq. (17) cease to be valid for configurations where the atom moves beyond the cross points $C$, because there the ground level becomes higher than the lowest energy of free electron states, which means that the trapped state may cease to exist or at least it should be considered as a virtual state, something like that of a disintegrating $\alpha$-particle. In this sense the adiabatic potential $E_l'$ in (5) might be considered as a complex number, or we might add some term to the perturbation of Eq. (5) which would represent the instability of the ground state for large amplitudes of the atom. To be rigorous we must also be careful about the form of the wave functions. However, the writer prefers not to investigate these points at present, because such an investigation would inevitably introduce additional ambiguous assumptions.

In our theory, the rate of thermal ionization is governed essentially by the dependence of vibrational modes on the electronic states. As mentioned before, this idea is in sharp contrast to the theory of Goodman, Lawson, and Schiff.[4] The fractional change of frequency $\rho$, (40), is to be calculated from the quantum mechanical basis. Such a calculation, too ambitious for our simplified model, would be very important for a more quantitative theory. Hence we must content ourselves with a rough estimate. In $N$-type semiconductors of silicon and germanium, the impurity atom has one more electron than the atom of the mother crystal does. In this state we may suppose, as a crude approximation, that the bond degree between the impurity atom and its neighbors is 5/4. If we assume that the force constant of covalent bonds is proportional to the bond degree, the ratio of the vibrational frequencies of the central atom in the ground and in the ionized state will be $(5/4)^{\frac{1}{2}}$, which gives $\rho \approx 1-(4/5)^{\frac{1}{2}}=0.108$. This suggests that it is not unreasonable to assume $\rho$ to be the order of magnitude 0.1.

In Figs. 2 and 3 we have plotted $W_t(x_0)$ as a function of $x_0$ and $\beta$, where for illustration we chose arbitrarily $\rho=0.1$. It will be seen that we have the right to expect much larger rates of the thermal ionization process. $\nu_1$ is of the order of $10^{10}$ sec$^{-1}$, so taking $x_0=3$, $W_t$ will be $10^7$ sec$^{-1}$ for $\hbar\omega/kT=0.5$, $10^5$ sec$^{-1}$ for $\hbar\omega/kT\sim 1$, and $10^3$ sec$^{-1}$ for $\hbar\omega/kT\sim 2$. Of course these figures depend on $\rho$, but the effect of changing $\rho$ can easily be estimated from Eqs. (65) and (66).

Actually the wave function of the trapped electron is not so concentrated as assumed here, but it may extend over many atoms surrounding the impurity. This circumstance requires a generalization of the model to include many atoms, which might be very complicated.[7]

We have hitherto discussed only the direct transition from the ground state to the ionized states. There may be some excited states of trapped electrons. However, it is not clear at present whether such excited levels may play the role of a staircase for the liberation of the electron, and consequently result in an increase of the rate of ionization. Analogy to the theory of recombination in discharge processes will help in developing the theory in this direction. Unfortunately, however, the latter appears to be in a rather unsatisfactory state from a quantum mechanical point of view.

Finally, it seems necessary to add remarks about the role of the temperature radiation for the establishment of the equilibrium distribution of electrons. In fact one may expect it to be dominant in some cases. Let us consider the dipole transition of a hydrogen-like $1s$-state to a $2p$-state in a medium with dielectric constant $\kappa$ at temperature $T$. The transition probability is given by

$$w_{1s\rightarrow 2p}=0.94\times 10^9 \kappa^{-7/2}(e^{h\nu/kT}-1)^{-1}\ \text{sec}^{-1}, \tag{70}$$

where $h\nu$ is the energy of excitation, which has been assumed to be $(3/8)(e^2/\kappa^2 a_0)$, $a_0$ being the Bohr radius.

On the other hand, the total cross section of photoionization by light of frequency $\nu$ is given by

$$\phi=64\times 137^3 \kappa^{3/2}\phi_0(I/h\nu)^{7/2}, \tag{71}$$

if roughly estimated by the Born approximation, where $\phi_0$ is the classical cross section of an electron, that is, $6.5\times 10^{-25}$ cm$^2$. It should be mentioned here that the radiation field is considered, both in Eq. (70) and Eq. (71), as that with velocity $v=c/\sqrt{\kappa}$ instead of $c$. The total rate of photoionization caused by the temperature radiation is given by

$$W_{\text{rad}}=\int_{\nu=I/h}^{\infty}\phi(\nu)\frac{8\pi\nu^2 d\nu}{v^2(e^{h\nu/kT}-1)}, \tag{72}$$

which is roughly approximated by

$$W_{\text{rad}}\sim 1.5\times 10^{-16}\kappa^{5/2}(kT/\lambda_0^2 h)e^{-I/kT}, \tag{73}$$

if $I \gg kT$, and by

$$W_{\text{rad}}\lesssim 1.5\times 10^{-16}\kappa^{5/2}c^{-2}(kT/h)^3\times\text{const.}, \tag{74}$$

if $I \ll kT$. In Eq. (73) $\lambda_0$ is the maximum wavelength of the photoionization in vacuum, and the constant in (74) is the integral $\int_0^\infty x^2(e^x-1)^{-1}dx$.

These expressions should be compared with the ionization rate $W_t$ caused by the multiphonon jump discussed above. Generally speaking, the energy $I$ of photoionization may be different from $\epsilon_0$ for the thermal ionization, but in the case of nonpolar crystals these two may be considered as the same. For illustration, if we take $\kappa=16$, Eq. (73) or Eq. (74) gives $W_{\text{rad}}\sim 10^5$ sec$^{-1}$ at room temperatures. We cannot give any definite conclusion whether this rate will prevail in the multiphonon process, but it will be seen that this gives a lower limit for the relation frequency of germanium rectifiers. It should be noted that the high dielectric constant favors photoionization, through the increase of the cross section and also through the decrease of the ionization energy.

The excitation probability (70) also gives a pretty large rate for the numerical example above mentioned. It will be $\sim e^{-h\nu/kT}\times 10^5$ sec$^{-1}$, which is the order of $\sim 10^4$ sec$^{-1}$ at room temperatures. However, it seems likely that this process plays a more important role for low temperatures, $h\nu \gg kT$. If the rate of attaining equilibrium between the excited level and the ionized states is assumed to be much larger than that between the ground and the excited levels, the probability (70) is rate-determining, and it may compete with the multiphonon process, which depends in fact on the magnitudes of the photo-exciting energy and the thermal ionization energy and also on the magnitude of $\rho$, or more generally on the difference of vibrational modes in different electronic states.

However, it should be noticed that the rates caused by temperature radiation are very small if the excitation energy exceeds 1 ev or so. So we are forced to believe that the thermal excitation energies may sometimes be very small. For example, Dutton, Heller, and Maurer[9] took this point of view for the explanation of their experiment on KCl, which showed that free charges are liberated from $V_1$ and $F$ centers at $-132°$ in KCl crystals irradiated by x-rays at liquid nitrogen temperature. These authors concluded that the thermal ionization energy of $V_1$ is only one-tenth of its optical excitation energy, which seems somewhat surprising.

The writer wishes to suggest another possible explanation. In this kind of experiment it seems important to notice that the crystal is not in a state of thermal equilibrium, so that the relaxation process taking place in heating may possibly supply energy to liberate free charges from deep traps. To clarify these points, further experiments would be required.

This work was undertaken three years ago but has been completed during the author's visit in the United States. On this occasion, he wishes to express his gratitude for the opportunity to work for a year at the Institute for the Study of Metals of the University of Chicago. Also, he wishes to thank Professor M. Kotani of Tokyo University for his interest in this work.

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[9] Dutton, Heller, and Maurer, Phys. Rev. 84, 363 (1951).

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# Measurement of Neutron Densities with Crystals of NaI(Tl)

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Crystals of NaI(Tl) were irradiated in a nuclear reactor and the induced activity in sodium and iodine registered with a photomultiplier tube. It was found that an absolute measurement of the activities can be made in this way. Since sodium is an almost pure "one over $v$" absorber the neutron density can be determined from its activity.

Comparisons have also been made between the sodium and iodine cross sections for capture of thermal neutrons. With the sodium cross section equal to 0.47 barn, the cross section of iodine was found to be 5.00 barns.

WE consider an element with only one stable isotope which, after neutron capture, gives a radioactive isotope decaying with a single period. The number of radioactive nuclei formed when such an element is irradiated in a neutron flux will be

$$B=K\nu\cdot\int_0^\infty n(v)\cdot v\sigma(v)dv, \tag{1}$$

where

$$K=(1/\lambda)(1-e^{-\lambda t}). \tag{2}$$

$\lambda$ is the radioactivity constant of the isotope formed, $t$ the time of irradiation, $\nu$ the number of nuclei exposed to irradiation, $n(v)$ the neutron density as a function of neutron velocity, and $\sigma(v)$ the cross section of the stable isotope for neutron capture. In the region of thermal energies we shall usually have

$$\sigma(v)=(\sigma_0\cdot v_0/v), \tag{3}$$

with $v_0=2.2\cdot 10^5$ cm/sec and $\sigma_0$ the value of the cross section at this velocity. In the region above thermal energies there will often be one or more resonances, and we can put

$$\sigma(v)=(\sigma_0 v_0/v)+\sigma_r(v), \tag{4}$$

where $\sigma_r(v)$ stands for the pure resonance part of the cross section. It is assumed that all resonances are outside the thermal region, so that $\sigma_r(v)=0$ for all thermal velocities. We may then write

$$B=K\nu\sigma_0 v_0 N+K\nu\int_0^\infty n(v)v\sigma_r(v)dv, \tag{5}$$

where

$$N=\int_0^\infty n(v)dv. \tag{6}$$

If we work with a pure "one over $v$" absorber we can determine $N$, the total neutron density, from Eq. (5)