

Electron Capture by a Lattice Vacancy in Si

AKIRA MORITA*

Department of Physics, Purdue University, Lafayette, Indiana

(Received July 17, 1959)

The electron-capture cross section of the deep trap due to a lattice vacancy in Si is calculated by taking into account the distortion of the lattice vibrations by the lattice vacancy. It is assumed that the trap is a neutral center for electron capture. The results show that although the distortion effect enlarges the calculated cross section by three orders of magnitude at 300°K, it is not enough to explain the magnitudes of observed cross sections.

1. INTRODUCTION

THE appearance of some deep levels, as well as shallow levels, in Si and Ge bombarded by high-energy particles has been reported by many authors. These deep levels have been attributed to the presence of lattice vacancies, interstitial atoms, and clusters of these produced by bombardment. James and Lark-Horovitz¹ have proposed that an interstitial atom produces two donor levels and a lattice vacancy produces two acceptor levels, and have explained bombardment effects on Si and Ge. Coulson and Kearsley² have studied the electronic structure of an isolated vacancy in diamond crystals and have shown that color centers in irradiated diamonds are probably neutral isolated vacancies. Their result suggests that in Si and Ge a neutral isolated vacancy (V^0) may be more stable than a negatively ionized vacancy (V^-) plus a positive hole at the top of the valence band. Figure 1 shows this situation schematically. In the figure we have assumed that the energy difference between V^0 and V^- is less than the energy gap.

The deep traps produced by bombardment are responsible for recombination processes in bombarded Si and Ge. Wertheim³ has measured the lifetime of minority carriers in electron-bombarded Si, and has shown that for the trap level located at 0.16 eV below the conduction band, the capture cross sections at 300°K are

$$\sigma_p = 1.8 \times 10^{-15} \text{ cm}^2 \quad \text{and} \quad \sigma_n = 1.9 \times 10^{-15} \text{ cm}^2,$$

and for the trap level located at 0.27 eV above the

valence band,

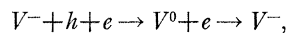
$$\sigma_p = 8.0 \times 10^{-13} \text{ cm}^2 \quad \text{and} \quad \sigma_n = 9.5 \times 10^{-15} \text{ cm}^2.$$

Curtis⁴ has performed the lifetime measurement on *n*-type Ge samples bombarded by 14-MeV neutrons and has shown that for the trap level located at 0.32 eV above the valence band, the capture cross sections at room temperature are

$$\sigma_p = 6 \times 10^{-15} \text{ cm}^2 \quad \text{and} \quad \sigma_n = 2.2 \times 10^{-17} \text{ cm}^2.$$

These recombination processes are expected to consist of captures by Coulomb attractive potential (probably with the larger cross sections) and by a neutral center. Because of the rather large cross sections of these traps, the possibility of Coulomb repulsive centers may be excluded.

The following tentative model is proposed for recombination mechanism in bombarded *n*-type Si and Ge; that is



where h and e stand for a free electron and a free hole. This is the simplest model compatible with considerations mentioned above. Now the following must be noted: The primary defects produced by bombardment may be vacancies, interstitial atoms and/or very close vacancy-interstitial pairs. It is not unlikely, however, that secondary annealing processes, the mechanisms of which have not yet been understood completely, have transformed these primary defects into more complicated ones. Even so, it seems desirable to obtain as much information as possible from the isolated vacancy model. One can then know how it could be improved.

The aim of the present paper is to investigate the capture cross section by such an isolated neutral vacancy in Si. Lax and Gummel⁵ have developed a general theory of thermal capture of electrons in nonpolar crystals and have applied it to calculate the capture cross section of deep levels in Si. They have found that the capture cross sections strongly depend on the effective mass of trapped electrons through the trapped state wave functions. The calculated cross sections are of order 10^{-27} cm^2 for $m^* = 0.38m_0$ to 10^{-20} cm^2 for

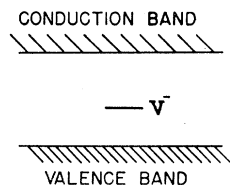


FIG. 1. Energy level of an isolated vacancy. The energy difference between the bottom of the conduction band and V^- gives the electron-ionization energy of a negatively ionized isolated vacancy. The energy difference between V^- and the top of the valence band gives the hole-ionization energy of a neutral isolated vacancy.

* On leave from the Department of Physics, Tohoku University, Sendai, Japan.

¹ H. M. James and K. Lark-Horovitz, *Z. physik Chem.* **198**, 107 (1951).

² C. A. Coulson and M. J. Kearsley, *Proc. Roy. Soc. (London)* **A241**, 433 (1957).

³ G. K. Wertheim, *Phys. Rev.* **105**, 1730 (1957); **110**, 1272 (1958); and **111**, 1500 (1958).

⁴ O. L. Curtis, Jr., *J. Appl. Phys.* **30**, 1174 (1959).

⁵ H. Gummel and M. Lax, *Ann. Phys.* **2**, 28 (1957).

$m^* = m_e$. These values are too small to explain the experimental results. Observed cross sections of deep traps in Si and Ge involving binding energies many times the Debye energy are in the range of 10^{-15} cm² to 10^{-13} cm² and those of neutral centers in the range of 10^{-17} cm² to 10^{-15} cm². The reason that they have obtained such small cross sections is as follows. As is mentioned by Lax,⁶ direct transition to the ground states of these traps requires simultaneous emission of many phonons. Such a probability is very small in these materials, where the interaction of electrons with lattice vibration is rather weak. Thus the calculated cross sections are smaller by five to ten orders of magnitude than the geometrical ones which are determined by the average radius of their ground-state wave functions and are of order 10^{-15} cm².

In order to explain such large observed cross section, Lax has introduced the idea of "giant traps." In his new model of giant traps he assumes the existence of many excited states of large orbit. Capturing to one of these excited states occurs initially and then a cascade process involving successive emission and absorption of single phonons follows until the electron enters the ground state or escapes. By taking into account this process, he has computed cross section comparable with the observed ones.

The existence of many excited states depends on the behavior of the potential associated with the trap. It is to be expected for traps with Coulomb attractive potential. However, we cannot always expect it for neutral traps. For such cases we must look for another kind of trapping mechanism.

As is shown by several authors,⁷⁻¹⁰ the introduction of a lattice defect such as a lattice vacancy, an interstitial atom, or a substitutional foreign atom into an otherwise perfect crystal distorts the normal modes of lattice vibrations. The lattice defects can also produce localized lattice vibrational modes under certain conditions. An electron trapped at a defect will have rather strong interaction with such distorted normal modes and localized modes, because these distortions are concentrated around the defect. Thus we can expect that the distortions produced by a lattice defect will have rather large influences on carrier capture by the defect. In the present paper we investigate such an effect for electron-capture by a lattice vacancy in Si.

In the next section we discuss the distortion of lattice vibrations produced by a lattice vacancy, by taking the rock-salt type crystal as an example. In Sec. 3 we calculate the electron capture cross section

of a lattice vacancy in Si by using the results obtained in Sec. 2.

2. LATTICE VIBRATION IN A CRYSTAL WITH A LATTICE VACANCY

Generally the equation of a lattice vibration in a perfect crystal is expressed by

$$\sum_{j, \mathbf{r}'} L_{\mathbf{r}\mathbf{r}'}^{ij} \chi^j(\mathbf{r}') - \omega^2 \chi^i(\mathbf{r}) = 0, \quad i, j = x, y, z, \quad (1)$$

or, in the matrix form, by

$$(L - \omega^2) \chi = 0, \quad (1')$$

where $\chi^i(\mathbf{r})$ means the i -component of the displacement of the atom relative to its equilibrium position \mathbf{r} and ω is the circular frequency of the normal lattice vibration, which is the eigenvalue of Eq. (1). As is well known, the eigenfunction (the normal lattice vibration) of (1) or (1') is given by

$$\chi = q_s(\boldsymbol{\tau}) U_{s\tau}(\mathbf{r}) = N^{-1/2} q_s(\boldsymbol{\tau}) e_s(\boldsymbol{\tau}) \exp i \boldsymbol{\tau} \cdot \mathbf{r}, \quad s = 1, \dots, 3n, \quad (2)$$

and its eigenvalue by

$$\omega_s^2(\boldsymbol{\tau}) = \sum_{j, \mathbf{r}'} L_{\mathbf{r}\mathbf{r}'}^{ij} U_s^j(\mathbf{r}') \{U_s^i(\mathbf{r})\}^{-1}, \quad (3)$$

where $q_s(\boldsymbol{\tau})$ and $e_s(\boldsymbol{\tau})$ are the complex amplitude and the unit polarization vector, respectively, of the s th normal mode of wave vector $\boldsymbol{\tau}$, which extends over the N values in the first Brillouin zone, and n the number of atoms in unit cell.

Now, let us consider an imperfect crystal which contains a single lattice vacancy and let us express the perturbing part to the equation of lattice vibration due to the lattice defect by Δ . Then we have, instead of (1'),

$$(L + \Delta - Z) \chi = 0, \quad (4)$$

where we put $\omega^2 = Z$. A solution of (4) in the continuous spectrum regions of (1) is given as the solution of the equation

$$\begin{aligned} \chi_{s,\tau} &= q_s(\boldsymbol{\tau}) U_{s,\tau}(\mathbf{r}) + \frac{1}{Z - L + i\epsilon} \Delta \chi_{s,\tau} \\ &= q_s(\boldsymbol{\tau}) U_{s,\tau}(\mathbf{r}) + i\pi \delta(Z - L) \Delta \chi_{s,\tau} + \frac{P}{Z - L} \Delta \chi_{s,\tau}, \end{aligned} \quad (5)$$

where $\delta(x)$ is Dirac's δ -function, ϵ is a infinitesimally small positive quantity, and P means that the principal value must be taken in each integration containing the operator $P(Z - L)^{-1}$.

Sometimes a lattice defect may produce localized modes of lattice vibration with new discrete frequencies outside the continuous spectrum regions. Such a localized mode, if any, is given as the solution of the equation

$$\chi = [1/(Z - L)] \Delta \chi, \quad (6)$$

where Z is outside the continuous spectrum regions.

We show two kinds of lattice defect in a two-dimensional rock-salt type crystal in Fig. 2, where the springs

⁶ M. Lax, *Proceedings of the International Conference on Semiconductors, Rochester, 1958* [J. Phys. Chem. Solids 8, 66 (1959)].

⁷ I. M. Lifshitz, Suppl. Nuovo cimento No. 3, 591 (1958).

⁸ Mazur, Montroll, and Potts, J. Wash. Acad. Sci. 46, 2 (1956).

⁹ E. W. Montroll and R. B. Potts, Phys. Rev. 100, 525 (1955); 102, 72 (1956).

¹⁰ Maradudin, Mazur, Montroll, and Weiss, Revs. Modern Phys. 30, 175 (1958).

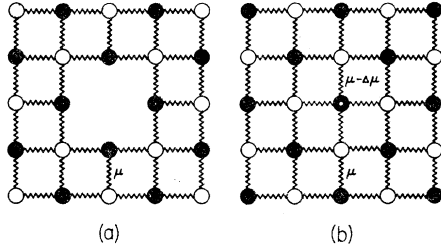


FIG. 2. Simplified models of lattice defects in a two dimensional rock-salt type crystal: (a) a lattice vacancy, (b) a substitutional impurity atom. Springs stand for central forces binding the nearest neighbors. In (a) all springs have the same force constant μ . In (b) springs binding the impurity atom with its nearest neighbors have the force constant $\mu - \Delta\mu$ and the rest have the force constant μ .

stand for the central forces binding nearest neighbors and μ for their force constant. Figure 2(a) shows a lattice vacancy and Fig. 2(b) the case in which the force constant between the atom under consideration and its nearest neighbors is reduced by $\Delta\mu$. We may consider that the behavior of lattice vibration around a lattice vacancy [Fig. 2(a)] is the same as that of Fig. 2(b) in which $\Delta\mu = \mu$. To be more exact, we must take into account the influences of binding forces between the atom under consideration and its more distant neighboring atoms. In a nonpolar crystal, however, such long range binding forces usually are weak. In what follows, therefore, we neglect them. Thus we may write down the matrix elements of Δ in a crystal with a lattice vacancy as

$$\begin{aligned} \Delta_{0,0}^{ii} &= -2\mu/M, & \Delta_{0,\alpha(i)}^{ii} &= \mu/M, \\ \Delta_{\alpha(i),\alpha(i)}^{ii} &= -\mu/M, & \Delta_{\alpha(i),0}^{ii} &= \mu/M, \text{ for } i=x, y, z, \end{aligned} \quad (7)$$

and otherwise

$$\Delta_{\mathbf{r},\mathbf{r}'}^{ii} = 0,$$

where the lattice vacancy is located at the origin and $\alpha(i)$ means the coordinate of the nearest neighbor site of the vacancy in the i -direction.

According to the investigations by Montroll and others, we may conclude that in the case of Fig. 2(b) localized modes do not appear, at least from acoustical modes. We are interested in thermal capture of a slow electron in a nonpolar crystal such as Si in which the interaction of a slow electron with acoustical longitudinal modes is most important. In such a case we need consider only the Eq. (5) for acoustical longitudinal modes.

Now let us define $\bar{\chi}_\tau$ by

$$\bar{\chi}_\tau = U_\tau + i\pi\delta(\omega^2 - L)\Delta\bar{\chi}_\tau, \quad (8)$$

namely

$$\bar{\chi}_\tau = \frac{1}{1 - i\pi\delta(\omega^2 - L)\Delta} U_\tau = \int f(\tau, \tau') \delta(\omega^2 - \omega'^2) U_{\tau'} d^3\tau', \quad (9)$$

where, as hereafter, we suppress the suffix s for the

acoustical longitudinal mode. We put

$$\chi_\tau/q_\tau = \bar{\chi}_\tau + \chi_\tau', \quad (10)$$

and substitute it into (5). Then we obtain

$$\chi_\tau' = A(\bar{\chi}_\tau + \chi_\tau') + B\chi_\tau', \quad (11)$$

where

$$A = P(\omega_\tau^2 - L)^{-1}\Delta \quad \text{and} \quad i\pi\delta(\omega_\tau^2 - L)\Delta = B. \quad (12)$$

From (11), we get

$$\chi_\tau' = \left(\frac{1}{1 - B - A} \right) A \bar{\chi}_\tau. \quad (13)$$

By neglecting higher order terms with respect to Δ in (13), we have

$$\chi_\tau/q_\tau = \int f(\tau, \tau') \delta(\omega_\tau^2 - \omega_{\tau'}^2) (1 + A) U_{\tau'} d^3\tau'. \quad (14)$$

Now let us introduce the quantities

$$\begin{aligned} B_{ab}^0 &= (\psi_a(\mathbf{r}) | \nabla \cdot U_\tau(\mathbf{r}) | \psi_b(\mathbf{r})), \\ B_{ab} &= (\psi_a(\mathbf{r}) | \nabla \cdot \chi_\tau(\mathbf{r})/q_\tau | \psi_b(\mathbf{r})), \\ B_{ab}' &= (\psi_a(\mathbf{r}) | \nabla \cdot (1 + A) U_\tau | \psi_b(\mathbf{r})), \\ B_{ab}'' &= (\psi_a(\mathbf{r}) | \nabla \cdot \bar{\chi}_\tau/q_\tau | \psi_b(\mathbf{r})), \end{aligned} \quad (15)$$

for convenience in the following calculations. When these B 's are independent of the direction of the vector τ ,¹¹ we get

$$B_{ab}(\tau) = B_{ab}'(\tau) \int f(\tau, \tau') \delta(\omega_\tau^2 - \omega_{\tau'}^2) d\tau' = g(\tau) B_{ab}'(\tau). \quad (16)$$

$g(\tau)$ is determined as follows. From (9) we have

$$\begin{aligned} B_{ab}^0(\tau) &= \int f(\tau, \tau') \delta(\omega_\tau^2 - \omega_{\tau'}^2) d\tau' \\ &= B_{ab}^0(\tau) \sum_{\tau'} [U_{\tau'}, (1 + B + B^2 + \dots) U_\tau]. \end{aligned} \quad (17)$$

If we put

$$\sum_{\tau'} (U_{\tau'}, B U_\tau) = i\alpha(\tau), \quad (18)$$

with a real quantity $\alpha(\tau)$, we can show

$$\sum_{\tau'} (U_{\tau'}, B^n U_\tau) = \{i\alpha(\tau)\}^n. \quad (19)$$

Substituting (19) into (17), we obtain

$$\int f(\tau, \tau') \delta(\omega_\tau^2 - \omega_{\tau'}^2) d^3\tau' = \frac{1}{1 + i\alpha(\tau)}. \quad (20)$$

¹¹ This is not the case. Strictly speaking, B 's depend on the crystallographic direction of τ , because Δ has the crystallographic symmetry of the crystal. However, the following calculation may be a good approximation for the averaged value of $B(\tau)$ with respect to the direction of τ .

$B_{ab}'(\tau)$ is expressed, with the term of B_{ab}^0 , by

$$B_{ab}'(\tau) = B_{ab}^0(\tau) \times \left(1 + \frac{N}{(2\pi)^3} \int \frac{(U_{\tau'}, \Delta U_{\tau})}{\omega_{\tau'}^2 - \omega_{\tau}^2} \frac{B_{ab}^0(\tau')}{B_{ab}^0(\tau)} d^3\tau' \right), \quad (21)$$

where the integration extends over the first Brillouin zone. Thus we can express $B_{ab}(\tau)$ with the term of $B_{ab}^0(\tau)$ by using (16), (18), (20), and (21). The integral in the right-hand side of (20) may seem to become infinity at $\omega^2=0$ and ω_m^2 which is the maximum circular frequency of the acoustical longitudinal modes. This is not the case, as shown in the following. If we define

$$j_{ab}(\omega^2, \tau) F(\omega^2) = \int (U_{\tau'}, \Delta U_{\tau}) \frac{B_{ab}^0(\tau')}{B_{ab}^0(\tau)} \delta(\omega^2 - \omega_{\tau'}^2) d^3\tau', \quad (22)$$

where $F(\omega^2)d\omega^2$ is the number of normal modes in the range between ω^2 and $\omega^2 + d(\omega^2)$. Then we can rewrite (21) as

$$B_{ab}'(\tau) = B_{ab}^0(\tau) \times \left[1 + j_{ab}(\omega_{\tau}^2, \tau') F(\omega_{\tau}^2) \ln \left(\frac{\omega_{\tau}^2}{\omega_m^2 - \omega_{\tau}^2} \right) + \int_0^{\omega_m^2} \frac{j_{ab}(\omega^2, \tau) F(\omega^2) - j_{ab}(\omega_{\tau}^2, \tau) F(\omega_{\tau}^2)}{\omega_{\tau}^2 - \omega^2} d(\omega^2) \right]. \quad (23)$$

We know that for a small value of ω^2

$$F(\omega^2) \propto \omega.$$

From the general property of the equation of lattice vibration, we can expect that

$$\omega_m^2 - \omega^2 \propto (\tau_m - \tau)^2,$$

near $\omega^2 = \omega_m^2$. This means that

$$F(\omega^2) \propto (\omega_m^2 - \omega^2)^{\frac{1}{2}},$$

near $\omega^2 = \omega_m^2$. Therefore, (23) does not contain any

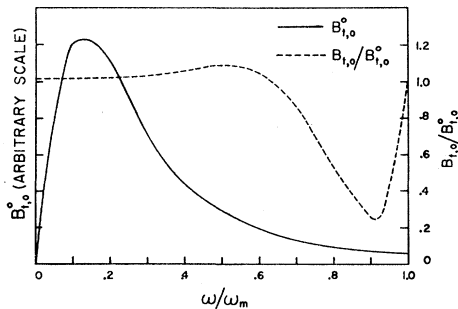


FIG. 3. Matrix element, B_{i0}^0 , and ratio, B_{i0}/B_{i0}^0 , are plotted against the reduced frequency.

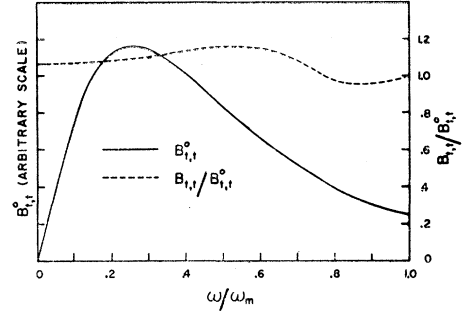


FIG. 4. Matrix element, B_{i1}^0 , and ratio, B_{i1}/B_{i1}^0 , are plotted against the reduced frequency.

difficulty of divergence at $\omega^2=0$ and ω_m^2 . However, it is usually very difficult to calculate the exact form of $F(\omega^2)$ from the equation of lattice vibration. In what follows, therefore, we use the Debye approximation to the lattice vibration except with the second term in the right-hand side of (23). In that term we use

$$F(\omega^2) = \frac{V}{(2\pi)^3} \frac{v^3}{-\omega}, \quad \text{for } \omega^2 < \omega_m^2/2$$

$$F(\omega^2) = \frac{V}{(2\pi)^3} \frac{v^3}{-(\omega_m^2 - \omega^2)^{\frac{1}{2}}}, \quad \text{for } \omega^2 > \omega_m^2/2, \quad (24)$$

where v is the sound velocity. Although this approximation is not so good for $\omega > \omega_m/2$, the error introduced by it is expected to be small. This is because, as will be shown in Figs. 3 and 4, the magnitude of $B_{ab}^0(\tau)$ is small in a region near $\omega = \omega_m$. This means the contributions for electron capture from this region are small.

In Figs. 3 and 4, we show the matrix elements B_{ab}^0 and B_{ab} as a function of $x = \omega/\omega_m$ when ψ_a is the electronic wave function of the trapped ground state or of the bottom of the conduction band and ψ_b that of the trapped ground state.¹²

3. CALCULATION OF CROSS SECTION

In this section we calculate the cross section of electron capture by a neutral lattice vacancy in Si according to the model mentioned in the preceding sections. Now we make the following assumptions to simplify the calculation without losing our physical picture.

(a) An unperturbed conduction electron is described by a plane wave with effective mass m^* :

$$\psi_{\mathbf{k}}(\mathbf{r}) = V^{-\frac{1}{2}} e^{i\mathbf{k} \cdot \mathbf{r}}, \quad E(\mathbf{k}) = (\hbar^2/2m^*)k^2; \quad (25)$$

that is, we assume the simple structure of the conduction band.

(b) We take a hydrogenic wave function as the unperturbed trapped state wave function.

$$\psi_t(r) = (\alpha^3/\pi)^{\frac{1}{2}} e^{-\alpha r}. \quad (26)$$

¹² For these electronic wave functions, see the next section.

As is shown by Lax and Gummel, the cross section of a deep trap strongly depends on the trapped state wave function. However, it is a very difficult problem to know the exact form of the potential associated with deep traps.¹³ Also we cannot expect that the effective mass approximation is good for deep traps. We are rather interested in knowing the relative change of the cross section by taking into account the distortion of the lattice vibration produced by a lattice vacancy.

(c) We assume that the distortion of the acoustical longitudinal modes produced around a lattice vacancy in Si is described by the results obtained in the preceding section, although a silicon is not a rock-salt type crystal.

(d) We assume that an electron interacts only with the longitudinal acoustic mode, and also that the deformation potential approximation is applicable to such an interaction.

In the following we consider two cases. In one of them, (I), we neglect the distortion of the normal modes of lattice vibration due to the lattice vacancy, but assume the same binding energy for the trapped electron as that in the case (II). In the other case, (II), we take into account the influence of the distortion of the normal modes on both the lattice relaxation energy and the capture process.

The Hamiltonian corresponding to the case (II) is

$$H = H_e + H_{\text{vib}} + H_{\text{int}},$$

$$H_{\text{vib}} = \sum_{\tau} \left(-\frac{\hbar^2}{2M} \frac{\partial^2}{\partial q_{\tau}^2} + \frac{1}{2} M \omega_{\tau}^2 q_{\tau}^2 \right), \quad (27)$$

$$H_{\text{int}} = E_1 \text{div} \sum_{\tau} \chi_{\tau}(r),$$

and

H_e = the electronic Hamiltonian.

Now according to Lax and Gummel, we can define ξ and λ , and also $f(\omega)$, $h(\omega)$, and $g(\omega)$ by using $B_{ab}(\tau)$ defined by (15).¹⁴ Then we define S_{II} by

$$\omega_0 = \int \omega' f(\omega') \exp(S_{\text{II}} \omega') d\omega' = \phi_{\text{II}}(S_{\text{II}}), \quad (28)$$

where $\hbar\omega_0$ is the thermal ionization energy of the trapped state, $\hbar\omega_i$, plus the energy of the conduction electron, $E(\mathbf{k})$.

Now let us put

$$E_{\text{II}}(\omega_0) = \omega_0 S_{\text{II}} - \int_0^{S_{\text{II}}} \phi_{\text{II}}(S') dS', \quad (29)$$

¹³ Strictly speaking, one should treat a neutral isolated vacancy as a four-electron system and a negatively ionized isolated vacancy as a five-electron system according to Coulson and Kearsley.

¹⁴ In the present paper we use the same notations as the Lax and Gummel paper as far as possible. We do not repeat the details of the calculation which are given in their paper.

and define

$$f_{ex}^{\text{II}}(\omega_0) = [2\pi d\phi_{\text{II}}(S)/dS]_{S=S_{\text{II}}} \exp[-E_{\text{II}}(\omega_0)]. \quad (30)$$

Then according to Lax and Gummel, the transition probability from a state k in the conduction band to the trapped state is given by

$$W_{t,k}^{\text{II}} = (2\pi/\hbar^2) f_{ex}^{\text{II}}(\omega_0) \left(\int_{-\omega_m}^{\omega_m} h(\omega) \exp(S_{\text{II}} \omega) d\omega + \left| \int_{-\omega_m}^{\omega_m} g(\omega) [\exp(S_{\text{II}} \omega) - 1] d\omega \right|^2 \right). \quad (31)$$

In case (I), by replacing B_{ab} with B_{ab}^0 and using the same ω_0 , we have, instead of (31),

$$W_{t,k}^{\text{I}} = (2\pi/\hbar^2) f_{ex}^{\text{I}}(\omega_0) \left(\int_{-\omega_m}^{\omega_m} h^0(\omega) \exp(S_{\text{I}} \omega) d\omega + \left| \int_{-\omega_m}^{\omega_m} g^0(\omega) [\exp(S_{\text{I}} \omega) - 1] d\omega \right|^2 \right), \quad (31')$$

where $h^0(\omega)$ and $g^0(\omega)$ represent the quantities defined by replacing B_{ab} with B_{ab}^0 in the expressions of $h(\omega)$ and $g(\omega)$, and S_{I} is defined by

$$\omega_0 = \int \omega' f^0(\omega') \exp(S_{\text{I}} \omega') d\omega' = \phi_{\text{I}}(S_{\text{I}}). \quad (28')$$

The capture cross section is given by

$$\sigma^{(\alpha)} = \frac{\int V W_{t,k}^{(\alpha)} \exp[-E(k)/k_0 T] d^3 k}{\int (\hbar k/m^*) \exp[-E(k)/k_0 T] d^3 k}, \quad \alpha = \text{I or II}. \quad (32)$$

In order to perform the integration in (32), we have to know the k -dependency of $W_{t,k}$. A k -dependency comes through the k -dependencies of ξ and λ which are rather weak and may be neglected. Another dependency comes from $\omega_0 = \omega_i + (1/\hbar)E(k)$. Thus we get

$$\sigma^{(\alpha)} \approx V W_{t,0}^{(\alpha)} (\pi^{\frac{1}{2}}/2) (m^*/2k_0 T)^{\frac{1}{2}} (1 + S_{\alpha} k_0 T/\hbar)^{-\frac{1}{2}}. \quad (33)$$

4. NUMERICAL RESULTS AND DISCUSSION

The numerical constants of Si used in our calculation are as follows. The sound velocity in Si is $v = 8.3 \times 10^5$ cm/sec. The constant measuring the strength of the interaction is $E_1 = 15$ eV. The mean effective mass of a conduction electron is $m^* = 0.25 m_e$.

Usually it is difficult to know the detailed behavior of the potential associated with deep traps. Also the effective mass approximation is not expected to be good approximation for the deep traps. This is the reason that we assume the hydrogenic wave function

for the trapped state. For the present, therefore, we do not have a reasonable way to determine the constant α . We tentatively take $1/\alpha=7$ a.u. and the thermal ionization energy $\hbar\omega_i=0.85$ ev.¹⁵ μ appearing in the expression of Δ is determined as follows. If one neglects long range forces, the relation between the compressibility β and the energy change produced by a volume change gives¹⁶

$$\mu/a=3\beta=C_{11}+2C_{12},$$

where a is the nearest neighbor distance and C_{11} and C_{12} the elastic constants, the observed values of which are 1.674×10^{12} dyne/cm² and 0.6523×10^{12} dyne/cm² respectively.

Using these numerical values, we got $\sigma^{(I)}\approx 10^{-23}$ cm² and $\sigma^{(II)}\approx 10^{-20}$ cm² at 300°K. This result shows that

¹⁵ This value is equal to the energy gap between the bottom of the conduction band and the trap level located at 0.27 ev above the valence band.

¹⁶ See, for example, F. Seitz, *Modern Theory of Solids* (McGraw-Hill Book Company, Inc., New York, 1940).

the distortion of the lattice vibration due to a lattice vacancy can enlarge the cross section by three orders of magnitude. Although the influence of the distortion of lattice vibration for the capture cross section is rather strong, it is not enough to explain the magnitudes of observed cross sections, which are of order 10^{-15} cm² to 10^{-17} cm². It thus appears that it may be possible to explain observed capture cross sections only by attributing to the deep traps a more complex structure than an isolated vacancy.

ACKNOWLEDGMENT

The present author wishes to express his cordial thanks to the late Professor K. Lark-Horovitz and Professor H. M. James for their hospitality at the Department of Physics, Purdue University. Thanks are also due to Professor James for many stimulating discussions and to Dr. B. V. Paranjape for his reading of the original manuscript. He also gratefully acknowledges the assistance of the Fulbright Commission during 1958-1959.

Low-Temperature Magnetic Remanence, Molecular Field, and Approach to Saturation of Holmium Metal

WARREN E. HENRY

United States Naval Research Laboratory, Washington, D. C.

(Received July 31, 1959)

Magnetization approaching absolute magnetic saturation has been achieved for polycrystalline holmium metal. At 1.3°K and 70 000 gauss, the magnetic moment is approaching 4.0 Bohr magnetons per atom of holmium in contrast to the 10 Bohr magnetons per atom expected on the basis of the spectroscopically determined quantum numbers. The actual results are explained on the basis of crystalline electric field splitting of the ground term of holmium and application of the Pauli exclusion principle. In the liquid helium range, there is a pronounced hysteresis; i.e., the moment at 10 000 gauss is 50% higher in decreasing fields than in increasing fields. The remanence is 0.22 Bohr magneton per atom of holmium at 4.2°K and 0.42 Bohr magneton per atom at 1.3°K. A sample motion technique was used to measure the magnetic moment of the 5-gram sample. The equipment was calibrated with iron and nickel.

INTRODUCTION

PREVIOUS magnetic studies on holmium metal have been carried out by Bommer¹ and by Rhodes, Legvold, and Spedding.² Bommer found that if he used the Curie-Weiss law

$$\chi=C/(T-\Delta), \quad (1)$$

with two adjustable parameters, C and Δ , he could fit his susceptibility data for 5 points (195°K, 294°K, 364°K, 428°K, and 515°K), but his 90°K point did not fit. Néel³ had been able to calculate the predicted Curie temperatures of the rare-earth elements from

the formula

$$\theta=16WS^2(J+1)/kJ, \quad (2)$$

where W is an interaction energy term, characteristic of rare earths, S the spin, J the total magnetic quantum number, and k the Boltzmann constant. This predicted value of θ is 86°K for holmium. Bommer found that if he took the Néel value for θ [Δ in Eq. (1)], he could fit his 5 points with a Curie constant, $C=14.3$. When Bommer used the formula

$$\mu=A[\chi(T-\Delta)]^{\frac{1}{2}}, \quad (3)$$

where A is $(3k)^{\frac{1}{2}}$, he calculated a moment of 10.6 Bohr magnetons. Rhodes, Legvold, and Spedding, applying Eq. (3) to low field susceptibility data in the high-temperature range, got μ_{eff} of 10.9 Bohr magnetons

¹ H. Bommer, *Z. anorg. u. allgem. Chem.* **242**, 277 (1939).

² Rhodes, Legvold, and Spedding, *Phys. Rev.* **109**, 1547 (1958).

³ L. Néel, *Compt. rend.* **206**, 49 (1938).