

## Theory of Electron Emission Widths\*

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An expression for the reduced width of an autoionizing level is derived using the  $R$ -matrix theory. The electron emission widths are calculated as a function of channel radius. It is shown that certain selection rules cause some of the partial widths to vanish. Thus, measurements can provide very useful information about the type of coupling. The electronic radial wave functions are obtained by a self-consistent-field calculation. The calculation also shows that the penetrability is not too sensitive to the change in atomic electrical polarizability and the core radius.

### I. INTRODUCTION

IT is well known in atomic spectroscopy that there are certain energy levels which lie above the ionization limit.<sup>1</sup> These discrete levels, because of the interaction with the states in the continuum, undergo spontaneous ionization. We are interested in calculating the widths of these autoionizing levels.

According to  $R$ -matrix theory<sup>2</sup> the partial width  $\Gamma_{\lambda c}$  for a particular energy level  $\lambda$  and decay mode  $c$  is given by the expression

$$\Gamma_{\lambda c} = 2P_c \gamma_{\lambda c}^2, \quad (1)$$

where  $P_c$  is a dimensionless quantity called the penetrability and  $\gamma_{\lambda c}^2$  is called the reduced width and has the dimensions of energy. We shall derive an expression for the reduced-width amplitude  $\gamma_{\lambda c}$  in Sec. II.

The details of the computer programs which are needed to obtain the numerical values of the partial widths  $\Gamma_{\lambda c}$  are given in a technical note.<sup>3</sup>

### II. DERIVATION OF THE EXPRESSION FOR THE REDUCED WIDTH AMPLITUDE

The derivation of the reduced-width amplitude will be carried out in  $L$ - $S$  coupling, which is valid for not too heavy atoms. We consider an atomic system having  $N+1$  electrons which breaks up into an electron-ion pair. Let the set of quantum numbers  $LSM_L M_S$  or  $LSJM$  label the energy states of the atom and let the primed set label the states of the residual system. Then the separate conservation of  $\mathbf{L}$  and  $\mathbf{S}$  gives the selection rules

$$\mathbf{S} = \mathbf{S}' + \frac{1}{2}, \quad \mathbf{L} = \mathbf{L}' + \mathbf{I}, \quad (2)$$

where  $\mathbf{I}$  is the orbital angular momentum quantum number of the outgoing electron. The conservation of  $\mathbf{J}$  gives the selection rule

$$\mathbf{J} = \mathbf{J}' + \mathbf{I} + \frac{1}{2}. \quad (3)$$

\* Research supported by the U. S. Atomic Energy Commission.  
<sup>1</sup> C. E. Moore, *Atomic Energy Levels* (U. S. Government Printing Office, Washington, D. C., 1949), U. S. Natl. Bur. Std. Circular 467, Vol. 1.

<sup>2</sup> A. M. Lane and R. G. Thomas, *Rev. Mod. Phys.* **30**, 257 (1958).

<sup>3</sup> Nazakat Ullah, Brookhaven National Laboratory Report BNL 79 (T-303), 1963 (unpublished).

We shall now construct the channel spin-wave function  $\psi_{cs\nu}$  of the  $R$ -matrix theory by vector coupling the wave function of the residual system  $|L'S'J'M'\rangle$  and the elementary spin function  $|\frac{1}{2}m_s\rangle$ .

$$\psi_{cs\nu} = \sum_{M'+m_s=\nu} (J'\frac{1}{2}M'm_s | s\nu) |L'S'J'M'\rangle |\frac{1}{2}m_s\rangle, \quad (4)$$

where the channel spin quantum number  $\mathbf{s} = \mathbf{J}' + \frac{1}{2}$  and  $\nu$  is its projection. The wave function  $|L'S'J'M'\rangle$  can be expressed as a linear combination of the wave functions  $|L'S'M_L M_S'\rangle$  as

$$|L'S'J'M'\rangle = \sum_{M_L'+M_S'=M'} (L'S'M_L M_S' | J'M') \times |L'S'M_L M_S'\rangle. \quad (5)$$

The channel surface wave functions  $\varphi_{csl\nu m}$  are defined as

$$\varphi_{csl\nu m} = r_c^{-1} \psi_{cs\nu} Y_l^m, \quad (6)$$

where  $r_c$  is the relative separation of the electron-ion pair and  $Y_l^m$  is a normalized spherical harmonic. The channel surface wave function in the  $sJM$  scheme is obtained by vector coupling  $\psi_{cs\nu}$  and  $Y_l^m$ . Using (4), (5), and (6),  $\varphi_{cslJM}$  can be written as

$$\begin{aligned} \varphi_{cslJM} = r_c^{-1} \sum_{\nu+m=M} \sum_{M'+m_s=\nu} \sum_{M_L'+M_S'=M'} (sl\nu m | JM) \\ \times (J'\frac{1}{2}M'm_s | s\nu) (L'S'M_L M_S' | J'M') \\ \times |L'S'M_L M_S'\rangle |\frac{1}{2}m_s\rangle Y_l^m. \end{aligned} \quad (7)$$

The wave function  $X_{\lambda JM}$  of  $(N+1)$  electrons can be written as a linear combination of the  $L$ - $S$  coupled wave functions  $|LSM_L M_S\rangle$  as

$$X_{\lambda JM} = \sum_{M_L+M_S=M} (LSM_L M_S | JM) |LSM_L M_S\rangle. \quad (8)$$

The reduced width amplitude  $\gamma_{\lambda c}$  is given by

$$\gamma_{\lambda c} = \left( \frac{\hbar^2}{2M_c a_c} \right)^{1/2} \int \varphi_c^* X_{\lambda JM} dS_c, \quad (9)$$

where  $M_c$  is the reduced mass,  $a_c$  the channel radius,  $dS_c$  is an element of channel surface, and  $\varphi_c$  denotes the channel surface wave function  $\varphi_{cslJM}$  which is properly antisymmetrized. To antisymmetrize  $\varphi_{cslJM}$ ,

given by (7), we assume that the outgoing  $(N+1)$ st electron is inequivalent to the remaining  $N$  electrons, and the wave function of  $N$  electrons  $|L'S'M_L'M_S'\rangle$  is already antisymmetric. By applying the antisymmetrizing operator  $A = [1/(N+1)^{1/2}] \sum_p (-1)^p P$  to expression (7), in which the permutation operator  $P$  permutes the  $(N+1)$ st electron with the remaining  $N$  electrons, we get the properly antisymmetrized channel surface wave function. We make a further simplifying assumption that the state of  $N$  electrons is not seriously distorted by the addition of the  $(N+1)$ st electron. Then the  $L$ - $S$  coupled wave function  $|LSM_L M_S\rangle$  of  $(N+1)$  electrons can be expressed in terms of the wave function  $|L'S'M_L'M_S'\rangle$  of  $N$  electrons and the wave function  $|l\frac{1}{2}mm_s\rangle$  of the  $(N+1)$ st electron. Therefore,  $X_{\lambda JM}$  can be written as

$$X_{\lambda JM} = \sum_{M_L+M_S=M} \sum_{M_L'+m=M_L} \sum_{M_S'+m_s=M_S} (LSM_L M_S | JM) \times (L' M_L' m | L M_L) (S' \frac{1}{2} M_S m_s | S M_S) A \times |L'S'M_L'M_S'\rangle |l\frac{1}{2}m m_s\rangle. \quad (10)$$

We need to evaluate the following integral:

$$\int A |L'S'M_L'M_S'\rangle |l\frac{1}{2}m_s\rangle Y_l^m A |L'S'M_L'M_S'\rangle \times |l\frac{1}{2}m m_s\rangle d\tau_1 \cdots d\tau_N, \quad (11)$$

where the integration is over the configuration space of  $N$  electrons. Since the antisymmetrizing operator  $A$  is self-adjoint, the integral (11) can be written as

$$\int |L'S'M_L'M_S'\rangle |l\frac{1}{2}m_s\rangle Y_l^m A^2 |L'S'M_L'M_S'\rangle \times |l\frac{1}{2}m m_s\rangle d\tau_1 \cdots d\tau_N.$$

Further,  $A^2 - (N+1)^{\frac{1}{2}} A = 0$ ; therefore, the above integral reduces to

$$(N+1)^{\frac{1}{2}} \int |L'S'M_L'M_S'\rangle |l\frac{1}{2}m_s\rangle Y_l^m A |L'S'M_L'M_S'\rangle \times |l\frac{1}{2}m m_s\rangle d\tau_1 \cdots d\tau_N.$$

If we also integrate over the angular coordinates of  $(N+1)$ st electron and use the orthogonality of  $N$ -electron functions, then this integral reduces to  $R_{N+1}(a_c)$ , where  $R_{N+1}(a_c)$  is the radial wave function of  $(N+1)$ st electron evaluated at the channel radius. Substituting the expressions for  $\varphi_c$  and  $X_{\lambda JM}$  in expression (9), replacing the integral by its value  $R_{N+1}(a_c)$ , and expressing the summation over magnetic quantum numbers in terms of Racah coefficients, we find

$$\gamma_{\lambda c} = \left(\frac{\hbar^2 a_c}{2M_c}\right)^{1/2} R_{N+1}(a_c) (-1)^{S+S'-s-J'} \times [(2J'+1)(2S+1)(2s+1)(2L+1)]^{1/2} \times W(L'S's\frac{1}{2}; J'S) W(SL'Jl; sL). \quad (12)$$

TABLE I. Parameters  $A_i, a_i$  for the basis orbitals  $\eta_i$ .

$\eta_i$	$l$	$A_i$	$a_i$ (a.u.)
$\eta_1$	0	0	7.658
$\eta_2$	0	1	2.995
$\eta_3$	0	1	1.497
$\eta_4$	0	2	1.800
$\eta_5$	0	2	0.900
$\eta_6$	1	0	2.968
$\eta_7$	1	0	1.484
$\eta_8$	1	1	1.800
$\eta_9$	1	1	0.900

III. ELECTRONIC RADIAL WAVE FUNCTIONS

The electronic radial wave functions  $R_{nl}(r)$  are obtained by a self-consistent-field calculation. The parameters in the radial wave functions are determined by a variational calculation, in which the radial wave functions  $R_{nl}(r)$  are expressed as a linear combination of basis orbitals  $\eta_i$

$$R_a = \sum_{i=1}^M X_{a_i} \eta_i, \quad (13)$$

where  $a$  is written for  $nl$ .

The orbitals  $\eta_i$  are of the form

$$\eta_i = r^{l+A_i} e^{-a_i r}, \quad (14)$$

where  $A_i$  is an integer and  $a_i$  a variable parameter. To determine these parameters for the unoccupied Hartree-Fock orbitals, the energy of the lowest excited state relative to the ground state is minimized. The various states of the atomic system having a definite value of  $L$  and  $S$  are constructed by the use of a projection operator technique.<sup>4</sup> The details of the self-consistent-field calculation and the various formulas for the evaluation of matrix elements of the Hamiltonian between Slater determinants are given by Nesbet.<sup>5</sup>

The numerical calculation is carried out for the oxygen atom. The lowest excited state  $^5S$  was constructed from the excited configuration  $(2p)^3(3s)$ . Its energy was minimized relative to the ground state  $^3P$  of the oxygen atom. The parameters for  $3s$  and  $3p$  electrons are shown in Table I, and the coefficients  $X$  are shown in Table II. Using these values the energy of the  $^5S$  excited state turns out to be  $84\,622.83\text{ cm}^{-1}$  compared to an experimental value of  $86\,625.35\text{ cm}^{-1}$ , and the energy of the  $^5P$  excited state turns out to be  $100\,400.85$

TABLE II. Coefficients  $X_{a_i}$  for  $3s$  and  $3p$  electrons.

$R_a$	$X_{a1}$	$X_{a2}$	$X_{a3}$	$X_{a4}$	$X_{a5}$
$3s$	0.05447	-0.34707	1.06127	-1.34775	1.25635
	$ X_{a6}$	$X_{a7}$	$X_{a8}$	$X_{a9}$	
$3p$	-0.61580	2.13333	-2.35741	1.30707	

<sup>4</sup> R. K. Nesbet, J. Math. Phys. 2, 701 (1961).

<sup>5</sup> R. K. Nesbet, Proc. Roy. Soc. (London) A230, 312 (1955).

$\text{cm}^{-1}$  compared to an experimental value of 86 625.35  $\text{cm}^{-1}$ .

#### IV. CALCULATION OF PENETRABILITY

The penetrability  $P_c$  is given by

$$P_c = \frac{kr}{F^2 + G^2} \Big|_{r=a_c}, \quad (15)$$

where  $k$  is the magnitude of the propagation vector in the c.m. system, and  $F, G$  are the two linearly independent solutions of the radial wave equation of the relative motion

$$\left\{ \frac{d^2}{dr_c^2} - \frac{l(l+1)}{r_c^2} - \frac{2M_c}{\hbar^2} [V(r_c) - E] \right\} U(r_c) = 0, \quad (16)$$

where  $V(r_c)$  is the electron-ion potential energy,  $E$  is the energy of the outgoing electron in the c.m. system, and  $U(r_c)$  is either  $F$  or  $G$ .

The regular solution  $F_l$  starts from zero at the origin and has the asymptotic form

$$F_l \xrightarrow{r \rightarrow \infty} \sin[kr - \gamma \ln 2kr + \eta_l - \frac{1}{2}l\pi], \quad (17)$$

where  $\gamma$  is the Coulomb parameter  $ZZ'e^2/\hbar v$ ,  $v$  being the relative velocity, and  $\eta_l$  the total phase shift. The irregular solution  $G_l$  is the solution which is  $\frac{1}{2}\pi$  out of phase with  $F_l$  at infinity. To get the values of  $F_l$  and  $G_l$ , Eq. (16) is integrated numerically. The logarithmic derivative of the inside solution is matched to that of the outside Coulomb solution at the boundary which determines the phase shift  $\eta_l$ .

We shall now calculate the electron-ion potential which is to be used in Eq. (16). The charge density for the ion can be written as

$$\rho(\mathbf{r}) = Ze\delta(\mathbf{r}) - \sum_{i=1}^{Z-1} eP_i(\mathbf{r}), \quad (18)$$

where  $Z$  is the atomic number,  $\delta(\mathbf{r})$  is the three-dimensional Dirac delta function, and  $P_i(\mathbf{r})$  is the probability density for the  $i$ th electron. It is given by

$$P_i(\mathbf{r}) = \int |\psi(\mathbf{r}_1, \dots, \mathbf{r}_{i-1}, \mathbf{r}, \mathbf{r}_{i+1}, \dots, \mathbf{r}_{Z-1})|^2 \times d\tau_1 \dots d\tau_{i-1} d\tau_{i+1} \dots d\tau_{Z-1}. \quad (19)$$

From (16) and (17) we get

$$\int \rho(\mathbf{r}) d^3r = e,$$

as it should be.

The potential  $\varphi(\mathbf{r})$  due to the ion at  $\mathbf{r}$  satisfies Poisson's equation

$$\nabla^2 \varphi = -4\pi\rho, \quad (20)$$

and is given by

$$\varphi(\mathbf{r}) = \int \frac{\rho(\mathbf{r}') d^3r'}{|\mathbf{r} - \mathbf{r}'|}. \quad (21)$$

Using (18) and expanding  $1/|\mathbf{r} - \mathbf{r}'|$ ,  $\varphi(\mathbf{r})$  can be written as

$$\varphi(\mathbf{r}) = \frac{Ze}{r} - e \sum_{i=1}^{Z-1} \sum_{k=0}^{\infty} \sum_{m=-k}^{+k} \frac{4\pi}{2k+1} Y_k^m(\theta, \varphi) \times \int \frac{r_{<}^k}{r_{>}^{k+1}} Y_k^{m*}(\theta', \varphi') P_i(\mathbf{r}') d^3r', \quad (22)$$

where  $r_{<}, r_{>}$  is the smaller or the larger of  $r, r'$ .

We now average  $\varphi(\mathbf{r})$  over the angles and simplify it using the determinantal functions. This gives the following expression for the electron-ion potential energy  $V(r)$ :

$$V(r) = -\frac{Ze^2}{r} + e^2 \sum_{i=1}^{Z-1} \left[ \frac{1}{r} \int_0^r |R_j(r')|^2 r'^2 dr' + \int_r^\infty |R_j(r')|^2 r' dr' \right] - \frac{\alpha}{2(r^2 + b^2)^2}, \quad (23)$$

where the last term is added to take into account the electrical polarization;  $\alpha$  is the polarizability and  $b$  is

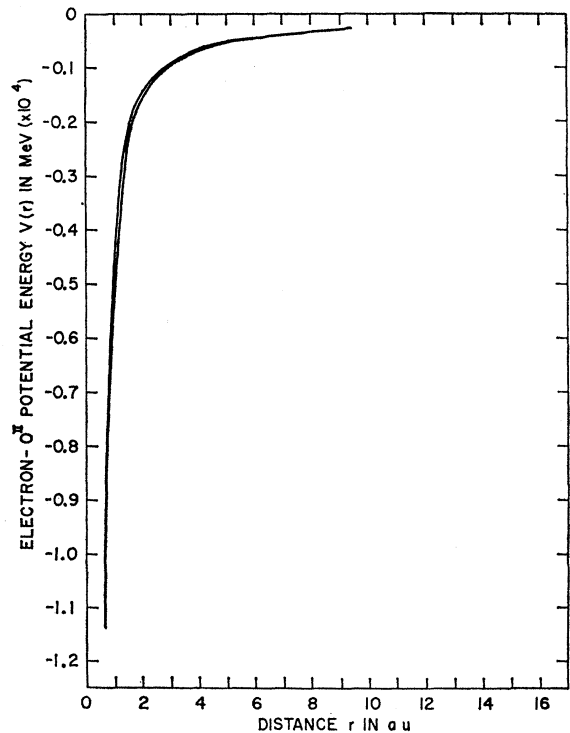


FIG. 1. Electron-Orbital potential energy  $V(r)$  as a function of  $r$ .  $\alpha$  is varied from 3.47 to 5.59 and  $b$  from 1.23 to 3.23 a.u. The values of  $V(r)$  for different sets of values of  $\alpha$  and  $b$  lie between the two curves shown in the figure.

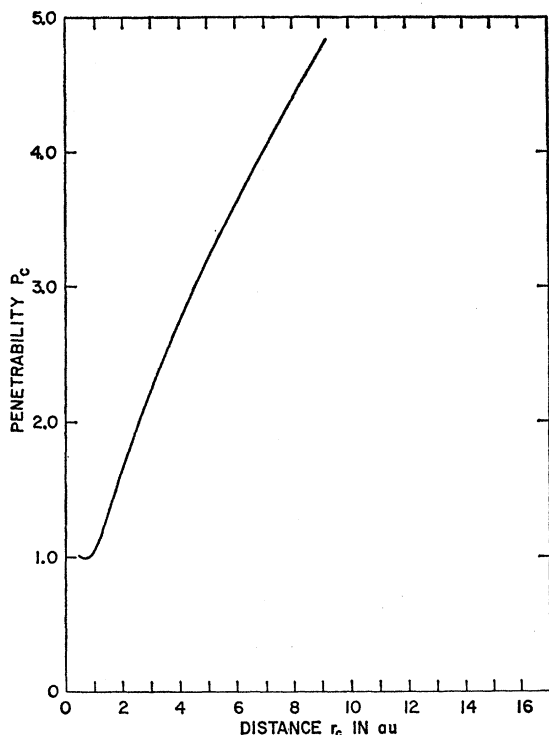


FIG. 2. Penetrability  $P_c$  versus separation distance  $r_c$ .  
 $\alpha = 3.47$   $b = 1.23$  a.u.

the core radius. To get a simpler expression for  $V(r)$ ,  $R_j(r')$ 's are replaced by approximate radial orbitals obtained by Slater's method.<sup>6</sup> Thus, for the  $e$ -OII system,  $V(r)$  can be written as

$$V(r) = -\frac{1}{r} - \frac{1}{r} (2e^{-15.4r} + 5e^{-4.9r}) - 15.4e^{-15.4r} - 1.02e^{-4.9r} \\ \times (18 + 29.4r + 24.01r^2) - \frac{\alpha}{2(r^2 + b^2)^2}, \quad (24)$$

where we have used atomic units (a.u.). One a.u. of energy = 27.210 eV and 1 a.u. of distance =  $5.292 \times 10^{-9}$  cm.

## V. RESULTS AND CONCLUSIONS

The potential energy  $V(r)$  calculated for various values of  $\alpha$  and  $b$  is shown in Fig. 1. These values were used in the ABACUS-2 code to print out the phase shifts and the numerical values of  $F_i$ . The values of the irregular function were obtained by a separate FORTRAN program. The numerical calculation shows that the penetrability  $P_c$  is not very sensitive to the values of  $\alpha$  and  $b$ . In subsequent calculations  $\alpha$  was taken to be 3.47 a.u. and  $b$  was taken to be 1.23 a.u. A plot of  $P_c$  for this set of values of  $\alpha$  and  $b$  is shown in Fig. 2 for  $p$  waves.

<sup>6</sup> H. Eyring, J. Walter, and G. Kimball, *Quantum Chemistry* (John Wiley & Sons, Inc., New York, 1957), p. 162.

TABLE III. Values of  $\Gamma_{\lambda c}$  as a function of channel radius  $a_c$ .

Kinetic energy of $3p$ electron (eV) $a_c$ (a.u.)	1.1865	2.8797	1.2978	1.1623	1.0709
	$\Gamma_{\lambda c}$ in eV				
1.228	0.4439	0.4294	0.4485	0.0298	0.3984
1.984	0.0274	0.0272	0.0280	0.0019	0.0247
2.740	1.5790	1.5773	1.5987	0.1059	1.4187
3.496	3.6534	3.6638	3.6666	0.2433	3.2755
4.252	3.9666	4.0222	3.9770	0.2637	3.5458
5.007	2.9686	3.0663	2.9992	0.1982	2.6485
5.763	1.7933	1.8859	1.8290	0.1204	1.5993
6.520	0.9471	1.0069	0.9702	0.0638	0.8452
7.275	0.4572	0.4879	0.4670	0.0307	0.4082
8.031	0.2066	0.2209	0.2096	0.0138	0.1843
8.787	0.0886	0.0952	0.0893	0.0059	0.0789

Because of the selection rules described in Sec. II, a number of levels which lie above the series limit in OI have zero width. Thus, all of the autoionizing levels which emit a  $3s$  electron have zero widths. The calculation shows that a number of excited states which are obtained from the configuration  $(2p)^3(3p)$  can emit a  $3p$  electron. The values of partial widths for these levels are obtained as a function of channel radius. These values are shown in Table III. The values of  $\Gamma_{\lambda c}$  continue to decrease with increasing channel radius, not shown in Table III. Figure 3 shows a plot of  $\Gamma_{\lambda c}$  as a function of channel radius  $a_c$  for the emission of a  $3p$  electron of kinetic energy 1.152 eV.

In  $R$ -matrix theory the channel radius is arbitrary, the only requirement being that it exceeds a certain minimum value. This undesirable aspect of the theory has been pointed out by Wigner.<sup>7</sup> For neutron emission a minimum value of the channel radius is taken to be the radius of the nuclear potential well. Lane<sup>8</sup> has used this value as the channel radius for the calculation of neutron emission widths and has discussed the errors arising because of the rather arbitrary choice of the channel radius. In case of electron emission widths, even the minimum value of the channel radius cannot be fixed as in the nuclear case. The problem of choosing an appropriate channel radius for electron emission is completely unsolved at present.

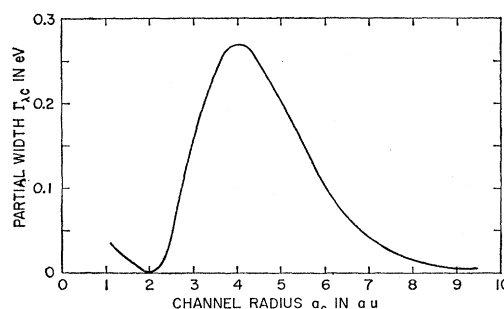


FIG. 3. Partial width  $\Gamma_{\lambda c}$  as a function of channel radius  $a_c$  for the emission of a  $3p$  electron of K.E. 1.162 eV.

<sup>7</sup> E. P. Wigner, Review of Collision Theory (to be published).

<sup>8</sup> A. M. Lane, Proc. Phys. Soc. (London) A66, 977 (1953).

The selection rules on  $L$  and  $S$  cause a number of partial widths to vanish. The measurements of these widths can therefore give information about the type of coupling.

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## Neutron Coherent-Scattering Amplitudes of Ga, In, As, and Sb†

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Neutron-diffraction data obtained from the compounds GaAs, GaSb, InAs, and InSb lead to the following neutron coherent-scattering amplitudes:  $f_{\text{Ga}} = (0.72 \pm 0.01) \times 10^{-12}$  cm,  $f_{\text{In}} = (0.39 \pm 0.01) \times 10^{-12}$  cm,  $f_{\text{As}} = (0.64 \pm 0.01) \times 10^{-12}$  cm, and  $f_{\text{Sb}} = (0.54 \pm 0.01) \times 10^{-12}$  cm. The data were also used to evaluate the Debye characteristic temperature for the compounds in use; the resulting Debye temperatures are 175°K for InSb, 240°K for InAs, 235°K for GaSb, and 247°K for GaAs. The neutron wavelength employed was 1.391 Å.

### I. INTRODUCTION

INFORMATION on neutron coherent-scattering amplitudes is still lacking for a few of the naturally occurring elements. The present experiment was instigated to determine the scattering amplitudes primarily of Ga and In. During the course of the experiment, it was discovered that In had been measured previously<sup>1</sup>; however, it is believed that the accuracy of the present result is an improvement over the earlier measurement. As a consequence of the particular compounds used in the measurements for Ga and In, values for the scattering lengths of Sb and As could also be determined. Measurements on the latter elements have been previously reported<sup>2</sup> but, again, the accuracy is somewhat better in the present experiment.

The intermetallic compounds, GaAs, GaSb, InAs, and InSb, were employed in the present measurements on account of their common cubic structure and their availability in semiconductor purity. The customary usage of the metal sesquioxides in this type of measurement was not employed in this instance on account of their more complex structure and unresolved diffraction patterns. Since the Sb and As scattering amplitudes are not known as accurately as that of O, two compounds of each element were used in order to improve the accuracy of the Ga and In measurements.

† Work performed under the auspices of the U. S. Atomic Energy Commission.

<sup>1</sup> S. S. Sidhu, L. Heaton, and M. H. Mueller, *J. Appl. Phys.* **30**, 1323 (1959).

<sup>2</sup> C. G. Shull and E. O. Wollan, *Phys. Rev.* **81**, 527 (1951).

### II. EXPERIMENTAL

The measurements were made on one of the neutron diffractometers at the Omega West Reactor. The neutron beam reflected from the (111) planes of a Pb monochromating crystal had a cross-sectional area of  $1\frac{1}{2} \times 1\frac{1}{2}$  in., an intensity of  $10^6$  neutrons/cm<sup>2</sup>-sec at the sample position, and a wavelength of 1.391 Å. The compounds were contained in a 3-in.-diam disk-type holder made of Ti-Zr alloy. The total wall thickness of the holder was 0.050 in. and the neutron transmission of the empty holder was 95%.

Pertinent physical data entering into subsequent calculations are given in Table I for each compound. The measured neutron transmissions given in Table I were obtained by placing the sample in the diffracted neutron beam from the (111) planes of a pressed nickel-powder sample; these measured values were used to determine the absorption correction for the samples. The calcu-

TABLE I. Physical data on samples used in the present experiment.

Compound	Theoretical density (gm/cm <sup>3</sup> )	Sample thickness (gm/cm <sup>2</sup> )	Measured transmission <sup>a</sup>	Calculated transmission <sup>a</sup>	Lattice constant (Å)
GaAs	5.37	1.03	0.87	0.88	5.636
GaSb	5.62	0.79	0.90	0.91	6.096
InAs	5.67	0.94	0.56	0.58	6.058
InSb	5.78	0.91	0.64	0.65	6.476

<sup>a</sup> These values include the Ti-Zr sample holder.