R. W. Keyes

Hydrogen-like Impurity States in Axially Symmetric Crystals

The ionization energies of donors and acceptors in germanium and silicon have been successfully interpreted on the basis of hydrogen-like models. In its simplest form such a model merely changes the potential energy from $(-q^2/r)$ to $(-q^2/Kr)$, where K is the dielectric constant, and replaces the electron mass by an effective mass.[1] Several authors have extended the hydrogen-like model to the case of an effective mass tensor which is anisotropic but has an axis of rotational symmetry.[2-4] Explicit results were given only for cases in which the longitudinal effective mass M_l is greater than the transverse effective mass M_t. In addition, the method has been applied only to cubic crystals, in which the dielectric constant, and consequently, the potential of a point charge, are isotropic. However, interest has recently developed in cases in which the crystal has only one axis of three- or four-fold rotational symmetry. These are $CdAs_2$, a tetragonal crystal, and *p*-type germanium and silicon elastically strained along a symmetry axis. In these cases the dielectric constant tensor $\mathbf{K}$ has the form

$$\mathbf{K}=\begin{vmatrix} K_1 & 0 & 0 \\ 0 & K_1 & 0 \\ 0 & 0 & K_3 \end{vmatrix}, \tag{1}$$

where coordinate z is the symmetry axis. They differ in one other matter of detail from those considered in the references[2-4]: although the effective mass tensors have an axis of rotational symmetry, the transverse mass is greater than the longitudinal mass. The purpose of this note is to extend the method of the references to take account of the anisotropy of the dielectric constant tensor and to present numerical results for the case in which the transverse mass is greater than the longitudinal mass.

The conditions which the potential of a point charge in an anisotropic crystal must satisfy are

$$\nabla\cdot\mathbf{K}\cdot\nabla\phi=0 \tag{2}$$

and

$$\int_S d\mathbf{S}\cdot\mathbf{K}\cdot\nabla\phi=4\pi q\,, \tag{3}$$

where $\mathbf{K}$ is the dielectric constant tensor and $\mathbf{S}$ is any closed surface containing the point charge q. It is easily verified that the solution of (1), (2), and (3) is

$$\phi=-\frac{q}{[K_1K_3(x^2+y^2)+K_1^2z^2]^{1/2}}\,.$$

Here we introduce the "transverse Rydberg," E_t, as unit of energy and a corresponding quantity, a_t, as unit of length:

$$E_t\equiv M_tq^4/2\hbar^2K_1K_3 \tag{4}$$

$$a_t\equiv(K_1K_3)^{1/2}\hbar^2/M_tq^2\,. \tag{5}$$

In the cases under consideration the symmetry axis of the effective mass tensor is the same as that of the dielectric constant tensor. The present method would be inapplicable if this were not the case. Thus the Hamiltonian takes the dimensionless form

$$H=-\frac{1}{2}\left[\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{M_t}{M_l}\frac{\partial^2}{\partial z^2}\right]-\frac{2}{[x^2+y^2+(K_1/K_3)z^2]^{1/2}}\,.$$

This Hamiltonian is not separable, and exact solutions of the equation $H\psi=E\psi$ have not been found. In the references quoted[2-4] the energy of the lowest state (and of some of the excited states) was found approximately by the variational method. The trial function used in the references is also suitable here. For the lowest state it is

$$\psi_0=\pi(a_\parallel a_\perp^2)^{-1/2}\exp\left[-\left(\frac{x^2+y^2}{a_\perp^2}+\frac{z^2}{a_\parallel^2}\right)^{1/2}\right].$$

The parameters $a_\perp$ and $a_\parallel$ are to be determined as those which minimize the calculated energy. It is convenient to introduce a parameter α defined by

$$a_\parallel=a_\perp(K_3/K_1)^{1/2}(1+\alpha^2)^{1/2}\,. \tag{6}$$

The calculated energy then comes out to be

$$E=\frac{1}{3a_\perp^2}\left[2+\frac{\omega}{1+\alpha^2}\right]-\frac{2}{a_\perp\alpha}\sinh^{-1}\alpha\,, \tag{7}$$

where $\omega\equiv(M_t/M_l)(K_1/K_3)$. The hyperbolic trigonometric function results when $\omega>1$. If $\omega<1$ the $\sinh^{-1}\alpha$ should be replaced by $\sin^{-1}\alpha$, and the results given in the references are applicable. The minimum occurs when α is related to ω by

$$\omega=2\left[\sinh^{-1}\alpha-\frac{\alpha}{(1+\alpha^2)^{1/2}}\right]\left[\frac{\alpha}{(1+\alpha^2)^{3/2}}-\frac{\sinh^{-1}\alpha}{(1+\alpha^2)^{3/2}}\right]^{-1} \tag{8}$$

Table 1 **Parameters of hydrogen-like states.**

Material	*Carrier*	$M_t, M_l/M_0$	$-E(ev)$	$a_\parallel(A)$	$a_\perp(A)$
$CdAs_2$	electrons	0.58, 0.15[b]	0.047	20	12
$CdAs_2$	holes	0.346, 0.094[b]	0.029	32	20
Si(001)[a]	holes	0.264, 0.196[c]	0.0224	28	25
Si(111)[a]	holes	0.401, 0.128[c]	0.0242	30	20

[a] Crystallographic orientation of the axis of strain.
[b] M. H. Stevenson, to be published.
[c] J. C. Hensel and G. Feher, *Phys. Rev. Letters* **5**, 307 (1960).

and $a_\perp$ has the value

$$a_\perp = \frac{1}{3}\left[2+\frac{\omega}{1+\alpha^2}\right]\left(\frac{\sinh^{-1}\alpha}{\alpha}\right)^{-1}. \qquad (9)$$

$a_\parallel$ can be found from Eq. (6) and E from Eq. (7). The values of E, $a_\perp$, and $(K_1/K_3)^{1/2}a_\parallel$ in the units defined by Eqs. (4) and (5) are plotted as functions of ω in Figure 1.

The results of the application of this method to $CdAs_2$ and elastically strained p-type silicon are given in Table 1. The anisotropy of **K** is not known in either of these cases, and the values $K_1=K_3=10.0$ for $CdAs_2$ (Ref. 5) and $K_1=K_3=12$ for silicon have been used. The anisotropy of K is probably small in strained silicon, but may be appreciable in $CdAs_2$.

References

1. H. C. Torrey and C. A. Whitmer, *Crystal Rectifiers,* McGraw-Hill, New York, 1948, p. 66.
2. C. Kittel and A. H. Mitchell, *Phys. Rev.* **96,** 1488 (1955).
3. M. Lampert, *Phys. Rev.* **97,** 352 (1955).
4. W. Kohn and J. Luttinger, *Phys. Rev.* **97,** 1721; **98,** 915 (1955).
5. W. Turner and W. Reese, private communication.

Received October 28, 1960

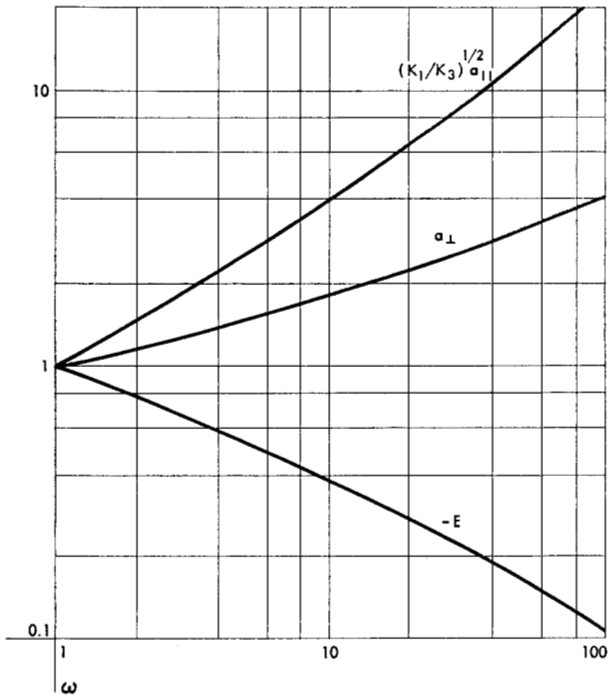

Figure 1 **Parameters of hydrogen-like states calculated according to Eqs. (6) to (9) in the units defined by Eqs. (4) and (5).**