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Shallow Donor Potential in Silicon

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The screened impurity potential of the shallow donor in Si, $\mathscr{V}_{\mathrm{d}}(\boldsymbol{r})$,[1] written as

$$\mathscr{V}_{\mathrm{d}}(\boldsymbol{r})=\int[v_{\mathrm{d}}(\boldsymbol{k})/\varepsilon(\boldsymbol{k})]\exp[-i\boldsymbol{k}\cdot\boldsymbol{r}]d\boldsymbol{k}/(2\pi)^3\,, \qquad (1)$$

where $v_{\mathrm{d}}(\boldsymbol{k})$ is the Fourier transform of the unscreened donor potential and $\varepsilon(\boldsymbol{k})$ is the wave-number-dependent dielectric function of Si. Recently, one of the present authors (H.N.) has investigated $\varepsilon(\boldsymbol{k})$ of semiconductors[2,3] and has found that the anisotropy of $\varepsilon(\boldsymbol{k})$ is not so serious. We also find that the inverse of the $\boldsymbol{k}$-dependent dielectric function of Si[2] is well approximated by the following spherical function (see Fig. 1(a)):

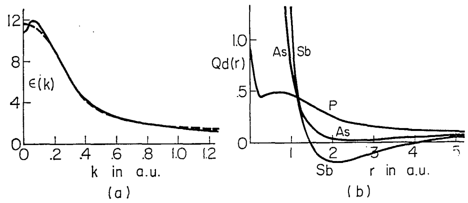

Fig. 1.(a) Isotropic dielectric function obtained by averaging $\varepsilon(\boldsymbol{k})$[2] over the directions of $\boldsymbol{k}$ (solid curve) and $\varepsilon(k)$ given by eq. (2) (dashed curve).
(b) $Q_{\mathrm{d}}(r)$ as a function of r for P, As and Sb donos in Si.

$$\left.\begin{aligned}&1/\varepsilon(k)=(Ak^2/k^2+\alpha^2)+(Bk^2/k^2+\beta^2)+(C\gamma^2/k^2+\gamma^2)\,,\\&\quad\alpha=0.7572,\ \beta=0.3123,\ \gamma=2.044\,,\\&\quad A=1.175,\ B=-0.175,\ C=1/\varepsilon^{(0)}=0.8547\,,\end{aligned}\right\} \qquad (2)$$

where $\varepsilon^{(0)}$ is the macroscopic dielectric constant of Si.

The unscreened potential $v_{\mathrm{d}}(\boldsymbol{r})$ due to the donor atom of Group V may be approximated by

$$v_{\mathrm{d}}(\boldsymbol{r})=V(\boldsymbol{r};Z_{\mathrm{d}}{}^{5+})-V(\boldsymbol{r};Z_{\mathrm{Si}}{}^{4+})\,, \qquad (3)$$

where $V(\boldsymbol{r};Z_{\mathrm{j}}{}^{n+})$ is the core potential of the free, n-fold ionized atom with atom number Z_{j} and is expressed to a good approximation as

$$V(\boldsymbol{r};Z_{\mathrm{j}}{}^{n+})=[n+(Z_{\mathrm{j}}-n)\exp(-\sigma_{\mathrm{j}}r)](-e^2/r)\,. \qquad (4)$$

Here σ_{j} is so determined as to give the best fit to the Hartree-Fock potential (see Table I).

Thus the screened donor potential is given by

Table I. Values of σ in atomic units (see eq. (4)).

Si^{4+}	P^{5+}	As^{5+}	Sb^{5+}
4.28	4.75	3.57	3.29

$$\mathscr{V}_d(r) \equiv (-e^2/r)Q_d(r) = (-e^2/r)\frac{2}{\pi}\int_0^\infty\left[\frac{1}{k^2}+\frac{Z_d-5}{k^2+\sigma_d^2}-\frac{Z_{Si}-4}{k^2+\sigma_{Si}^2}\right] \times\left[\frac{Ak^2}{k^2+\alpha^2}+\frac{Bk^2}{k^2+\beta^2}+\frac{C\gamma^2}{k^2+\gamma^2}\right]k\sin krdk\ , \tag{5}$$

and the results for P, As and Sb donors are shown in Fig. 1(b). As seen from the figure, the r-dependence of $Q_d(r)$ is rather complicated. In particular, $Q_{Sb}(r)$ becomes once negative and then approaches slowly to $1/\varepsilon^{(0)}$. This complicated behavior of $Q_d(r)$ comes from the dielectric screening effect on the core charge density, which is distributed over a small but finite range. This situation is demonstrated for a somewhat simplified case in what follows.

Let us consider as a model charge density of a donor atom in Si

$$\rho(r)=e[Z'\delta(r)-(Z'-1)\frac{\sigma^3}{8\pi}\exp(-\sigma r)]\ , \tag{6}$$

where $Z'=Z_d-Z_{Si}$ and σ is much larger than σ. As for $1/\varepsilon(k)$, we adopt the following simplification

$$1/\varepsilon(k)=(1/\varepsilon^{(0)})+(1-(1/\varepsilon^{(0)}))k^2/k^2+\alpha^2\ , \tag{7}$$

where α much is smaller than unity. This simplification may be allowed for the present purpose, since $A\cong1\gg|B|$, $\gamma^2\gg1$ and $\varepsilon^{(0)}\gg1$. Thus we have

$$\mathscr{V}_d(r)=(-e^2/r)\left\{\frac{1}{\varepsilon^{(0)}}\left[1+(Z'-1)\left(\frac{\sigma}{2}r+1\right)\exp(-\sigma r)\right]+\left(1-\frac{1}{\varepsilon^{(0)}}\right)\left[Z'-(Z'-1)\frac{\sigma^4}{(\sigma^2-\alpha^2)^2}\right]\exp(-\alpha r) +\left(1-\frac{1}{\varepsilon^{(0)}}\right)(Z'-1)\frac{\sigma^4}{(\sigma^2-\alpha^2)^2}\left[\frac{\sigma^2-\alpha^2}{2\sigma}r+1\right]\exp(-\sigma r)\right\}\ . \tag{8}$$

If the condition

$$Z'<(Z'-1)\sigma^4/(\sigma^2-\alpha^2)^2\ , \tag{9}$$

is satisfied, the second term in { } of (8) contributes to $Q_d(r)$ negatively. For a sufficiently heavy donor such that the condition (9) is easily satisfied, $Q_d(r)$ becomes negative for some range of r since the factor $\exp(-\sigma r)$ damps away faster than $\exp(-\alpha r)$ and $\varepsilon^{(0)}\gg1$.

The property of the screened impurity potential revealed in the present note plays the essential role in the theory of the shallow donor levels in Si. We have investigated the chemical shifts of the shallow donor levels in Si by using the donor potential (1), and the results will be published in a separate paper.[4]

References

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