7. Příměsové stavy - appendix pro Si:P

Rozbor vlivu symetrie krystalového pole na donorové stavy grupa (T_d)
Kohn-Luttinger, 1955

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Theory of Donor States in Silicon*

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By using the recently measured effective masses for *n*-type Si, $m_1=0.98\ m$ and $m_2=0.19$ m, approximate solutions of the resulting effective mass Schroedinger equation are obtained. The accuracy of the solutions was tested in the limiting cases where $m_2/m_1=1$ and 0 respectively. The nature of the resulting states and their degeneracy is discussed in some detail, taking into account the fact that the conduction band of Si has six equivalent minima. Experimentally measured ionization energies show that the effective mass theory is seriously in error in the case of the ground state. This error is attributed to failure of the effective mass theory near the donor nucleus, and allowance for this failure is made in the case of higher states. This leads finally to a theoretical spectrum for the electrons bound by P, As, or Sb donors.

Výsledek pro degeneraci nejnižších stavů:

TABLE II. Characters of tetrahedral point-group representations.

Representation \ Group element	E	$8C_3$	$3C_2$	$6\sigma_d$	$6S_4$
A_1	1	1	1	1	1
A_2	1	1	1	−1	−1
E	2	−1	2	0	0
T_1	3	0	−1	1	−1
T_2	3	0	−1	−1	1
$1s$	6	0	2	2	0

Comparison with the characters of the irreducible representations shows that $\{1s\}$ decomposes into

$$\{1s\}=A_1+E+T_1, \qquad (4.28)$$

Schéma energiových hladin a výsledky variačního výpočtu:

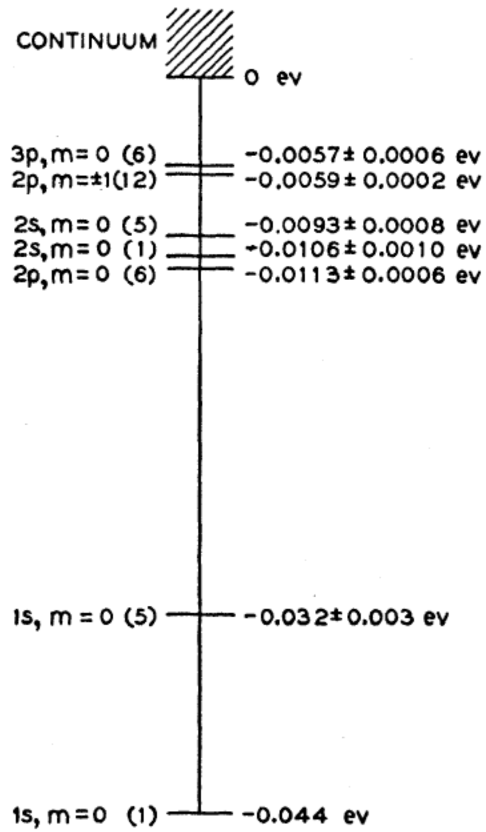


FIG. 3. Spectrum of bound states around a phosphorus-donor. Numbers in parentheses indicate number of approximately degenerate states; spin degeneracy is not included. See Table VII.

Podrobný popis výpočtů

6 ekvivalentních minim vodivostního pásu ve směru Δ v Brillouinově zóně;
stavové vektory elektronu v nich označíme symboly:

$|x\rangle$ pro minimum ve směru $[100]$,

$|y\rangle$ $[010]$,

$|z\rangle$ $[001]$,

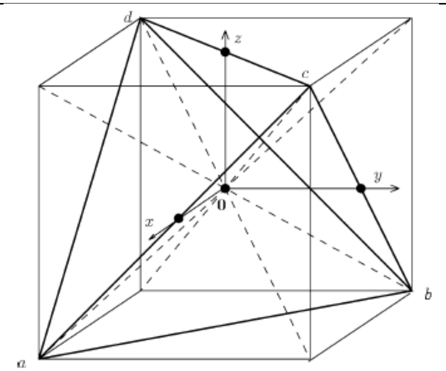
$|\bar{x}\rangle$ $[\bar{1}00]$,

$|\bar{y}\rangle$ $[0\bar{1}0]$,

$|\bar{z}\rangle$ $[00\bar{1}]$.

Umístění donorového atomu ve středu pravidelného čtyřstěnu je naznačeno v následujícím obrázku. Grupou symetrie je T_d (řádu 24) s třídami

E: identita,
$8C_3$: rotace kolem diagonál (čárkovaně),
$3C_2$: rotace kolem x,y,z,
$6S_4$: rotace kolem x,y,z o $\pm\pi/2$, pak inverze ($6IC_4$),
$6\sigma_d$: zrcadlení (diagonální roviny).



Pravidelný čtyřstěn s vrcholy abcd obsazenými atomy Si, ve středu O je donorový atom.

Aplikace operací symetrie T_d v šestirozměrném prostoru stavových vektorů

Tři operace C_2 (příspěvek do charakteru je 2 – je to počet vrcholů, které zůstávají na místě):

$$\begin{pmatrix}|x\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\\|\bar{x}\rangle\\|y\rangle\\|z\rangle\end{pmatrix}=C_{2x}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}=\begin{pmatrix}1&0&0&0&0&0\\0&0&0&0&1&0\\0&0&0&0&0&1\\0&0&0&1&0&0\\0&1&0&0&0&0\\0&0&1&0&0&0\end{pmatrix}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix},\quad \begin{pmatrix}|\bar{x}\rangle\\|y\rangle\\|\bar{z}\rangle\\|x\rangle\\|\bar{y}\rangle\\|z\rangle\end{pmatrix}=C_{2y}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}=\begin{pmatrix}0&0&0&1&0&0\\0&1&0&0&0&0\\0&0&0&0&0&1\\1&0&0&0&0&0\\0&0&0&0&1&0\\0&0&1&0&0&0\end{pmatrix}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix},\quad \begin{pmatrix}|\bar{x}\rangle\\|\bar{y}\rangle\\|z\rangle\\|x\rangle\\|y\rangle\\|\bar{z}\rangle\end{pmatrix}=C_{2z}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}=\begin{pmatrix}0&0&0&1&0&0\\0&0&0&0&1&0\\0&0&1&0&0&0\\1&0&0&0&0&0\\0&1&0&0&0&0\\0&0&0&0&0&1\end{pmatrix}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}.$$

Šest operací σ_d (příspěvek do charakteru je 2 – je to počet vrcholů, které zůstávají na místě):

$$\begin{pmatrix}|x\rangle\\|z\rangle\\|y\rangle\\|\bar{x}\rangle\\|\bar{z}\rangle\\|\bar{y}\rangle\end{pmatrix}=\sigma_{dx1}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}=\begin{pmatrix}1&0&0&0&0&0\\0&0&1&0&0&0\\0&1&0&0&0&0\\0&0&0&1&0&0\\0&0&0&0&0&1\\0&0&0&0&1&0\end{pmatrix}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix},\quad \begin{pmatrix}|x\rangle\\|\bar{z}\rangle\\|\bar{y}\rangle\\|\bar{x}\rangle\\|z\rangle\\|y\rangle\end{pmatrix}=\sigma_{dx2}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}=\begin{pmatrix}1&0&0&1&0&0\\0&0&0&0&0&1\\0&0&0&0&1&0\\0&0&0&1&0&0\\0&0&1&0&0&0\\0&1&0&0&0&0\end{pmatrix}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix},$$

$$\begin{pmatrix}|z\rangle\\|y\rangle\\|x\rangle\\|\bar{z}\rangle\\|\bar{y}\rangle\\|\bar{x}\rangle\end{pmatrix}=\sigma_{dy1}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}=\begin{pmatrix}0&0&1&0&0&0\\0&1&0&0&0&0\\1&0&0&0&0&0\\0&0&0&0&0&1\\0&0&0&0&1&0\\0&0&0&1&0&0\end{pmatrix}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix},\quad \begin{pmatrix}|\bar{z}\rangle\\|y\rangle\\|\bar{x}\rangle\\|z\rangle\\|\bar{y}\rangle\\|x\rangle\end{pmatrix}=\sigma_{dy2}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}=\begin{pmatrix}0&0&0&0&0&1\\0&1&0&0&0&0\\0&0&0&1&0&0\\0&0&1&0&0&0\\0&0&0&0&1&0\\1&0&0&0&0&0\end{pmatrix}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix},$$

$$\begin{pmatrix}|y\rangle\\|x\rangle\\|z\rangle\\|\bar{y}\rangle\\|\bar{x}\rangle\\|\bar{z}\rangle\end{pmatrix}=\sigma_{dz1}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}=\begin{pmatrix}0&1&0&0&0&0\\1&0&0&0&0&0\\0&0&1&0&0&0\\0&0&0&0&1&0\\0&0&0&1&0&0\\0&0&0&0&0&1\end{pmatrix}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix},\quad \begin{pmatrix}|\bar{y}\rangle\\|\bar{x}\rangle\\|z\rangle\\|y\rangle\\|x\rangle\\|\bar{z}\rangle\end{pmatrix}=\sigma_{dz2}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}=\begin{pmatrix}0&0&0&0&1&0\\0&0&0&1&0&0\\0&0&1&0&0&0\\0&1&0&0&0&0\\1&0&0&0&0&0\\0&0&0&0&0&1\end{pmatrix}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}.$$

Osm operací C_3 (příspěvek do charakteru je 0 – je to počet vrcholů, které zůstávají na místě):

(rotace kolem *Oc*)

$$\begin{pmatrix}|z\rangle\\|x\rangle\\|y\rangle\\|\bar{z}\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\end{pmatrix}=C_{3c}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}=\begin{pmatrix}0&0&1&0&0&0\\1&0&0&0&0&0\\0&1&0&0&0&0\\0&0&0&0&0&1\\0&0&0&1&0&0\\0&0&0&0&1&0\end{pmatrix}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}\ ,\ C_{3c}^2=\begin{pmatrix}0&1&0&0&0&0\\0&0&1&0&0&0\\1&0&0&0&0&0\\0&0&0&0&1&0\\0&0&0&0&0&1\\0&0&0&1&0&0\end{pmatrix}\ ,$$

(rotace kolem *Od*)

$$\begin{pmatrix}|z\rangle\\|\bar{x}\rangle\\|y\rangle\\|\bar{z}\rangle\\|x\rangle\\|\bar{y}\rangle\end{pmatrix}=C_{3d}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}=\begin{pmatrix}0&0&1&0&0&0\\0&0&0&1&0&0\\0&1&0&0&0&0\\0&0&0&0&0&1\\1&0&0&0&0&0\\0&0&0&0&1&0\end{pmatrix}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}\ ,\ C_{3d}^2=\begin{pmatrix}0&1&0&0&0&0\\0&0&0&0&0&1\\0&0&0&1&0&0\\0&0&0&0&1&0\\0&0&1&0&0&0\\1&0&0&0&0&0\end{pmatrix}\ ,$$

(rotace kolem *Oa*)

$$\begin{pmatrix}|\bar{z}\rangle\\|z\rangle\\|\bar{x}\rangle\\|y\rangle\\|x\rangle\\|\bar{y}\rangle\end{pmatrix}=C_{3a}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}=\begin{pmatrix}0&0&0&0&0&1\\0&0&1&0&0&0\\0&0&0&1&0&0\\0&1&0&0&0&0\\1&0&0&0&0&0\\0&0&0&0&1&0\end{pmatrix}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}\ ,\ C_{3a}^2=\begin{pmatrix}0&0&0&0&1&0\\0&0&0&1&0&0\\0&1&0&0&0&0\\0&0&1&0&0&0\\0&0&0&0&0&1\\1&0&0&0&0&0\end{pmatrix}\ ,$$

(rotace kolem *Ob*)

$$\begin{pmatrix}|z\rangle\\|\bar{z}\rangle\\|\bar{y}\rangle\\|y\rangle\\|x\rangle\\|\bar{x}\rangle\end{pmatrix}=C_{3b}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}=\begin{pmatrix}0&0&1&0&0&0\\0&0&0&0&0&1\\0&0&0&0&1&0\\0&1&0&0&0&0\\1&0&0&0&0&0\\0&0&0&1&0&0\end{pmatrix}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}\ ,\ C_{3b}^2=\begin{pmatrix}0&0&0&0&1&0\\0&0&0&1&0&0\\1&0&0&0&0&0\\1&0&0&0&0&0\\0&0&1&0&0&0\\0&1&0&0&0&0\end{pmatrix}\ ,$$

Šest operací S_4 (příspěvek do charakteru je 0 – je to počet vrcholů, které zůstávají na místě):

(rotace kolem x o π/2, pak I)

$$\begin{pmatrix} |\bar{x}\rangle \\ |z\rangle \\ |\bar{y}\rangle \\ |x\rangle \\ |\bar{z}\rangle \\ |y\rangle \end{pmatrix} = S_{4x+} \begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \\ |\bar{x}\rangle \\ |\bar{y}\rangle \\ |\bar{z}\rangle \end{pmatrix} = \begin{pmatrix} 0&0&0&1&0&0 \\ 0&0&0&0&1&0 \\ 0&0&0&0&0&1 \\ 1&0&0&0&0&0 \\ 0&1&0&0&0&0 \\ 0&0&1&0&0&0 \end{pmatrix} \begin{pmatrix} 1&0&0&0&0&0 \\ 0&0&0&0&0&1 \\ 0&1&0&0&0&0 \\ 0&0&0&1&0&0 \\ 0&0&1&0&0&0 \\ 0&0&0&0&1&0 \end{pmatrix} \begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \\ |\bar{x}\rangle \\ |\bar{y}\rangle \\ |\bar{z}\rangle \end{pmatrix} = \begin{pmatrix} 0&0&0&1&0&0 \\ 0&0&1&0&0&0 \\ 0&0&0&0&1&0 \\ 1&0&0&0&0&0 \\ 0&0&0&0&0&1 \\ 0&1&0&0&0&0 \end{pmatrix} \begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \\ |\bar{x}\rangle \\ |\bar{y}\rangle \\ |\bar{z}\rangle \end{pmatrix},$$

(rotace kolem x o -π/2, pak I)

$$\begin{pmatrix} |\bar{x}\rangle \\ |\bar{z}\rangle \\ |y\rangle \\ |x\rangle \\ |z\rangle \\ |\bar{y}\rangle \end{pmatrix} = S_{4x-} \begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \\ |\bar{x}\rangle \\ |\bar{y}\rangle \\ |\bar{z}\rangle \end{pmatrix} = \begin{pmatrix} 0&0&0&1&0&0 \\ 0&0&0&0&1&0 \\ 0&0&0&0&0&1 \\ 1&0&0&0&0&0 \\ 0&1&0&0&0&0 \\ 0&0&1&0&0&0 \end{pmatrix} \begin{pmatrix} 1&0&0&0&0&0 \\ 0&0&1&0&0&0 \\ 0&0&0&0&1&0 \\ 0&0&0&1&0&0 \\ 0&0&0&0&0&1 \\ 0&1&0&0&0&0 \end{pmatrix} \begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \\ |\bar{x}\rangle \\ |\bar{y}\rangle \\ |\bar{z}\rangle \end{pmatrix} = \begin{pmatrix} 0&0&0&1&0&0 \\ 0&0&0&0&0&1 \\ 0&1&0&0&0&0 \\ 1&0&0&0&0&0 \\ 0&0&1&0&0&0 \\ 0&0&0&0&1&0 \end{pmatrix} \begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \\ |\bar{x}\rangle \\ |\bar{y}\rangle \\ |\bar{z}\rangle \end{pmatrix},$$

(rotace kolem y o π/2, pak I)

$$\begin{pmatrix} |\bar{z}\rangle \\ |\bar{y}\rangle \\ |x\rangle \\ |z\rangle \\ |y\rangle \\ |\bar{x}\rangle \end{pmatrix} = S_{4x+} \begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \\ |\bar{x}\rangle \\ |\bar{y}\rangle \\ |\bar{z}\rangle \end{pmatrix} = \begin{pmatrix} 0&0&0&1&0&0 \\ 0&0&0&0&1&0 \\ 0&0&0&0&0&1 \\ 1&0&0&0&0&0 \\ 0&1&0&0&0&0 \\ 0&0&1&0&0&0 \end{pmatrix} \begin{pmatrix} 0&0&1&0&0&0 \\ 0&1&0&0&0&0 \\ 0&0&0&1&0&0 \\ 0&0&0&0&0&1 \\ 0&0&0&0&1&0 \\ 1&0&0&0&0&0 \end{pmatrix} \begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \\ |\bar{x}\rangle \\ |\bar{y}\rangle \\ |\bar{z}\rangle \end{pmatrix} = \begin{pmatrix} 0&0&0&0&0&1 \\ 0&0&0&0&1&0 \\ 1&0&0&0&0&0 \\ 0&0&1&0&0&0 \\ 0&1&0&0&0&0 \\ 0&0&0&1&0&0 \end{pmatrix} \begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \\ |\bar{x}\rangle \\ |\bar{y}\rangle \\ |\bar{z}\rangle \end{pmatrix},$$

(rotace kolem y o -π/2, pak I)

$$\begin{pmatrix} |z\rangle \\ |\bar{y}\rangle \\ |\bar{x}\rangle \\ |\bar{z}\rangle \\ |y\rangle \\ |x\rangle \end{pmatrix} = S_{4x-} \begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \\ |\bar{x}\rangle \\ |\bar{y}\rangle \\ |\bar{z}\rangle \end{pmatrix} = \begin{pmatrix} 0&0&0&1&0&0 \\ 0&0&0&0&1&0 \\ 0&0&0&0&0&1 \\ 1&0&0&0&0&0 \\ 0&1&0&0&0&0 \\ 0&0&1&0&0&0 \end{pmatrix} \begin{pmatrix} 0&0&0&0&0&1 \\ 0&1&0&0&0&0 \\ 1&0&0&0&0&0 \\ 0&0&1&0&0&0 \\ 0&0&0&0&1&0 \\ 0&0&0&1&0&0 \end{pmatrix} \begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \\ |\bar{x}\rangle \\ |\bar{y}\rangle \\ |\bar{z}\rangle \end{pmatrix} = \begin{pmatrix} 0&0&1&0&0&0 \\ 0&0&0&0&1&0 \\ 0&0&0&1&0&0 \\ 0&0&0&0&0&1 \\ 0&1&0&0&0&0 \\ 1&0&0&0&0&0 \end{pmatrix} \begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \\ |\bar{x}\rangle \\ |\bar{y}\rangle \\ |\bar{z}\rangle \end{pmatrix},$$

(rotace kolem z o π/2, pak I)

$$\begin{pmatrix}|y\rangle\\|\bar{x}\rangle\\|\bar{z}\rangle\\|\bar{y}\rangle\\|x\rangle\\|z\rangle\end{pmatrix}=S_{4z+}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}=\begin{pmatrix}0&0&0&1&0&0\\0&0&0&0&1&0\\0&0&0&0&0&1\\1&0&0&0&0&0\\0&1&0&0&0&0\\0&0&1&0&0&0\end{pmatrix}\begin{pmatrix}0&0&0&0&1&0\\1&0&0&0&0&0\\0&0&1&0&0&0\\0&1&0&0&0&0\\0&0&0&1&0&0\\0&0&0&0&0&1\end{pmatrix}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}=\begin{pmatrix}0&1&0&0&0&0\\0&0&0&1&0&0\\0&0&0&0&0&1\\0&0&0&0&1&0\\1&0&0&0&0&0\\0&0&1&0&0&0\end{pmatrix}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix},$$

(rotace kolem z o -π/2, pak *I*)

$$\begin{pmatrix}|\bar{y}\rangle\\|x\rangle\\|\bar{z}\rangle\\|y\rangle\\|\bar{x}\rangle\\|z\rangle\end{pmatrix}=S_{4z-}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}=\begin{pmatrix}0&0&0&1&0&0\\0&0&0&0&1&0\\0&0&0&0&0&1\\1&0&0&0&0&0\\0&1&0&0&0&0\\0&0&1&0&0&0\end{pmatrix}\begin{pmatrix}0&1&0&0&0&0\\0&0&0&1&0&0\\0&0&1&0&0&0\\0&0&0&0&1&0\\1&0&0&0&0&0\\0&0&0&0&0&1\end{pmatrix}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}=\begin{pmatrix}0&0&0&0&1&0\\1&0&0&0&0&0\\0&0&0&0&0&1\\0&1&0&0&0&0\\0&0&0&1&0&0\\0&0&1&0&0&0\end{pmatrix}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix},$$

Rozklad 6-rozměrné reducibilní reprezentace:

$R_6 = A_1 + E + T_2$.

Table A.32. Character table for group T_d (cubic)[a]

T_d ($\bar{4}3m$)		E	$8C_3$	$3C_2$	$6\sigma_d$	$6S_4$
$x^2+y^2+z^2$	A_1	1	1	1	1	1
	A_2	1	1	1	−1	−1
$(x^2-y^2, 3z^2-r^2)$	E	2	−1	2	0	0
(R_x, R_y, R_z) } $yz, zx, xy)$	T_1	3	0	−1	−1	1
(x, y, z)	T_2	3	0	−1	1	−1

[a] Note that (yz, zx, xy) transforms as representation T_1

	E	$8C_3$	$3C_2$	$6\sigma_d$	$6S_4$
R_6	6	0	2	2	0
$R_6 - A_1$	5	-1	1	1	-1
$R_6 - A_1 - E$	3	0	-1	1	-1
T_2	3	0	-1	1	-1

Prověříme, že stavové vektory z následujícího přehledu jsou bázemi odpovídajících ireducibilních reprezentací grupy T_d:

$$A_1:\ (|x\rangle+|\bar{x}\rangle+|y\rangle+|\bar{y}\rangle+|z\rangle+|\bar{z}\rangle)/\sqrt{6}\ ,$$
$$E:\ (|x\rangle+|\bar{x}\rangle-|y\rangle-|\bar{y}\rangle)/2\ ,\ (|x\rangle+|\bar{x}\rangle+|y\rangle+|\bar{y}\rangle-2|z\rangle-2|\bar{z}\rangle)/\sqrt{12}\ ,$$
$$T_2:\ (|x\rangle-|\bar{x}\rangle)/\sqrt{2}\ ,\ (|y\rangle-|\bar{y}\rangle)/\sqrt{2}\ ,\ (|z\rangle-|\bar{z}\rangle)/\sqrt{2}\ .$$

A_1 triviální.

E:
Tři operace C_2:

$$\begin{pmatrix}|x\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\\|\bar{x}\rangle\\|y\rangle\\|z\rangle\end{pmatrix}=C_{2x}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}\ ,\ \begin{pmatrix}|\bar{x}\rangle\\|y\rangle\\|\bar{z}\rangle\\|x\rangle\\|\bar{y}\rangle\\|z\rangle\end{pmatrix}=C_{2y}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}\ ,\ \begin{pmatrix}|\bar{x}\rangle\\|\bar{y}\rangle\\|z\rangle\\|x\rangle\\|y\rangle\\|\bar{z}\rangle\end{pmatrix}=C_{2z}\begin{pmatrix}|x\rangle\\|y\rangle\\|z\rangle\\|\bar{x}\rangle\\|\bar{y}\rangle\\|\bar{z}\rangle\end{pmatrix}\ ,$$

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$$\begin{pmatrix}|x\rangle+|\bar{x}\rangle-|y\rangle-|\bar{y}\rangle\\|x\rangle+|\bar{x}\rangle+|y\rangle+|\bar{y}\rangle-2|z\rangle-2|\bar{z}\rangle\end{pmatrix}=C_{2x}\begin{pmatrix}|x\rangle+|\bar{x}\rangle-|y\rangle-|\bar{y}\rangle\\|x\rangle+|\bar{x}\rangle+|y\rangle+|\bar{y}\rangle-2|z\rangle-2|\bar{z}\rangle\end{pmatrix}=\begin{pmatrix}1&0\\0&1\end{pmatrix}\begin{pmatrix}|x\rangle+|\bar{x}\rangle-|y\rangle-|\bar{y}\rangle\\|x\rangle+|\bar{x}\rangle+|y\rangle+|\bar{y}\rangle-2|z\rangle-2|\bar{z}\rangle\end{pmatrix}\ ,$$

$$\begin{pmatrix}|x\rangle+|\bar{x}\rangle-|y\rangle-|\bar{y}\rangle\\|x\rangle+|\bar{x}\rangle+|y\rangle+|\bar{y}\rangle-2|z\rangle-2|\bar{z}\rangle\end{pmatrix}=C_{2y}\begin{pmatrix}|x\rangle+|\bar{x}\rangle-|y\rangle-|\bar{y}\rangle\\|x\rangle+|\bar{x}\rangle+|y\rangle+|\bar{y}\rangle-2|z\rangle-2|\bar{z}\rangle\end{pmatrix}=\begin{pmatrix}1&0\\0&1\end{pmatrix}\begin{pmatrix}|x\rangle+|\bar{x}\rangle-|y\rangle-|\bar{y}\rangle\\|x\rangle+|\bar{x}\rangle+|y\rangle+|\bar{y}\rangle-2|z\rangle-2|\bar{z}\rangle\end{pmatrix}\ ,$$

$$\begin{pmatrix} |x\rangle+|\bar{x}\rangle-|y\rangle-|\bar{y}\rangle \\ |x\rangle+|\bar{x}\rangle+|y\rangle+|\bar{y}\rangle-2|z\rangle-2|\bar{z}\rangle \end{pmatrix} = C_{2z}\begin{pmatrix} |x\rangle+|\bar{x}\rangle-|y\rangle-|\bar{y}\rangle \\ |x\rangle+|\bar{x}\rangle+|y\rangle+|\bar{y}\rangle-2|z\rangle-2|\bar{z}\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} |x\rangle+|\bar{x}\rangle-|y\rangle-|\bar{y}\rangle \\ |x\rangle+|\bar{x}\rangle+|y\rangle+|\bar{y}\rangle-2|z\rangle-2|\bar{z}\rangle \end{pmatrix} ,$$

Šest operací σ_d:

$$\begin{pmatrix} |x\rangle \\ |z\rangle \\ |y\rangle \\ |\bar{x}\rangle \\ |\bar{z}\rangle \\ |\bar{y}\rangle \end{pmatrix} = \sigma_{dx1}\begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \\ |\bar{x}\rangle \\ |\bar{y}\rangle \\ |\bar{z}\rangle \end{pmatrix} , \begin{pmatrix} |x\rangle \\ |\bar{z}\rangle \\ |\bar{y}\rangle \\ |\bar{x}\rangle \\ |z\rangle \\ |y\rangle \end{pmatrix} = \sigma_{dx2}\begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \\ |\bar{x}\rangle \\ |\bar{y}\rangle \\ |\bar{z}\rangle \end{pmatrix} , \begin{pmatrix} |z\rangle \\ |y\rangle \\ |x\rangle \\ |\bar{z}\rangle \\ |\bar{y}\rangle \\ |\bar{x}\rangle \end{pmatrix} = \sigma_{dy1}\begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \\ |\bar{x}\rangle \\ |\bar{y}\rangle \\ |\bar{z}\rangle \end{pmatrix} , \begin{pmatrix} |\bar{z}\rangle \\ |y\rangle \\ |\bar{x}\rangle \\ |z\rangle \\ |\bar{y}\rangle \\ |x\rangle \end{pmatrix} = \sigma_{dy2}\begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \\ |\bar{x}\rangle \\ |\bar{y}\rangle \\ |\bar{z}\rangle \end{pmatrix} , \begin{pmatrix} |y\rangle \\ |x\rangle \\ |z\rangle \\ |\bar{y}\rangle \\ |\bar{x}\rangle \\ |\bar{z}\rangle \end{pmatrix} = \sigma_{dz1}\begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \\ |\bar{x}\rangle \\ |\bar{y}\rangle \\ |\bar{z}\rangle \end{pmatrix} , \begin{pmatrix} |\bar{y}\rangle \\ |\bar{x}\rangle \\ |z\rangle \\ |y\rangle \\ |x\rangle \\ |\bar{z}\rangle \end{pmatrix} = \sigma_{dz2}\begin{pmatrix} |x\rangle \\ |y\rangle \\ |z\rangle \\ |\bar{x}\rangle \\ |\bar{y}\rangle \\ |\bar{z}\rangle \end{pmatrix} .$$

tedy

$$\frac{1}{2}\begin{pmatrix} |x\rangle+|\bar{x}\rangle-|z\rangle-|\bar{z}\rangle \\ (|x\rangle+|\bar{x}\rangle+|z\rangle+|\bar{z}\rangle-2|y\rangle-2|\bar{y}\rangle)/\sqrt{3} \end{pmatrix} = \sigma_{dx1}\frac{1}{2}\begin{pmatrix} |x\rangle+|\bar{x}\rangle-|y\rangle-|\bar{y}\rangle \\ (|x\rangle+|\bar{x}\rangle+|y\rangle+|\bar{y}\rangle-2|z\rangle-2|\bar{z}\rangle)/\sqrt{3} \end{pmatrix}$$

$$= \begin{pmatrix} 1/2 & \sqrt{3}/2 \\ 1/2\sqrt{3} & -1/2 \end{pmatrix}\frac{1}{2}\begin{pmatrix} |x\rangle+|\bar{x}\rangle-|y\rangle-|\bar{y}\rangle \\ (|x\rangle+|\bar{x}\rangle+|y\rangle+|\bar{y}\rangle-2|z\rangle-2|\bar{z}\rangle)/\sqrt{3} \end{pmatrix} ,$$

atd.

Experimentální přiřazení infračervené absorpce přechodům mezi donorovými stavů, obsahuje také snížení symetrie jednoosým tlakem:

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Optical Determination of the Symmetry of the Ground States of Group-V Donors in Silicon*

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Excitation lines from the doublet, $1s(E)$, and the triplet, $1s(T_1)$, states have been measured at temperatures ~80, 59, and 30°K for P, As, and Sb donors in silicon. On the basis of the relative intensities of the lines with the same final state it is deduced that the $1s(E)$ state lies above the $1s(T_1)$ state for all three impurities investigated. At ~30°K the $1s(T_1) \rightarrow 2p_0, 2p_\pm$ transitions for antimony impurity resolved into a doublet. Uniaxial stress measurements for P and Sb, with compression **F** parallel to [100] or [110] and with the electric vector **E** either parallel or perpendicular to **F**, indicate that the lines with $1s(T_1)$ as their initial state do not exhibit any splittings or shift in their energies. On the other hand, the lines with $1s(E)$ as their initial state exhibit splittings with dichroic features. Experimental observations of the number and the positions of the stress-induced components and their polarization characteristics are consistent with the ordering in which $1s(E)$ lies above $1s(T_1)$.

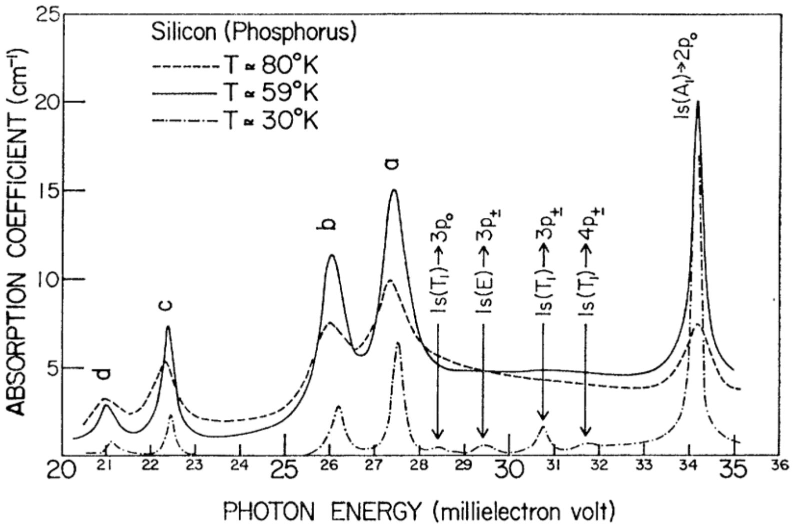


FIG. 1. Excitation spectrum of phosphorus donors in silicon. $N_D \simeq 5.2 \times 10^{15}$ cm^{-3}. At $\sim 30°$K the peak of the line $1s(A_1) \rightarrow 2p_0$ could not be located since, for the sample used, the transmission was very low.

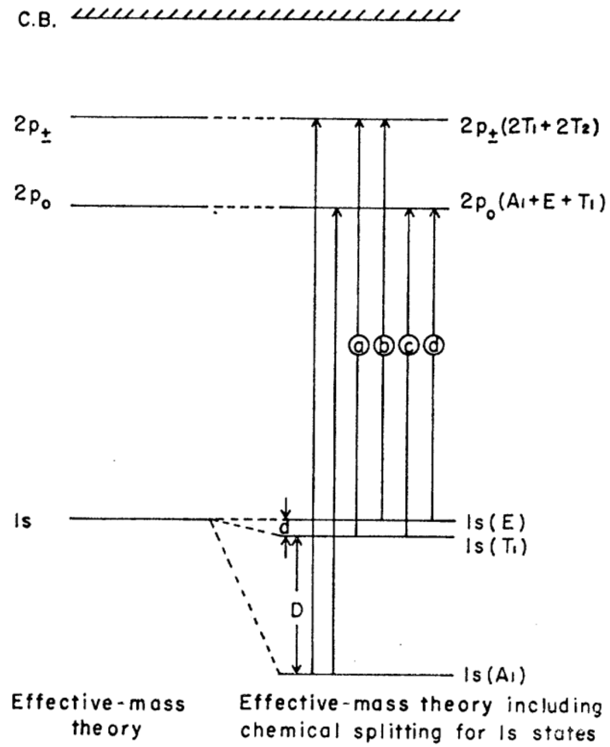
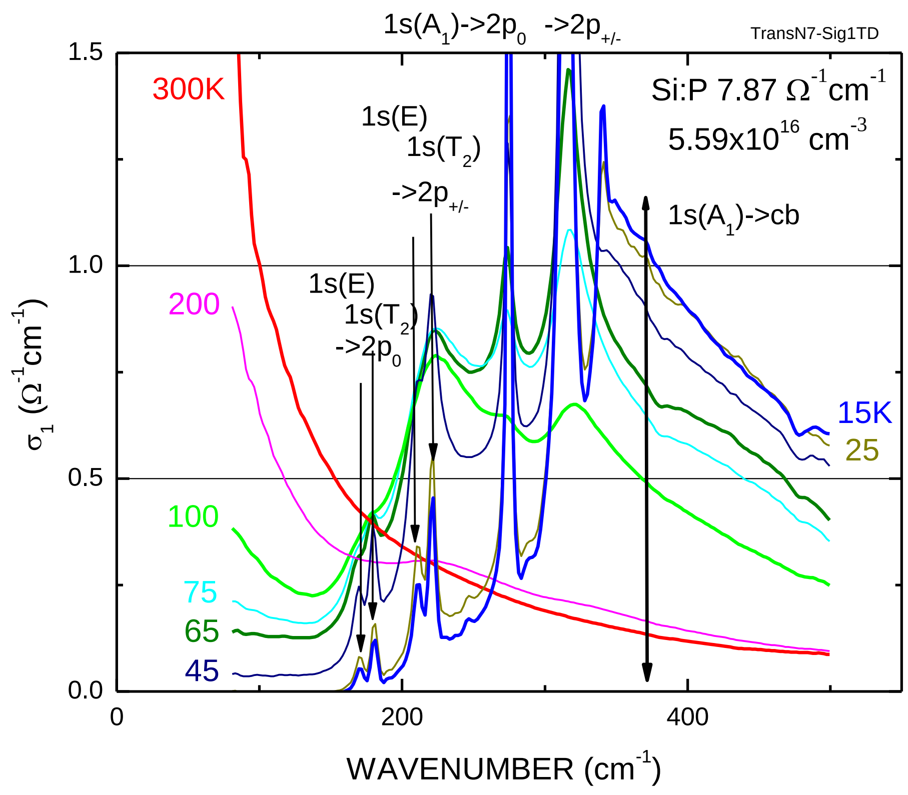


FIG. 2. Energy-level scheme (not to scale) for the transitions from the $1s$ states to the $2p_0$ and the $2p_\pm$ states. The letters next to a level indicate the irreducible representations of the donor-site symmetry, T_d, to which the level belongs. C.B. = conduction band.

Infračervená absorpce od nízké do vysoké teploty, postupná ionizace příměsových stavů, nakonec převládne obsazení vodivostního kontinua (měření UFKL 2008, FTIR Bruker IFS66, heliový kryostat, vzorky OnSemi Rožnov, zpráva LDDA). Rezistivita při RT je 127 mΩcm, ionizační energie pro přechod $1s(A_1)\rightarrow cb$ je 45 meV, ~365 cm^{-1}.



Reálná část vodivosti spočtená z transmisního spektra Si:P (5.59E16 cm^{-3}) při různých teplotách.