GRADUATE TEXTS IN PHYSICS

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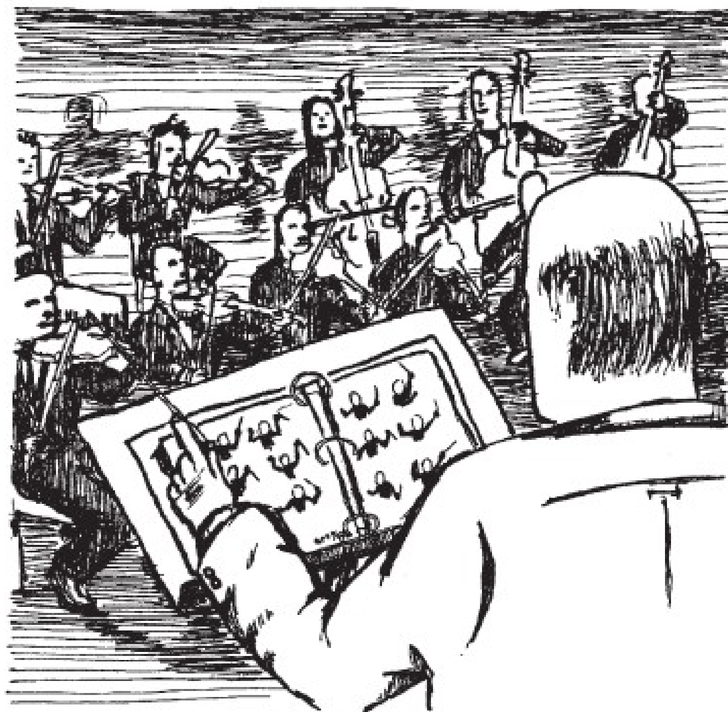
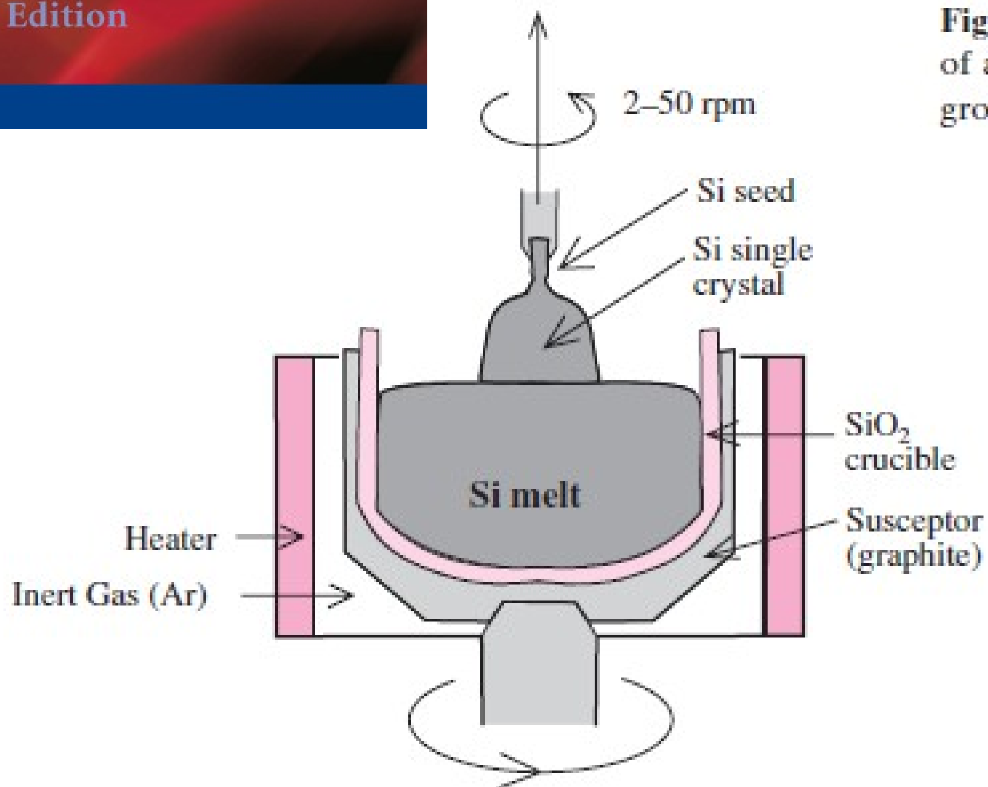
Fundamentals of Semiconductors

Physics and Materials Properties

Fourth Edition



A SEMI-CONDUCTOR



Jan Czochralski (23 October 1885 – 22 April 1953) was a Polish chemist who invented the Czochralski process, which is used for growing single crystals and in the production of semiconductor wafers. He is the most cited Polish scholar. He was also known for extraordinary physical strength.

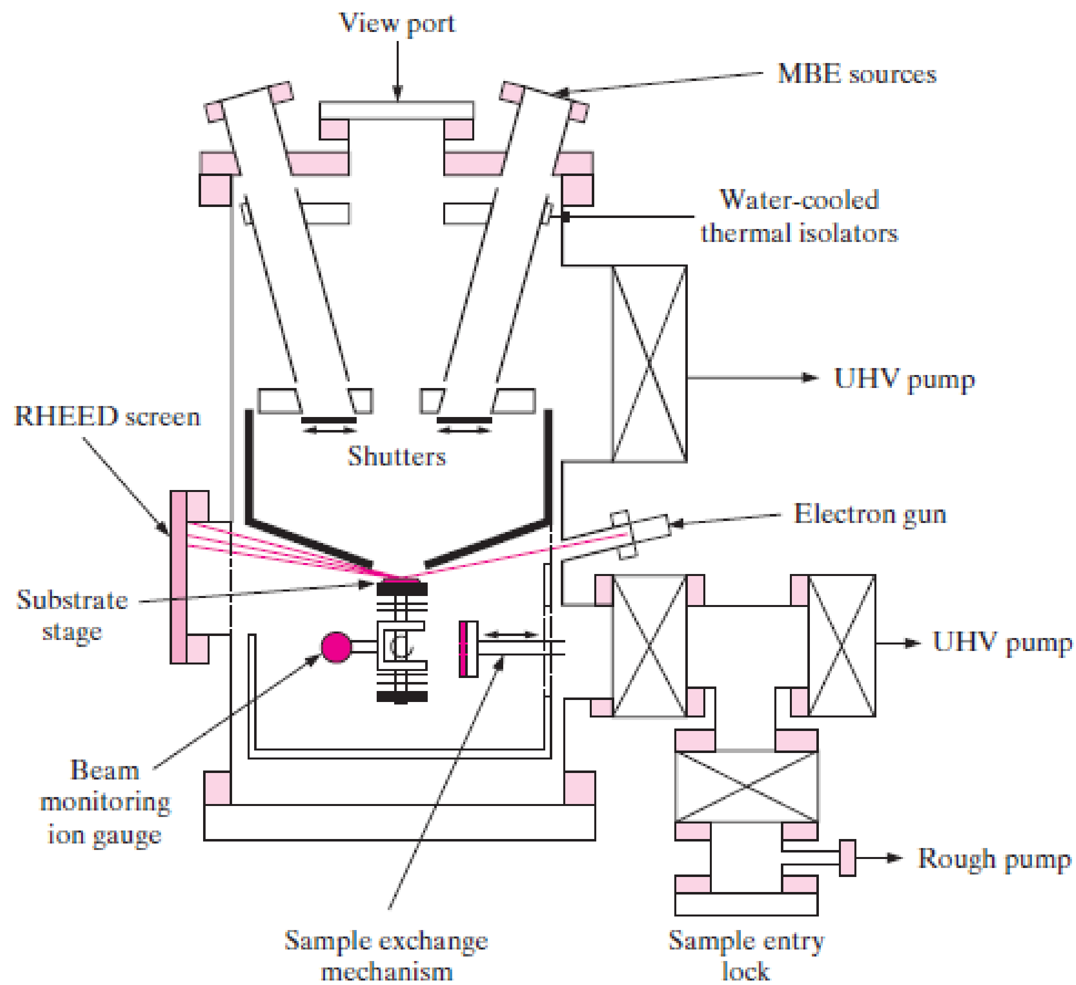
Czochralski was born in what was then Exin in the Prussian Province of Posen, German Empire (now Kcynia, Poland). Around 1900 he moved to Berlin, where he worked at a pharmacy. He was educated at Charlottenburg Polytechnic in Berlin, where he specialized in metal chemistry. Czochralski began working as an engineer for Allgemeine Elektrizitäts Gesellschaft (AEG) in 1907.

He discovered the Czochralski method in 1916, when he accidentally dipped his pen into a crucible of molten tin rather than his inkwell. He immediately pulled his pen out to discover that a thin thread of solidified metal was hanging from the nib. The nib was replaced by a capillary, and Czochralski verified that the crystallized metal was a single crystal. Czochralski's experiments produced single crystals a millimeter in diameter and up to 150 centimeters long. He published a paper on his discovery in 1918 in the Zeitschrift für Physikalische Chemie, a German chemistry journal, under the title "Ein neues Verfahren zur Messung der Kristallisationsgeschwindigkeit der Metalle" [A new method for the measurement of the crystallization rate of metals], since the method was at that time used for measuring the crystallization rate of metals such as tin, zinc and lead.[3] In 1950, Americans Gordon K. Teal and J.B. Little from Bell Labs would use the method to grow single germanium crystals, leading to its use in semiconductor production.

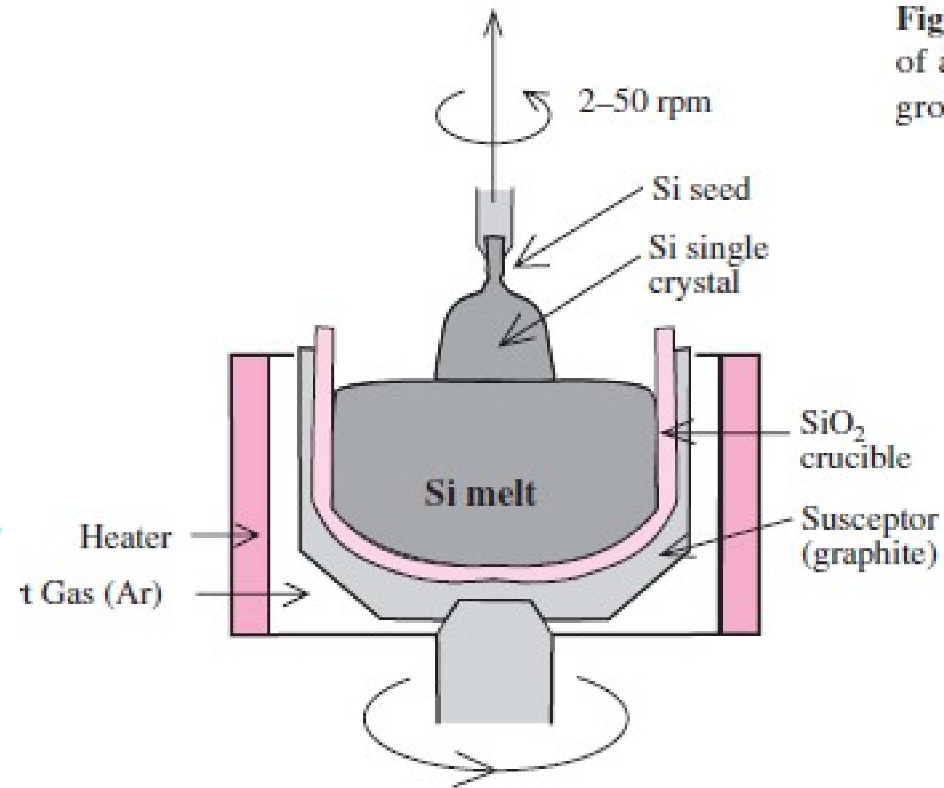
In 1917, Czochralski organized the research laboratory "Metallbank und Metallurgische Gesellschaft", which he directed until 1928. In 1919 he was one of the founding members of the German Society for Metals Science (Deutsche Gesellschaft für Metallkunde), of which he was president until 1925. In 1928, at the request of the president of Poland, Ignacy Mościcki, he moved to Poland and became the Professor of Metallurgy and Metal Research at the Chemistry Department of the Warsaw University of Technology.

After the war, he was stripped of his professorship by the communist regime due to his involvement with Germany during the war, although he was later cleared of any wrong doing by a Polish court. He returned to his native town of Kcynia, where he ran a small cosmetics and household chemicals firm until his death in 1953.

Techniki otrzymywania monokryształów oraz warstw



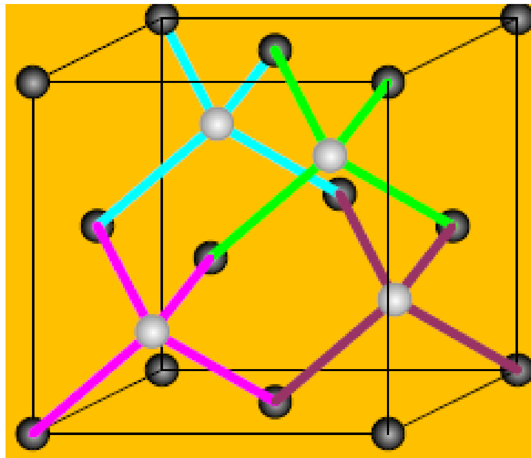
Molecular Beam Epitaxy (MBE)



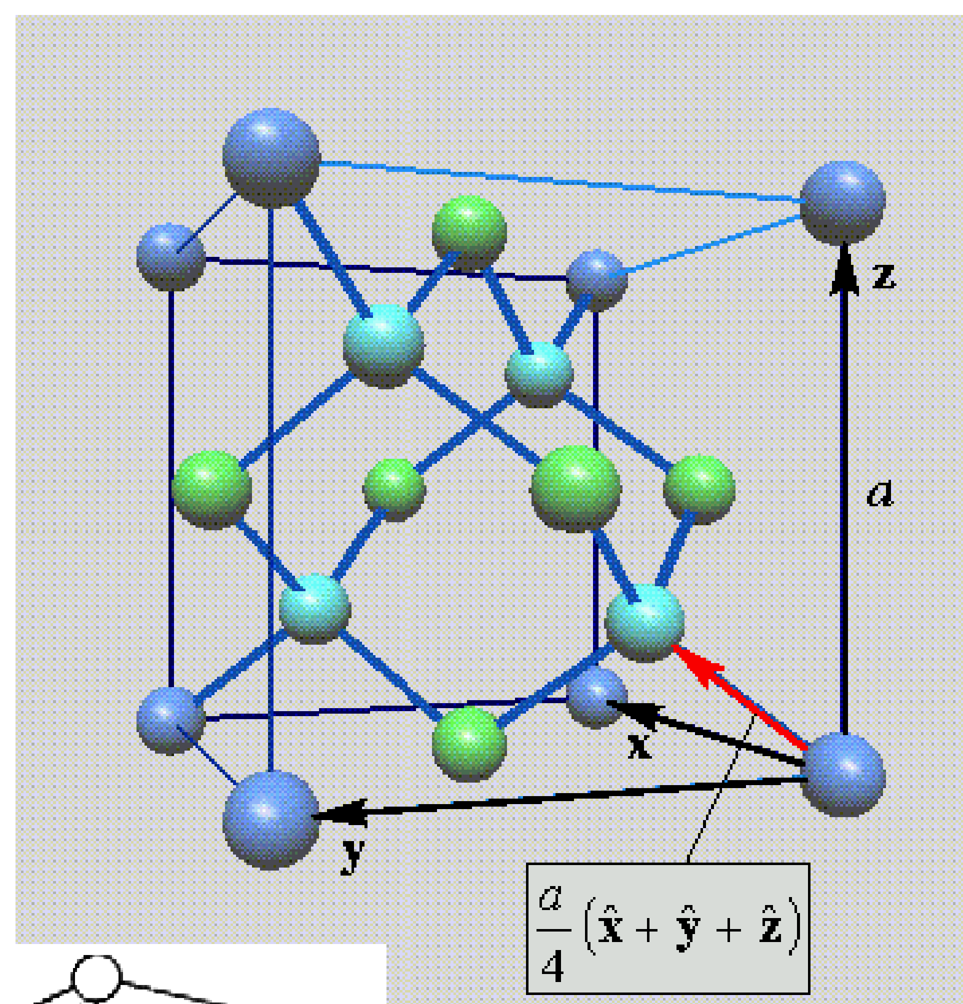
Metoda Czochralskiego –
„wyciągania" kryształów

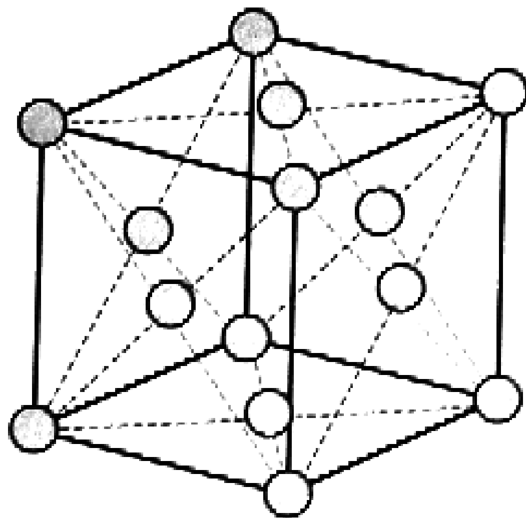
Struktura diamentu

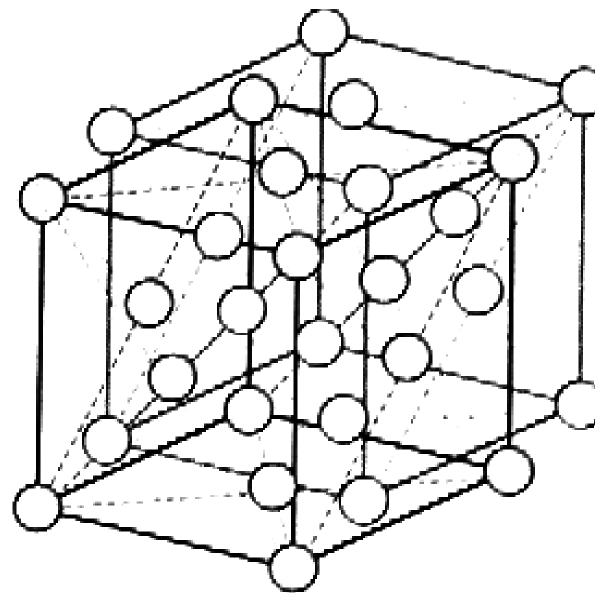
4 elektrony walencyjne tworzą bardzo silne wiązanie kowalencyjne z czterema najbliższymi atomami, <u>koordynacja tetraedyczna</u>



IIB	IIIA	IVA	VA	VIA
	5 B	6 C	7 N	8 O
	13 Al	14 Si	15 P	16 S
30 Zn	31 Ga	32 Ge	33 As	34 Se
48 Cd	49 In	50 Sn	51 Sb	52 Te







2 sieci fcc przesunięte o wektor (¼, ¼, ¼) wzdłuż diagonali

Struktura blendy cynkowej
ZnS (zinc-blend)

Atom Zn posiada koordynację 4 S i na odwrót
Atom S posiada koordynację 4 Zn atom
tworzą silne wiązanie kowalencyjne

IIB	IIIA	IVA	VA	VIA
	5 B	6 C	7 N	8 O
	13 Al	14 Si	15 P	16 S
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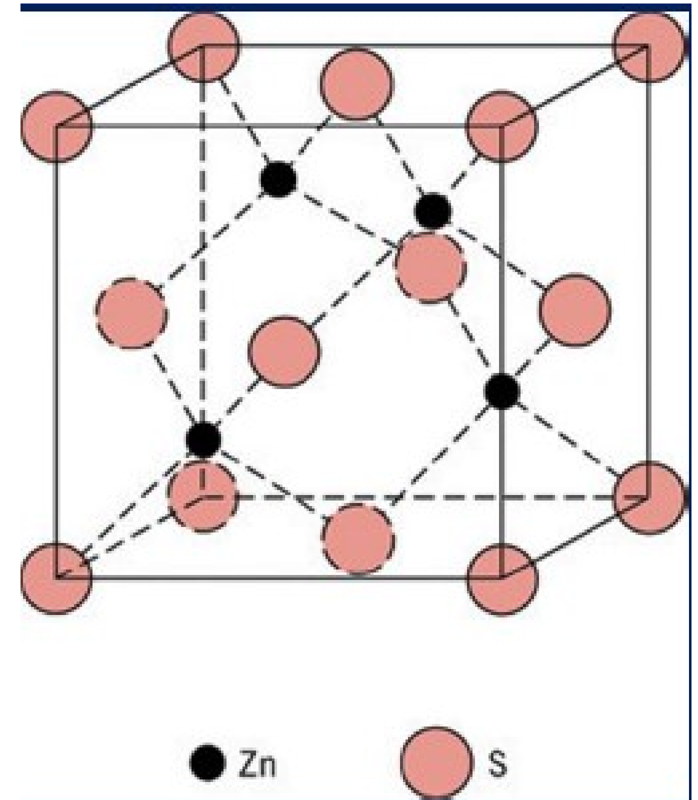


4 elektrony od Zn (s2) i S (p4) tworzą
pasmo walencyjne

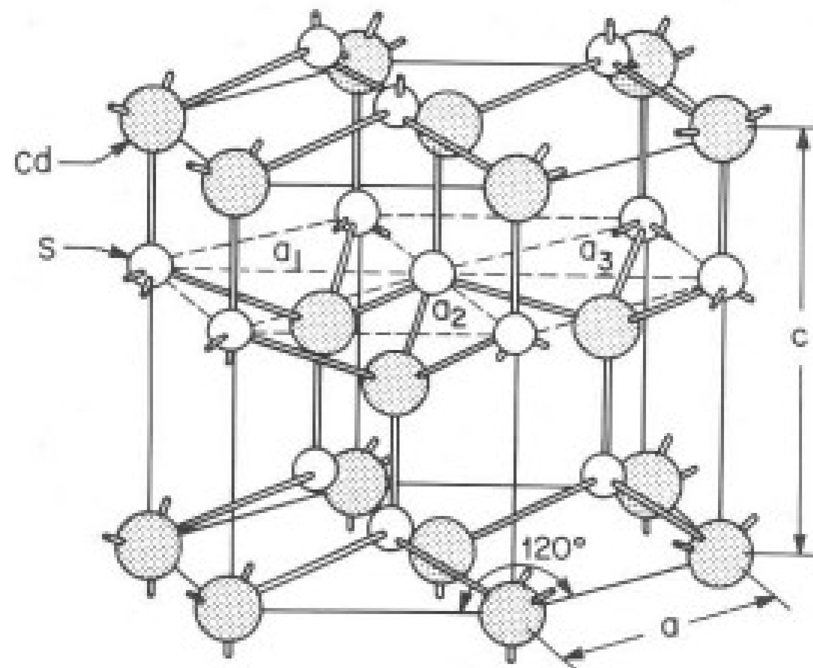
2 nierównoważne sieci fcc
przesunięte o wektor
(¼, ¼, ¼) wzdłuż diagonali

Zn: (0, 0, 0)
S: (¼, ¼, ¼)

ZnTe, CdTe
GaAs, GaN
SiC, Si-Ge

półprzewodniki „binarne” - związki
o strukturze blendy cynkowej

Heksagonalna struktura wurcytu ZnS (wurtzite)

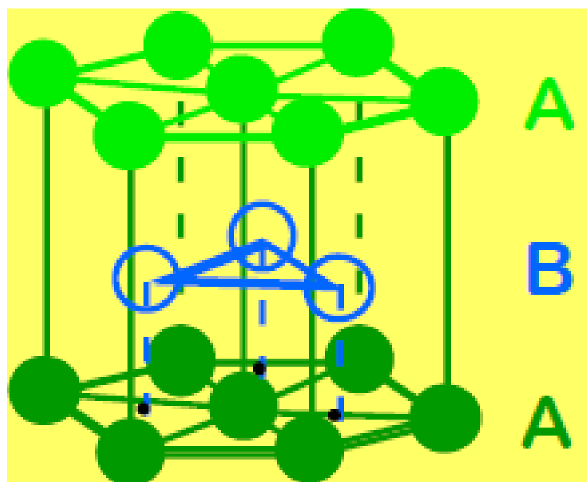


Atom Zn podobnie jak w sieci blendy posiada koordynację tetraedyczną atomów 4 S i na odwrót; tworzą silne wiązanie kowalencyjne

Wiele związków krystalizuje w dwóch formach wurcytu (heksagonalna) i blendy (kubiczna), np. **ZnS, CdS, SiC, GaN**

4 elektrony od Zn (s2, głębokie stany) i S (p4) tworzą pasmo walencyjne

2 sieci hcp przenikające się obsadzone przez dwa różne atomy np.
Zn: (0, 0, 0)
S: (¼, ¼, ¼)



IIB	IIIA	IVA	VA	VIA
	5 B	6 C	7 N	8 O
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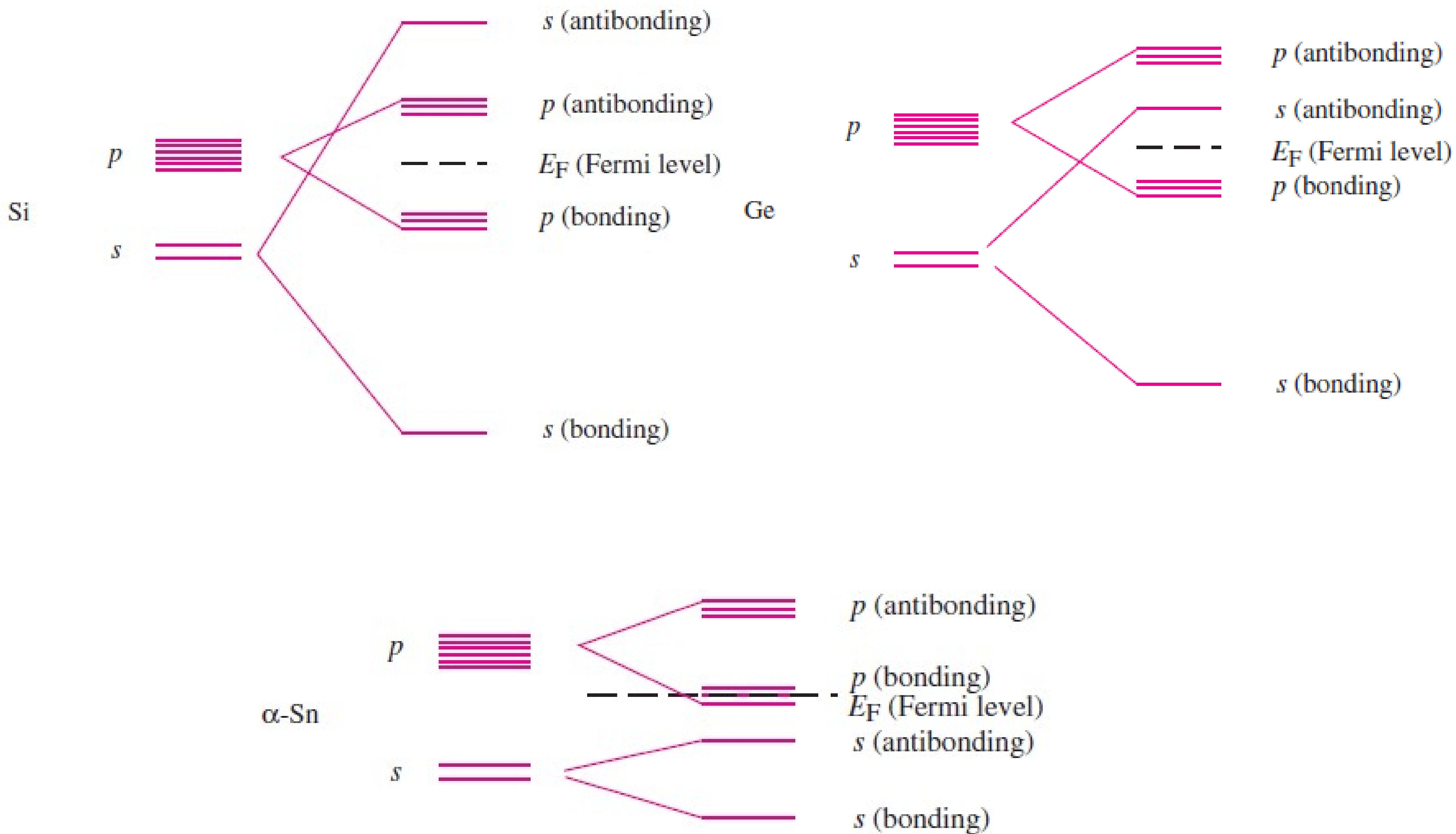
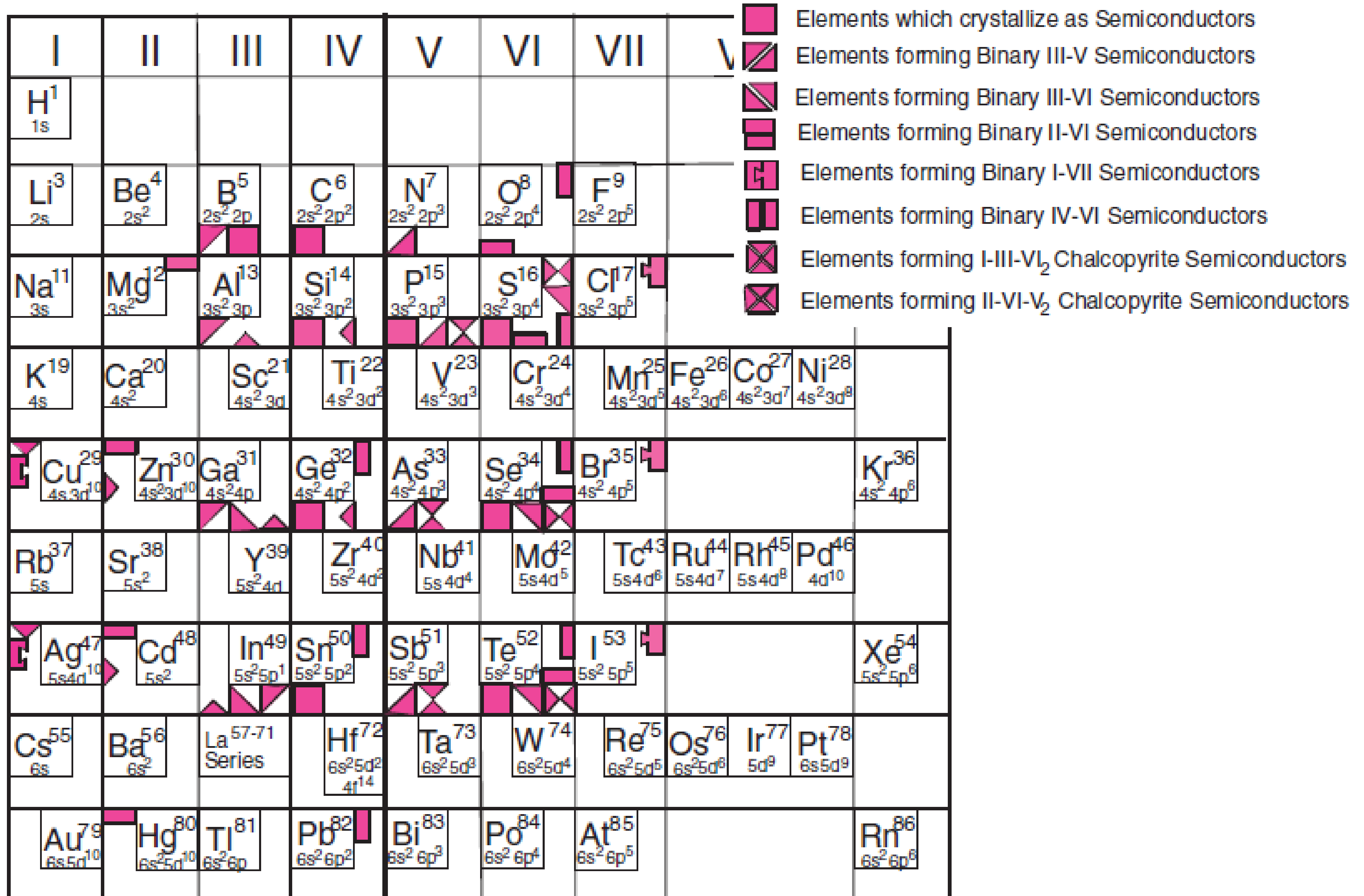
48 Cd	49 In	50 Sn	51 Sb	52 Te

Schemat poziomów energetycznych w kryształach Si/Ge/Sn od strony wiązań molekularnych

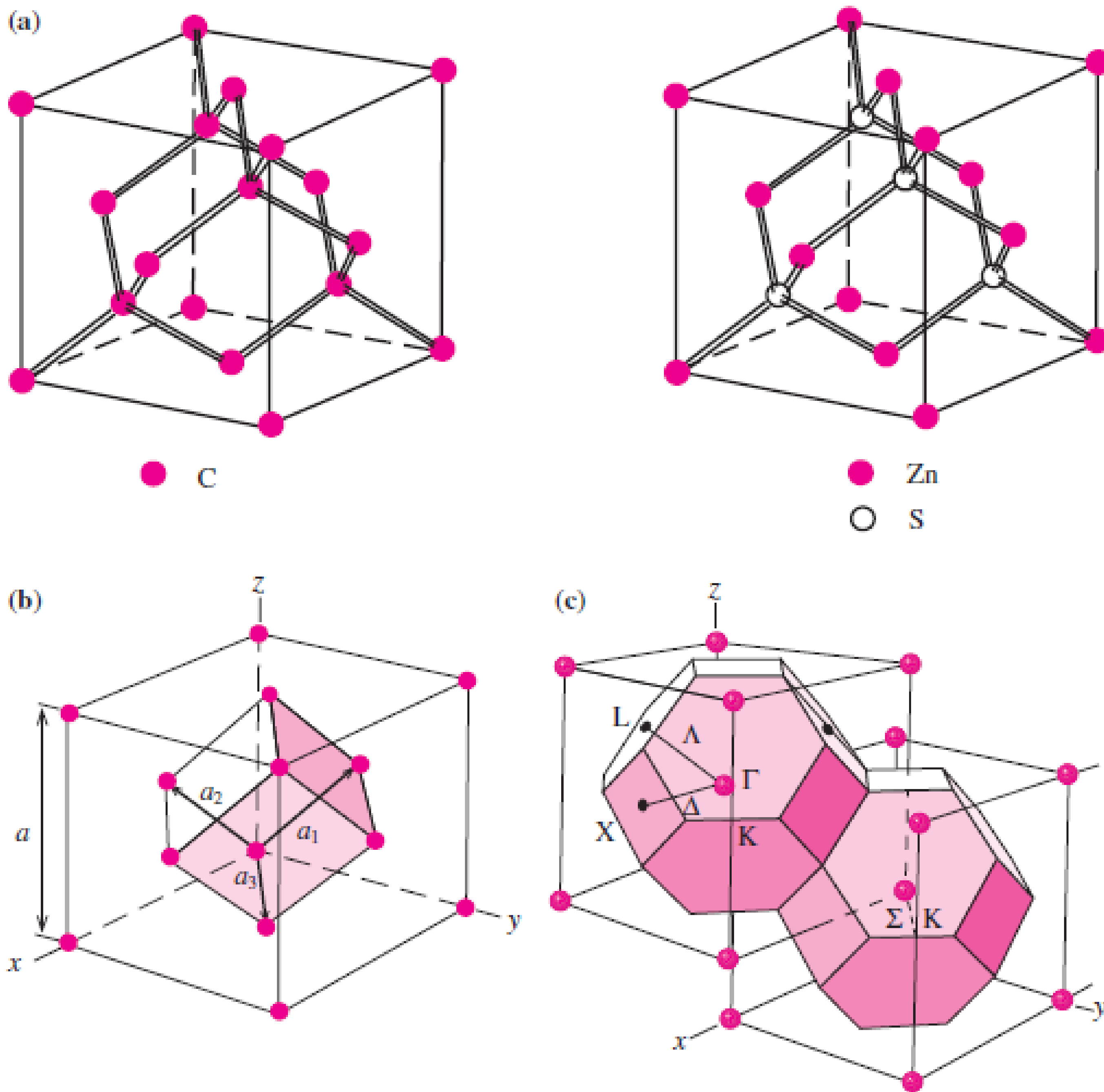


Periodic Table of "Semiconductor-Forming" Elements



P. Y. Yu & M. Cardona, Fundamentals of Semiconductors

Przestrzeń prosta i przestrzeń odwrotna dla przypadku struktur diamentu i blendy



Przypomnienie teorii grup i charakterów reprezentacji dla przypadku struktur o symetrii diamentu i blend (T_d, F-43m)

E:	identity
eight C_3 operations:	clockwise and counterclockwise rotations of 120° about the [111], [$\bar{1}$11], [1$\bar{1}$1], and [11$\bar{1}$] axes, respectively;
three C_2 operations:	rotations of 180° about the [100], [010], and [001] axes, respectively;
six S_4 operations:	clockwise and counterclockwise improper rotations of 90° about the [100], [010], and [001] axes, respectively;
six σ operations:	reflections with respect to the (110), (1$\bar{1}$0), (101), (10$\bar{1}$), (011), and (01$\bar{1}$) planes, respectively.

	$\{E\}$	$\{3C_2\}$	$\{6S_4\}$	$\{6\sigma\}$	$\{8C_3\}$	Basis functions
A_1	1	1	1	1	1	xyz
A_2	1	1	−1	−1	1	$x^4(y^2-z^2)+y^4(z^2-x^2)+z^4(x^2-y^2)$
E	2	2	0	0	−1	$\{(x^2-y^2), z^2-\frac{1}{2}(x^2+y^2)\}$
T_1	3	−1	1	−1	0	$\{x(y^2-z^2), y(z^2-x^2), z(x^2-y^2)\}$
T_2	3	−1	−1	1	0	$\{x, y, z\}$

Koster notation[a]	BSW notation	Molecular notation
Γ_1	Γ_1	A_1
Γ_2	Γ_2	A_2
Γ_3	Γ_{12}	E
Γ_4	Γ_{15}	T_2
Γ_5	Γ_{25}	T_1

nawiązanie do punktów wysokiej symetrii dla strefy Brillouina komórki fcc

Próba powiązania rozwiązań równań Blocha dla komórki blendy w przybliżeniu elektronów prawie swobodnych

Funkcja falowa $\Phi(x,y,z) = \exp[i(k_x x + k_y y + k_z z)]$

Relacja dyspersji $E = \hbar^2 k^2/2m$

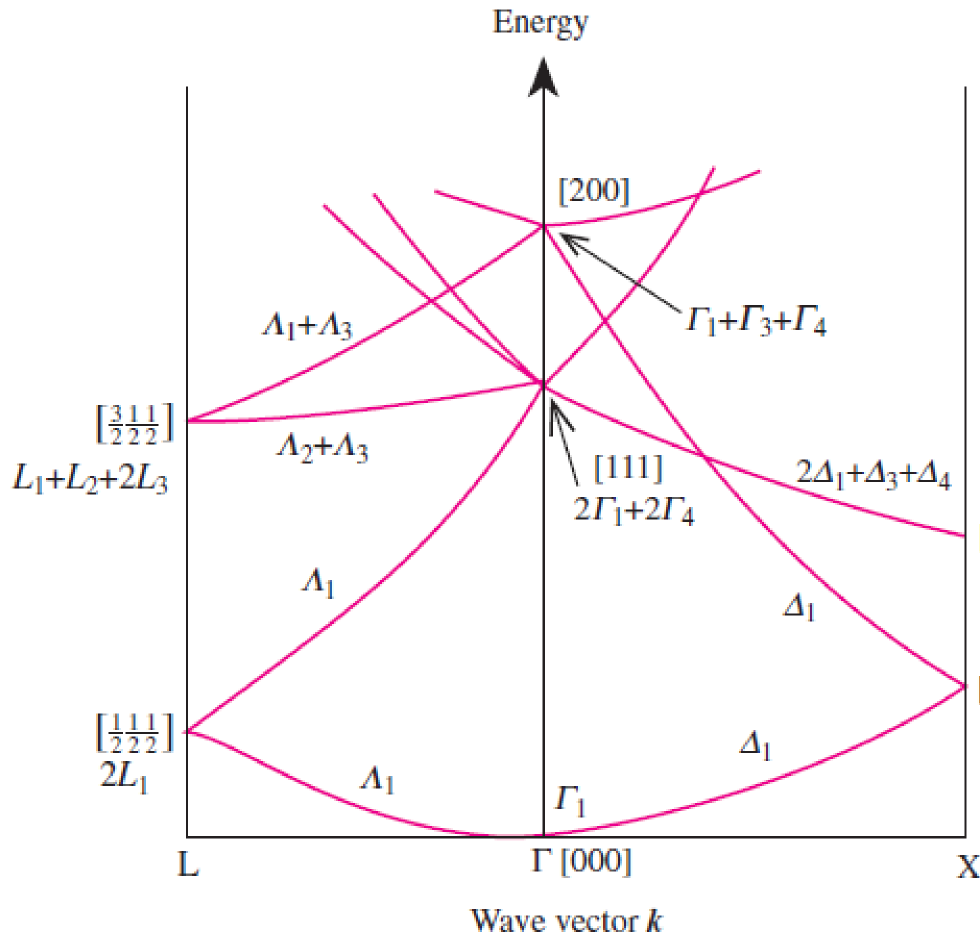
$(2\pi/a)(\pm 2,0,0)$, $(2\pi/a)(0,\pm 2,0)$, and $(2\pi/a)(0,0,\pm 2)$

Representation	Wave function
Γ_1	$\cos(4\pi x/a) + \cos(4\pi y/a) + \cos(4\pi z/a)$
Γ_3	$\cos(4\pi y/a) - \cos(4\pi z/a)$; $\cos(4\pi x/a) - (1/2)[\cos(4\pi y/a) + \cos(4\pi z/a)]$
Γ_4	$\sin(4\pi x/a)$; $\sin(4\pi y/a)$; $\sin(4\pi z/a)$

$(2\pi/a)(\pm 1,\pm 1,\pm 1)$

Representation	Wave function
Γ_1	$(1/\sqrt{8})(\{111\} + \{1\bar{1}\bar{1}\} + \{\bar{1}1\bar{1}\} + \{\bar{1}\bar{1}1\} + \{\bar{1}\bar{1}\bar{1}\} + \{\bar{1}11\} + \{1\bar{1}1\} + \{11\bar{1}\}) = (\sqrt{8})\cos(2\pi x/a)\cos(2\pi y/a)\cos(2\pi z/a)$
Γ_1	$(\sqrt{8})\sin(2\pi x/a)\sin(2\pi y/a)\sin(2\pi z/a)$
Γ_4	$(\sqrt{8})\{\sin(2\pi x/a)\sin(2\pi y/a)\cos(2\pi z/a)$; $\sin(2\pi x/a)\cos(2\pi y/a)\sin(2\pi z/a)$; $\cos(2\pi x/a)\sin(2\pi y/a)\sin(2\pi z/a)\}$
Γ_4	$(\sqrt{8})\{\sin(2\pi x/a)\cos(2\pi y/a)\cos(2\pi z/a)$; $\cos(2\pi x/a)\sin(2\pi y/a)\cos(2\pi z/a)$; $\cos(2\pi x/a)\cos(2\pi y/a)\sin(2\pi z/a)\}$.

Elektronowe pasma energetyczne dla komórki blendy (grupa T_d) w przybliżeniu elektronów prawie swobodnych

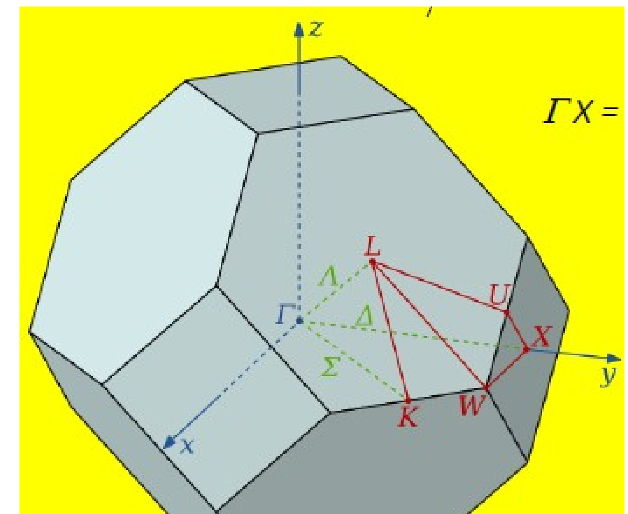


	$\{E\}$	$\{C_4^2(x)\}$	$\{2C_4^2(y,z)\}$	$\{2S_4\}$	$\{2m_d\}$
X_1	1	1	1	1	1
X_2	1	1	1	−1	−1
X_3	1	1	−1	−1	1
X_4	1	1	−1	1	−1
X_5	2	−2	0	0	0

X point:

$\exp[\pm i4\pi x/a]$; $\exp[\pm i4\pi y/a]$; and $\exp[\pm i4\pi z/a]$

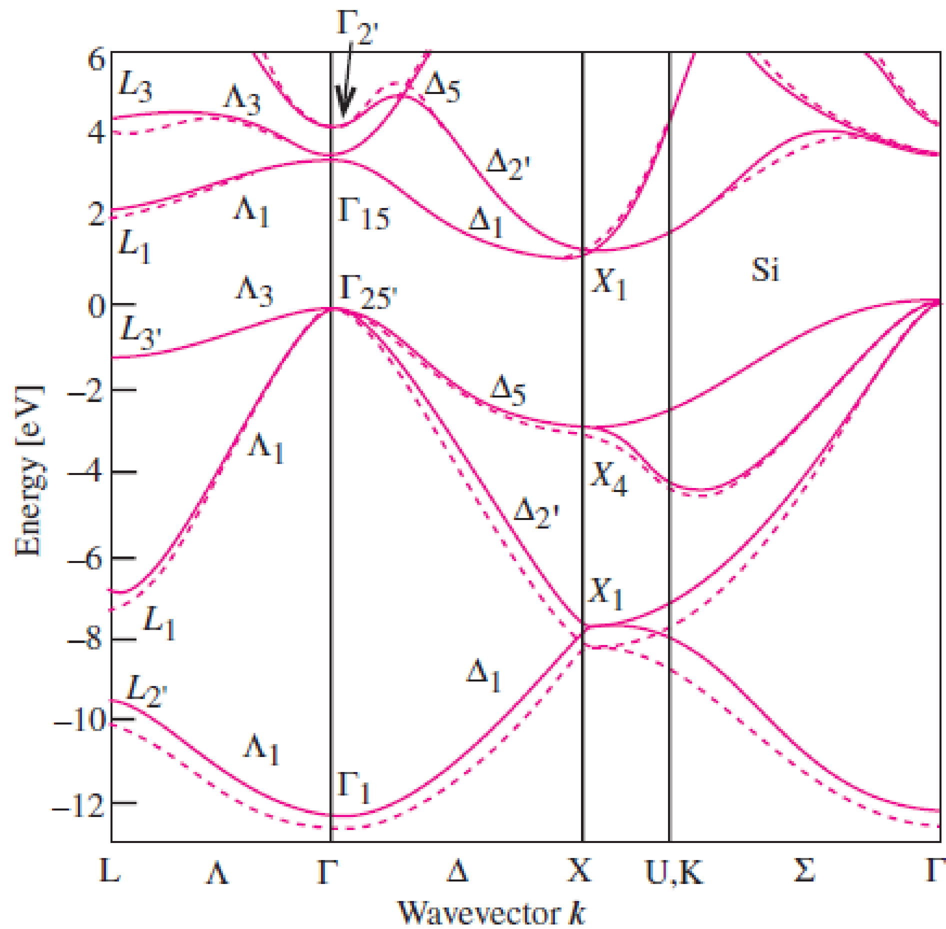
L point: $\exp[(i2\pi/a)(\pm x \pm y \pm z)]$

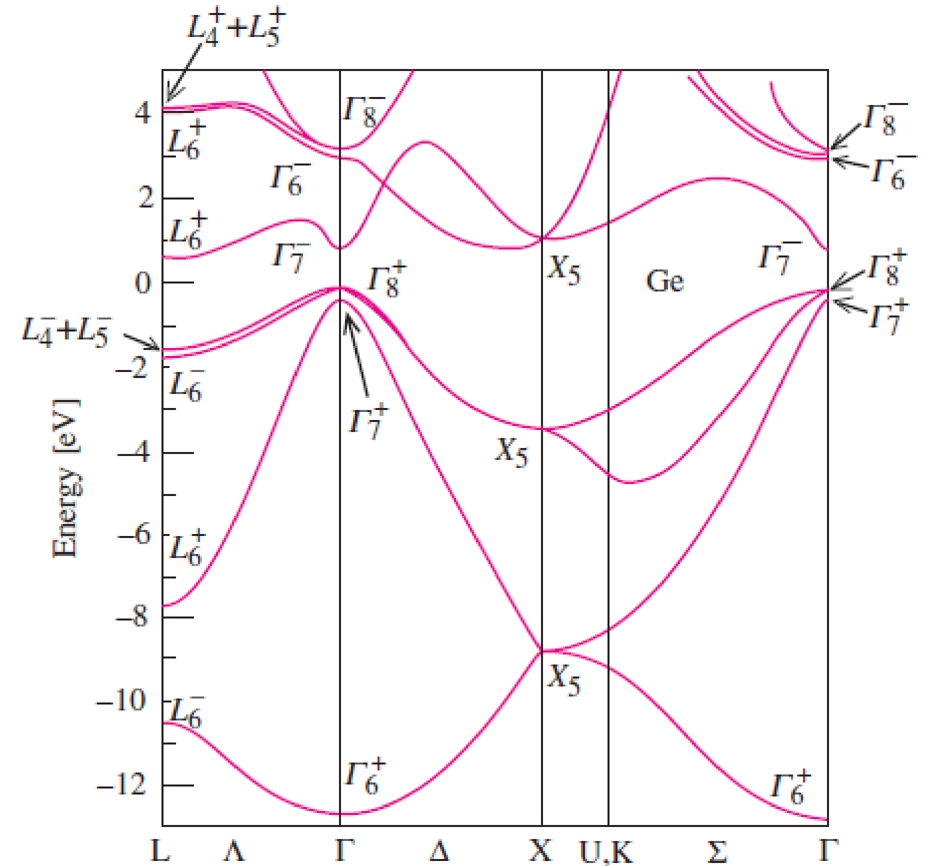


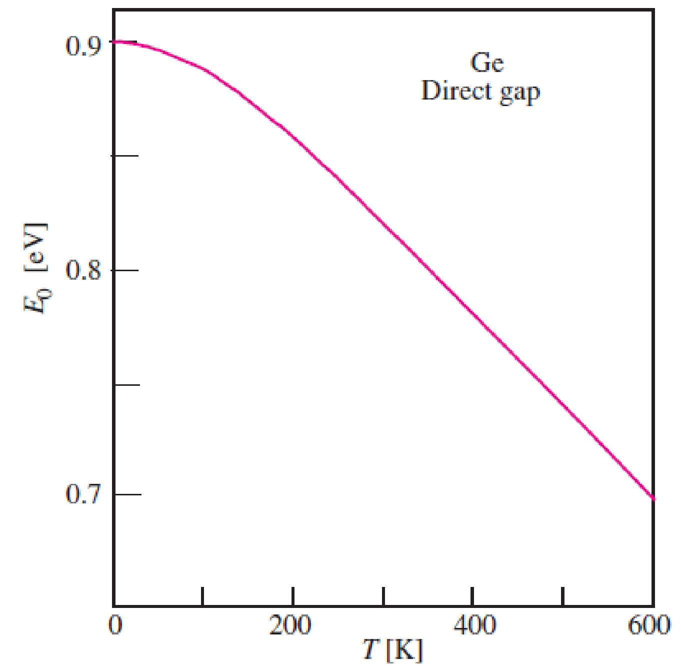
	$\{E\}$	$\{2C_3\}$	$\{3m\}$	Basis functions
Λ_1	1	1	1	1 or $x+y+z$
Λ_2	1	1	−1	$xy(x-y)+yz(y-z)+zx(z-x)$
Λ_3	2	−1	0	$\{(x-y); \sqrt{\frac{2}{3}}(z-\frac{1}{2}[x+y])\}$

Struktura elektronowa Si i Ge (+ poprawki na SO)

$$\mathcal{H}_{1e}\Phi_n(\boldsymbol{r}) = \left(\frac{p^2}{2m} + V(\boldsymbol{r})\right)\Phi_n(\boldsymbol{r}) = E_n\Phi_n(\boldsymbol{r}),$$



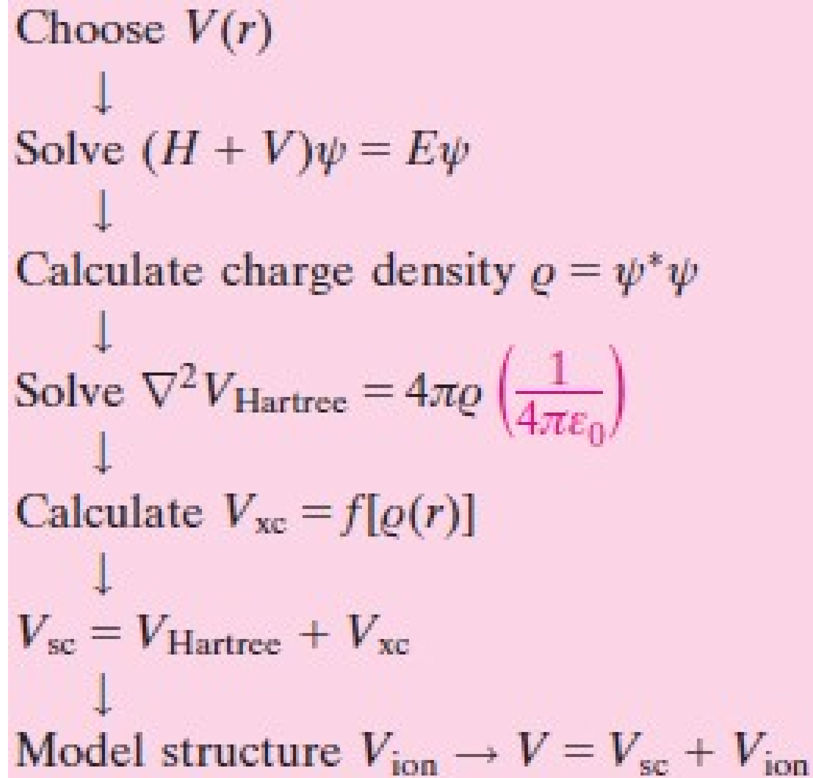




Metody obliczeń struktury elektronowej półprzewodników

$$\mathcal{H}_{1e}\Phi_n(\boldsymbol{r}) = \left(\frac{p^2}{2m} + V(\boldsymbol{r})\right)\Phi_n(\boldsymbol{r}) = E_n\Phi_n(\boldsymbol{r}),$$

Ogólny schemat obliczeń „samouzgodnionych”



Metoda **k·p**

$$\Phi_{nk} = \exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r})u_{nk}(\boldsymbol{r})$$

$$\left(\frac{p^2}{2m} + \frac{\hbar\boldsymbol{k}\cdot\boldsymbol{p}}{m} + \frac{\hbar^2k^2}{2m} + V\right)u_{nk} = E_{nk}u_{nk}$$

Γ point: $\boldsymbol{k}_0 = (0,0,0)$

$$\left(\frac{p^2}{2m} + V\right)u_{n0} = E_{n0}u_{n0} \quad (n = 1,2,3,\ldots)$$

Dla innych punktów k, rozwiązania można traktować jako zaburzenie wyrazem

$$\frac{\hbar\boldsymbol{k}\cdot\boldsymbol{p}}{m}$$

$$u_{nk} = u_{n0} + \frac{\hbar}{m}\sum_{n'\neq n}\frac{\langle u_{n0}\,|\,\boldsymbol{k}\cdot\boldsymbol{p}\,|\,u_{n'0}\rangle}{E_{n0} - E_{n'0}}u_{n'0}$$

Masy efektywne półprzewodników jako czynnik determinujący strukturę elektronową półprzewodników

$$u_{nk} = u_{n0} + \frac{\hbar}{m}\sum_{n'\neq n}\frac{\langle u_{n0}\,|\,\boldsymbol{k}\cdot\boldsymbol{p}\,|\,u_{n'0}\rangle}{E_{n0}-E_{n'0}}u_{n'0}$$

$$E_{nk} = E_{n0} + \frac{\hbar^2 k^2}{2m} + \frac{\hbar^2}{m^2}\sum_{n'\neq n}\frac{|\langle u_{n0}\,|\,\boldsymbol{k}\cdot\boldsymbol{p}\,|\,u_{n'0}\rangle|^2}{E_{n0}-E_{n'0}}.$$

$$E_{nk} = E_{n0} + \frac{\hbar^2 k^2}{2m^*}$$

$$\frac{1}{m^*} = \frac{1}{m} + \frac{2}{m^2 k^2}\sum_{n'\neq n}\frac{|\langle u_{n0}\,|\,\boldsymbol{k}\cdot\boldsymbol{p}\,|\,u_{n'0}\rangle|^2}{E_{n0}-E_{n'0}}$$

Dla symetrii Td półprzewodników o strukturze diamentu i blendy

$$\frac{1}{m_c^*} = \frac{1}{m} + \frac{2\,|\langle \Gamma_{1c}\,|\,\boldsymbol{k}\cdot\boldsymbol{p}\,|\,\Gamma_{4v}\rangle|^2}{m^2 E_0 k^2}$$

Wartość własna operatora pędu

$$\langle X\,|\,p_x\,|\,\Gamma_1\rangle = \langle Y\,|\,p_y\,|\,\Gamma_1\rangle = \langle Z\,|\,p_z\,|\,\Gamma_1\rangle = \mathrm{i}P$$

Masy efektywna elektronów/dziur

$$\frac{m}{m_c^*} \approx 1 + \frac{2P^2}{mE_0}$$

	Ge	GaN	GaAs	GaSb	InP	InAs	ZnS	ZnSe	ZnTe	CdTe
E_0 [eV]	0.89	3.44	1.55	0.81	1.34	0.45	3.80	2.82	2.39	1.59
m_c^*/m (exp)	0.041	0.17	0.067	0.047	0.073	0.026	0.20	0.134	0.124	0.093
m_c^*/m ((2.44))	0.04	0.17	0.078	0.04	0.067	0.023	0.16	0.14	0.12	0.08

Dobra zgodność z eksperymentem przyczyną stosowania tzw. przybliżenia „masy efektywnej" jako powszechnego podejścia do obliczeń kropek kwantowych, drutów i innych nanostruktur

Silny wpływ oddziaływania spin-orbita i przybliżenie „masy efektywnej” w znanych półprzewodników

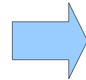
Hamiltonian oddziaływania SO

$$H_{so} = \frac{\hbar}{4c^2m^2}(\nabla V \times \boldsymbol{p}) \cdot \boldsymbol{\sigma},$$

Macierze Pauliego jako operatory spinowe

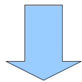
$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}; \ \sigma_y = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}; \ \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

Dla przypadku nierelatywistycznego



$$|lm_l\rangle = \begin{cases} |1\,1\rangle & = -(x+\mathrm{i}y)/\sqrt{2}, \\ |1\,0\rangle & = z, \\ |1\,{-1}\rangle & = (x-\mathrm{i}y)/\sqrt{2}. \end{cases}$$

Dla przypadku relatywistycznego



total angular momentum $\boldsymbol{j} = \boldsymbol{l} + \boldsymbol{s}$

$j = l + s = 3/2$ and $j = l - s = 1/2$.

(α = spin-up, β = spin-down)

$j, j-1, \ldots, -j+1, -j.$

$$|jm_j\rangle = \begin{cases} |3/2,\ 3/2\rangle = |1,\ 1\rangle\alpha \\ |3/2,\ 1/2\rangle = (1/\sqrt{3})(|1,\ 1\rangle\beta + \sqrt{2}|1,\ 0\rangle\alpha) \\ |3/2,\ -1/2\rangle = (1/\sqrt{3})(|1,\ -1\rangle\alpha + \sqrt{2}|1,\ 0\rangle\beta) \\ |3/2,\ -3/2\rangle = |1,\ -1\rangle\beta \\ |1/2,\ 1/2\rangle = (1/\sqrt{3})(|1,\ 0\rangle\alpha - \sqrt{2}|1,\ 1\rangle\beta) \\ |1/2,\ -1/2\rangle = (1/\sqrt{3})(|1,\ 0\rangle\beta - \sqrt{2}|1,\ -1\rangle\alpha) \end{cases}$$

$|X\rangle\alpha, |X\rangle\beta, |Y\rangle\alpha, |Y\rangle\beta, |Z\rangle\alpha$, and $|Z\rangle\beta$

$$|1,\ \ 1\rangle = -(|X\rangle + \mathrm{i}|Y\rangle)/\sqrt{2},$$
$$|1,\ \ 0\rangle = |Z\rangle,$$
$$|1, -1\rangle = (|X\rangle - \mathrm{i}|Y\rangle)/\sqrt{2}.$$

Punkt Γ

$$\Delta_0 = 3\lambda/2. \qquad H_{so} = \lambda \boldsymbol{l} \cdot \boldsymbol{s}$$

Masy efektywne i rozszczepienie SO Wybranych półprzewodników

$$\frac{1}{m^*_{hh}} = \frac{1}{\hbar^2}\left[-2A + 2B\left(1 + \frac{2|C|^2}{15B^2}\right)\right]$$

$$\frac{1}{m^*_{lh}} = \frac{1}{\hbar^2}\left[-2A - 2B\left(1 + \frac{2|C|^2}{15B^2}\right)\right]$$

	A	B	$\lvert C\rvert^2$	Δ_0 [eV]	m_{hh}/m_0 exp	m_{hh}/m_0 th	m_{lh}/m_0 exp	m_{lh}/m_0 th	m_{so}/m_0 exp	m_{so}/m_0 th
C[b]	−2.5	0.2	4.6	0.013[a]		0.66[e]		0.29[e]		0.39[b]
Si[e]	−4.28	−0.68	24	0.044	0.54	0.50	0.15	0.15	0.23	0.24
Ge	−13.38	−8.5	173	0.295	0.34	0.43	0.043	0.041	0.095	0.1
SiC[c]	−2.8	−1.016	5.8	0.014		0.6		0.25		0.36
GaN[d]	−5.05	−1.2	34	0.017		0.5[e]		0.13[e]		0.2
GaP[e]	−4.05	−0.98	16	0.08	0.57	0.51	0.18	0.16		0.25
GaAs	−6.9	−4.4	43	0.341	0.53	0.73	0.08	0.08	0.15	0.17
GaSb	−13.3	−8.8	230	0.75	0.8	0.98	0.05	0.04		0.15
InP[e]	−5.15	−1.9	21	0.11	0.58	0.44	0.12	0.11	0.12	0.2
InAs	−20.4	−16.6	167	0.38	0.4	0.4	0.026	0.026	0.14	0.10
InSb	−36.41	−32.5	43	0.81	0.42	0.48	0.016	0.013		0.12
ZnS	−2.54	−1.5		0.07						
ZnSe	−2.75	−1.0	7.5	0.43		1.09		0.145		
ZnTe	−3.8	−1.44	14.0	0.93						
CdTe	−4.14	−2.18	30.3	0.92						

[a] See: J. Serrano, M. Cardona, and T. Ruf, Solid State Commun. **113**, 411 (2000)
[b] See: M. Willatzen, M. Cardona, N.E. Christensen, *Linear Muffin-tin-orbital and* $\mathbf{k}\cdot\mathbf{p}$ *calculation of band structure of semiconducting diamond.* Phys. Rev. **B50**, 18054 (1994)
[c] See: M. Willatzen, M. Cardona, N.E. Christensen: *Relativistic electronic structure of 3C-SiC.* Phys. Rev. **B51**, 13150 (1995).

Schemat ewolucji elektronowej Si, Ge i Sn na podstawie podejścia TB

$$\mathcal{H}_0 = \sum_{j,l} h_l(\boldsymbol{r} - \boldsymbol{r}_{jl})$$

$$h_l \phi_{ml}(\boldsymbol{r} - \boldsymbol{r}_{jl}) = E_{ml} \phi_{ml}(\boldsymbol{r} - \boldsymbol{r}_{jl})$$

$$\Phi_{mlk} = \frac{1}{\sqrt{N}} \sum_j \exp(\mathrm{i}\boldsymbol{r}_{jl} \cdot \boldsymbol{k}) \phi_{ml}(\boldsymbol{r} - \boldsymbol{r}_{jl}).$$

$$\Psi_k = \sum_{m,l} C_{ml} \Phi_{mlk}.$$

$$\sum_{m,l} \left(H_{ml,m'l'} - E_k \delta_{mm'} \delta_{ll'} \right) C_{m'l'}(\boldsymbol{k}) = 0$$

$$\begin{aligned} H_{ml,m'l'}(\boldsymbol{k}) &= \sum_j^N \sum_{j'}^N \frac{\exp[\mathrm{i}(\boldsymbol{r}_{j'l'} - \boldsymbol{r}_{jl}) \cdot \boldsymbol{k}]}{N} \\ &\quad \times \langle \phi_{ml} \,|\, (\boldsymbol{r} - \boldsymbol{r}_{jl}) \,|\, H \,|\, \phi_{m'l'}(\boldsymbol{r} - \boldsymbol{r}_{j'l'}) \rangle \\ &= \sum_j^N \exp[\mathrm{i}(\boldsymbol{R}_j + \boldsymbol{r}_{l'} - \boldsymbol{r}_l) \cdot \boldsymbol{k}] \\ &\quad \times \langle \phi_{ml}(\boldsymbol{r} - \boldsymbol{r}_{jl}) \,|\, H \,|\, \phi_{m'l'}(\boldsymbol{r} - \boldsymbol{r}_{jl'}) \rangle. \end{aligned}$$

$$V_{ss} = 4V_{ss\sigma},$$

$$V_{sp} = 4V_{sp\sigma}/\sqrt{3},$$

$$V_{xx} = (4V_{pp\sigma}/3) + (8V_{pp\pi}/3),$$

$$V_{xy} = (4V_{pp\sigma}/3) - (4V_{pp\pi}/3),$$

$$\begin{aligned} H_{s1,s2} &= [\exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{d}_1) + \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{d}_2) + \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{d}_3) + \exp(\mathrm{i}\boldsymbol{k} \cdot \boldsymbol{d}_4)] \\ &\quad \times \langle S1 \,|\, \mathcal{H}_{\text{int}} \,|\, S2 \rangle, \end{aligned}$$

Schemat ewolucji elektronowej Si, Ge i Sn na podstawie podejścia TB

	S1	S2	X1	Y1	Z1	X2	Y2	Z2
S1	$E_s - E_k$	$V_{ss}g_1$	0	0	0	$V_{sp}g_2$	$V_{sp}g_3$	$V_{sp}g_4$
S2	$V_{ss}g_1^*$	$E_s - E_k$	$-V_{sp}g_2^*$	$-V_{sp}g_3^*$	$-V_{sp}g_4^*$	0	0	0
X1	0	$-V_{sp}g_2$	$E_p - E_k$	0	0	$V_{xx}g_1$	$V_{xy}g_4$	$V_{xy}g_3$
Y1	0	$-V_{sp}g_3$	0	$E_p - E_k$	0	$V_{xy}g_4$	$V_{xx}g_1$	$V_{xy}g_2$
Z1	0	$-V_{sp}g_4$	0	0	$E_p - E_k$	$V_{xy}g_3$	$V_{xy}g_2$	$V_{xx}g_1$
X2	$V_{sp}g_2^*$	0	$V_{xx}g_1^*$	$V_{xy}g_4^*$	$V_{xy}g_3^*$	$E_p - E_k$	0	0
Y2	$V_{sp}g_3^*$	0	$V_{xy}g_4^*$	$V_{xx}g_1^*$	$V_{xy}g_2^*$	0	$E_p - E_k$	0
Z2	$V_{sp}g_4^*$	0	$V_{xy}g_3^*$	$V_{xy}g_2^*$	$V_{xx}g_1^*$	0	0	$E_p - E_k$

$$g_1 = \cos(k_1\pi/2)\cos(k_2\pi/2)\cos(k_3\pi/2) - i\sin(k_1\pi/2)\sin(k_2\pi/2)\sin(k_3\pi/2),$$

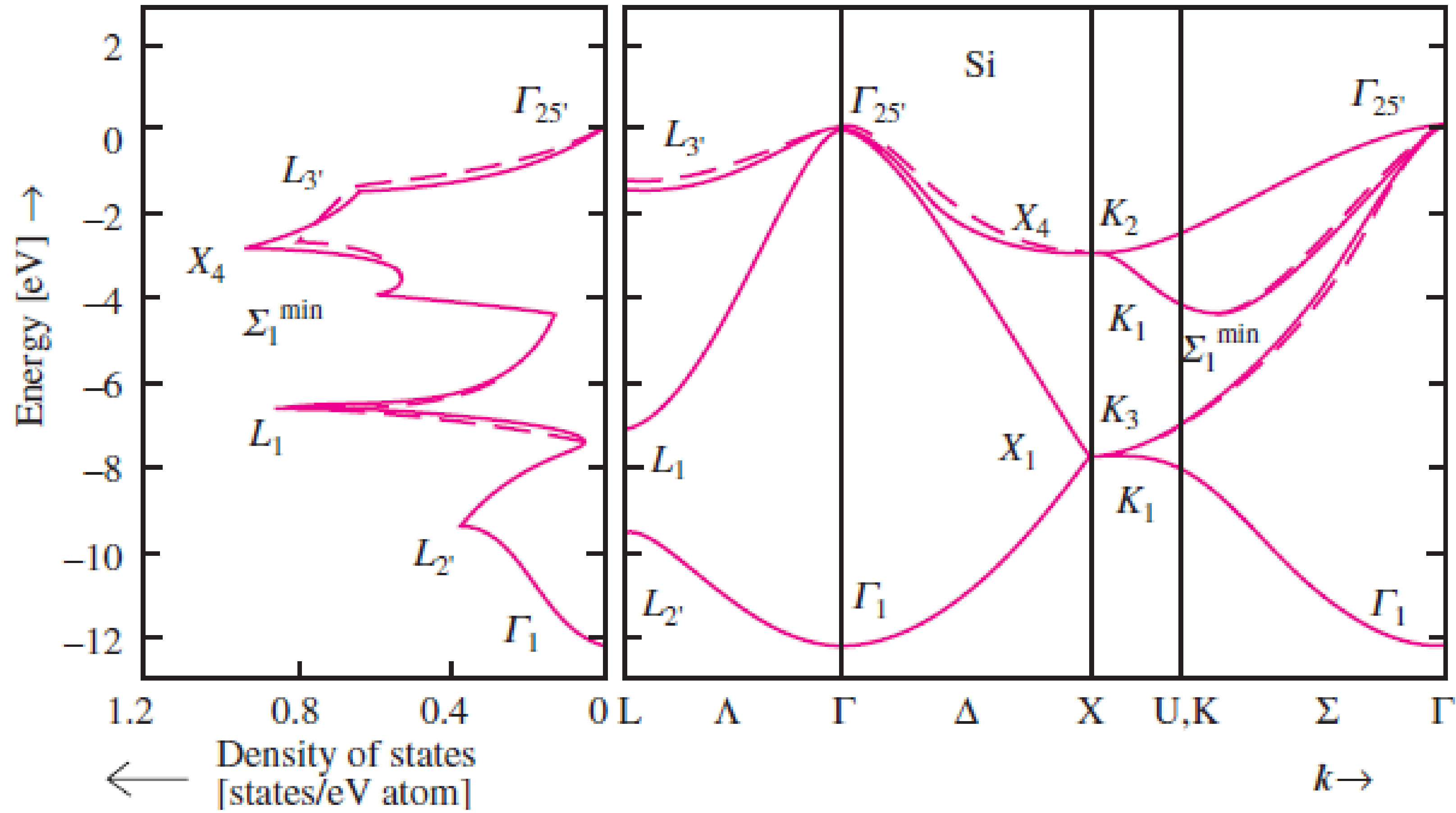
$$g_2 = -\cos(k_1\pi/2)\sin(k_2\pi/2)\sin(k_3\pi/2) + i\sin(k_1\pi/2)\cos(k_2\pi/2)\cos(k_3\pi/2)$$

$$g_3 = -\sin(k_1\pi/2)\cos(k_2\pi/2)\sin(k_3\pi/2) + i\cos(k_1\pi/2)\sin(k_2\pi/2)\cos(k_3\pi/2),$$

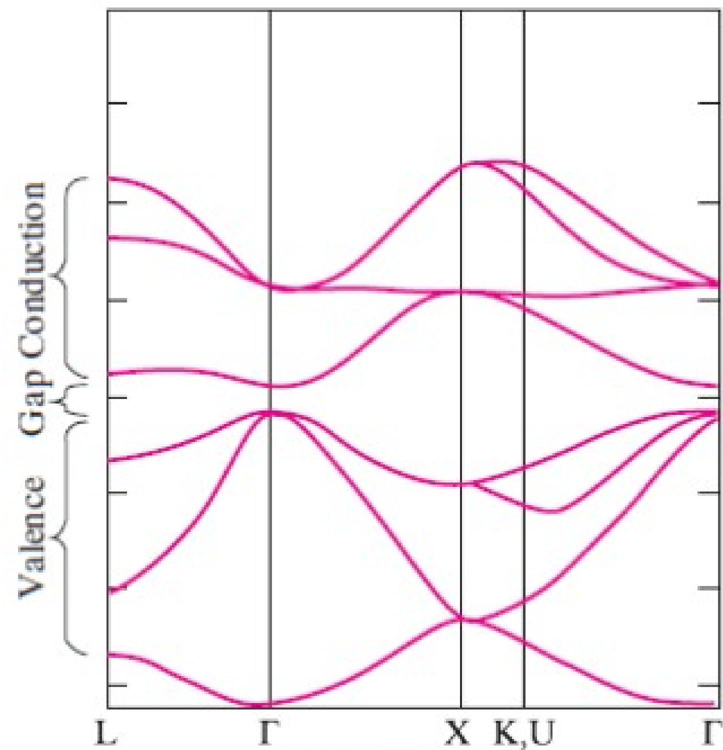
$$g_4 = -\sin(k_1\pi/2)\sin(k_2\pi/2)\cos(k_3\pi/2) + i\cos(k_1\pi/2)\cos(k_2\pi/2)\sin(k_3\pi/2),$$

	$E_p - E_s$	V_{ss}	V_{sp}	V_{xx}	V_{xy}
C	7.40	−15.2	10.25	3.0	8.3
Si	7.20	−8.13	5.88	3.17	7.51
Ge	8.41	−6.78	5.31	2.62	6.82

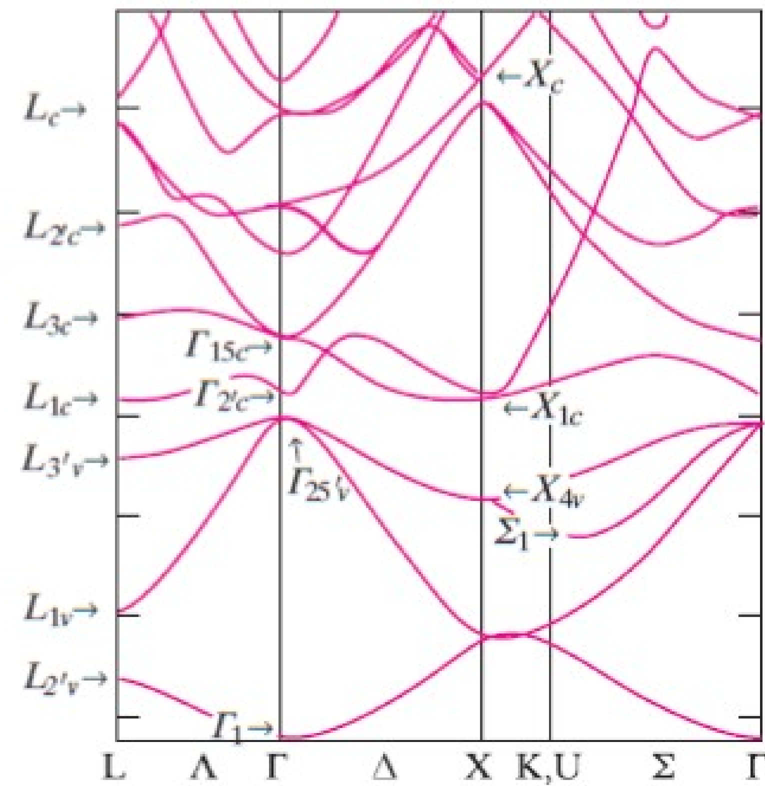
Schemat ewolucji elektronowej Si, Ge i Sn na podstawie podejścia TB



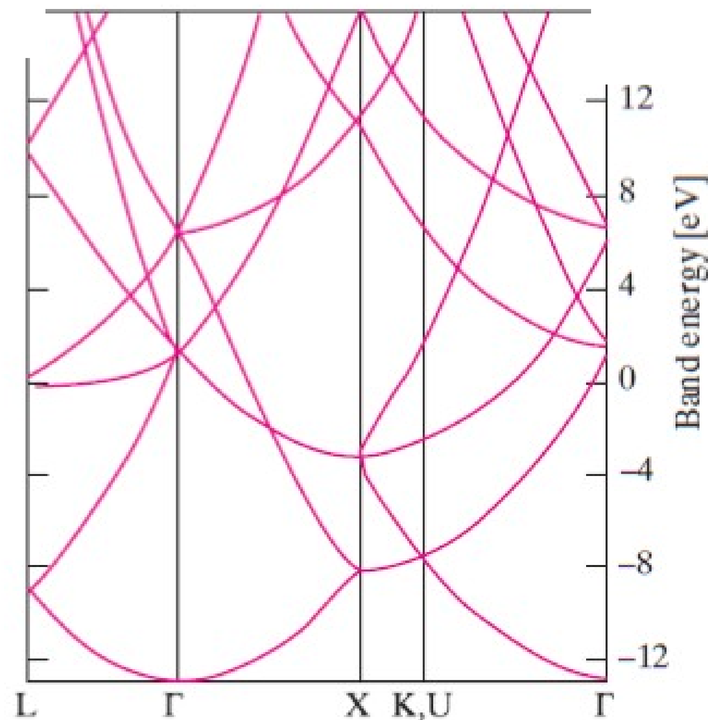
Porównanie pasm dla krzemu Si:
Free electron
TB-LCAO
DFT-advanced



(a) LCAO Bands



(b) True bands



(c) Free-electron bands