Materiale electrotehnice

1. Proprietati generale ale cristalelor

Prof.dr.ing.Florin Ciuprina

Structura disciplinei

Capitolul	Conținutul
	I Proprietati generale ale cristalelor
1	**Corpuri cristaline** Stari ale corpurilor Retele cristaline Defecte ale retelelor cristaline
2	**Electroni in cristale** Modele (clasic si cuantice) ale electronului. Benzi de energie asociate corpurilor cristaline. Clasificarea materialelor in conductori, semiconductori si izolatori.
	II Conductia electrica
3	**Conductia electrica a metalelor.** Conducția metalelor la temperaturi uzuale Supraconductibilitatea electrica.
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5	**Conductia electrica a izolatorilor solizi** Conductia in campuri slabe (Conductia electronica, Conductia ionica), Conductia in campuri intense (Străpungerea izolatorilor soliziși).
	III Proprietati dielectrice
6	**Polarizarea electrica** Tipuri de polarizare Polarizarea in campuri armonice. Pierderi in dielectrici.
	IV Proprietati magnetice
7	**Tipuri de magnetism**

Bibliografie

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- F. Ciuprina, *Materiale electrotehnice – fenomene si aplicatii*, Editura Printech, 2007
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- A. Ifrim, P. Notingher, *Materiale electrotehnice*, Editura Didactica si Pedagogica, 1992.
- L. Solymar, D. Walsh, *Electrical Properties of Materials*, Oxford University Press, 2004.
- B. Streetman, S. Banerjee, *Solid state Electronic Devices*, Prentice Hall, 2005
- http://www.superconductors.org/.

Mod de evaluare

- Laborator: 30p;
- Lucrări de control: 20p;
- Examen final (scris si oral):50p.

Cerinţele minimale pentru promovare:
- efectuarea tuturor lucrărilor de laborator,
- acumularea a 50 p şi
- acumularea a cel putin 20 p la examenul final.

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1. Corpuri cristaline

1.1. Stari ale corpurilor

1.2 Retele cristaline

1.3. Defecte ale retelelor cristaline

1. Corpuri cristaline

1.1. Stari ale corpurilor

1.2 Retele cristaline

1.3. Defecte ale retelelor cristaline

1.1. Stari ale corpurilor

A. La nivel macroscopic:

- Stare gazoasa
- Stare condensata - lichida
  - solida

Gaze: interactiuni slabe intre particulele constitutive (molecule, atomi), nu au nici forma si nici volum propriu.

Lichide: forte intermoleculare mai puternice dacat la gaze, au volume bine definite, dar nu au forme proprii.

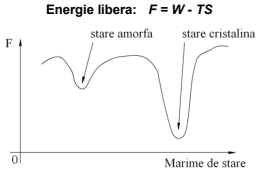
Solide: forte puternice intre particule (atomi, ioni, molecule), au forma si volum bine definite.

1.1. Stari ale corpurilor

B. La nivel microscopic:

- Stare cristalina
- Stare amorfa

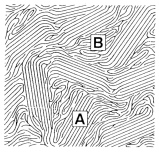
Energie libera: $F = W - TS$



Corpuri cristaline: ordine locala, ordine la distanta

Corpuri amorfe: ordine locala, dezordine la distanta

Corpuri partial cristaline: regiuni amorfe (B) si regiuni cristaline (A)



1.1. Stari ale corpurilor

Tipuri de cristale:

- ionice (NaCl)
- covalente (Ge, Si)
- metalice (Cu, Au, Ag)
- moleculare (cu legaturi Van der Waals, ex. parafina)
- cu legaturi de hidrogen

1. Corpuri cristaline

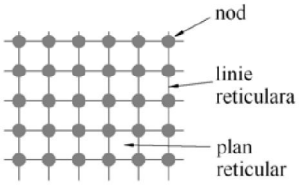
1.2. Retele cristaline

Retea cristalina:

succesiune regulata de puncte din spatiu, numite *noduri*.

Structura cristalina:

asociere nod - particula.



1.2. Retele cristaline

Sisteme cristaline:

Cubic $a = b = c$, $\alpha = \beta = \gamma = 90^\circ$

Tetragonal $a = b \neq c$, $\alpha = \beta = \gamma = 90^\circ$

Romboedric $a = b = c$, $\alpha = \beta = \gamma \neq 90^\circ$

Rombic $a \neq b \neq c$, $\alpha = \beta = \gamma = 90^\circ$

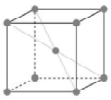
Monoclinic $a \neq b \neq c$, $\alpha = \gamma = 90^\circ \neq \beta$

Triclinic $a \neq b \neq c$, $\alpha \neq \beta \neq \gamma \neq 90^\circ$

Hexagonal $a = b \neq c$, $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$

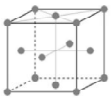
1.2. Retele cristaline

- 7 Sisteme cristaline ► 14 tipuri de retele (Bravais)
- cele mai importante tipuri de retele: CVC, CFC, HC



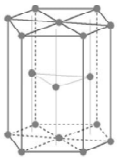
CVC

Cr, Mo, Ta, V, W,
Feα (<770 °C),
Feβ (770-912 °C),
Feδ (1394-1535 °C)



CFC

Cu, Au, Ag, Al, Ni, Pt,
Feγ (912-1394 °C)



HC

Co, Zn, Mg, Ti

1. Corpuri cristaline

1.3. Defecte ale retelelor cristaline

- Cristal ideal = fara defecte; la T = 0 K
- Cristal real = cu defecte; la T > 0 K

1.3. Defecte ale retelelor cristaline

- punctuale (zerodimensionale);
- liniare (unidimensionale);
- de suprafata (bidimensionale);
- de volum (tridimensionale).

1.3. Defecte ale retelelor cristaline

- Defecte punctuale:
  - nod vacant,
  - particula interstitiala
  - particula de impuritate (interstitiala, de substitutie)

Iacov Ilici Frenkel (1894-1952)
fizician rus

F-F' = defect Frenkel

$w_{dF} \approx 3$ eV ,(Al)

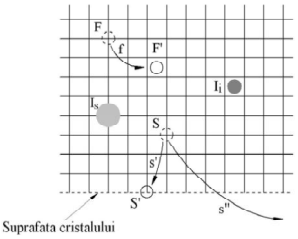
$N_F = \sqrt{NN'}e^{-\frac{w_{dF}}{2kT}}$

Walter Schottky (1886 -1976)
fizician german

S = defect Schottky

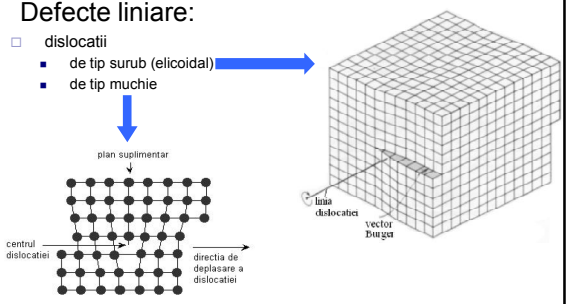
$w_{dS} \approx 0.75$ eV ,(Al)

$N_S = Ne^{-\frac{w_{dS}}{kT}}$



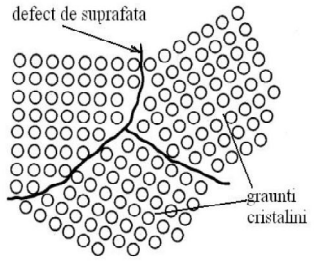
1.3. Defecte ale retelelor cristaline

- Defecte liniare:
  - dislocatii
    - de tip surub (elicoidal)
    - de tip muchie



1.3. Defecte ale retelelor cristaline

- Defecte de suprafata:



1.3. Defecte ale retelelor cristaline

- Defecte de volum:
  - cavitati,
  - incluziuni de corpuri straine,
  - fisuri

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2. Electroni in cristale

Conductia electrica

- fenomenul de deplasare ordonata a unor purtatori de sarcina electrica intr-un material sub actiunea campului electric
- se datoreaza:
  - electronilor (metale, semiconductori, izolatori);
  - ionilor (izolatori)

Conductivitatea electrica

- σ [S/m], $\sigma > 0$
- marime fizica ce caracterizeaza capacitatea unui material de a conduce curentul electric
- $\mathbf{J} = \sigma \mathbf{E}$ = legea conductiei electrice
- $\rho = 1/\sigma$ = rezistivitatea electrica, ρ [Ω m]

Conductivitatea electrica a materialelor

Ce sunt electronii?

Modele - clasic

- cuantice

2. Electroni in cristale

2.1. Modelul clasic al electronului

2.2 Modele cuantice. Unde asociate electronilor

2.3. Sisteme de particule. Numere cuantice

2.4. Starile electronilor in cristale

2.5. Repartitia electronilor pe nivelurile benzilor permise

2. Electroni in cristale

2.1. Modelul clasic al electronului

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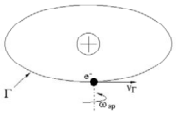
Conductia electrica

ELECTRON =
bilă minusculă, de rază $r \approx 2,82 \cdot 10^{-5}$ Å,

Ernest Rutherford (1871-1937)
fizician britanic

Niels Bohr (1885-1962)
fizician danez



a) $\mathbf{E} = 0$

$\mathbf{v} = \mathbf{v}_T$

b) $\mathbf{E} \neq 0$

$\mathbf{v} = \mathbf{v}_T + \mathbf{v}_D$

$$\tau_c = \frac{\tilde{l}}{v}$$

$$\mathbf{v_D} = \mathcal{M}\mathbf{E} \quad v_D = v_{D_0} \exp\left(-\frac{t}{\tau}\right)$$

2. Electroni in cristale

2.2 Modele cuantice. Unde asociate electronilor

electron ⟷ $w = hf = \frac{h\omega}{2\pi} = \hbar\omega,$ $p = \frac{h}{\lambda} = \frac{h}{2\pi}\frac{2\pi}{\lambda} = \hbar K,$ $\mathbf{p} = \hbar\mathbf{K}.$ ⟷ unda

Louis de Broglie (1892 - 1987)
fizician francez

Erwin Schrödinger (1887 - 1961)
fizician german

$\Psi(\mathbf{r},t)$ sau $\psi(\mathbf{r})$ – functie de unda = solutie a ec. Schrödinger:

$$-\frac{\hbar^2}{2m}\Delta\Psi + U\Psi = j\hbar\frac{\partial\Psi}{\partial t} \qquad |\Psi(\mathbf{r},t)|^2 = \mathcal{P}(\mathbf{r},t)$$

$$-\frac{\hbar^2}{2m}\Delta\psi + U\psi = w\psi \qquad |\psi(\mathbf{r})|^2 = \mathcal{P}(\mathbf{r})$$

2. Electroni in cristale

2.3 Sisteme de particule. Numere cuantice

Sisteme de particule

- nuclee + electroni = sistem de N particule.
- starile sistemului sunt descrise de functia de unda ψ_s, solutie a ecuatiei Schrödinger:

$$\sum_{i=1}^{N}\left[-\frac{\hbar^2}{2m_i}\left(\frac{\partial^2\psi_s}{\partial x_i^2}+\frac{\partial^2\psi_s}{\partial y_i^2}+\frac{\partial^2\psi_s}{\partial z_i^2}\right)\right]+U_s(x_1,\ldots,z_N)\psi_s=w_s\psi_s$$

$|\psi_s|^2=\psi_s\psi_s^*$ = densitatea de probabilitate a prezentei primei particule a sistemului in vecinatatea unui punct dat $M_1(x_1, y_1, z_1)$, a celei de a doua particule in vecinatatea punctului $M2(x_2, y_2, z_2)$ etc.

- $\psi_s=\Pi\psi_u$, ψ_u = expresii aproximative

2.3 Sisteme de particule. Numere cuantice

Numere cuantice

ψ_u depind in starile stationare de 4 numere cuantice:

- **numar cuantic principal** n
  - determina valorile energiei electronului
  - $n = 1, 2, 3, \ldots$
- **numar cuantic secundar** l
  - determina valorile momentului cinetic orbital si ale momentului magnetic orbital ale electronului
  - $l = 0, 1, 2, 3, \ldots,$ n-1
- **numar cuantic magnetic** m_l
  - determina valorile proiectiei momentului cinetic orbital si ale proiectiei momentului magnetic orbital pe o directie arbitrara (adesea directia campului magnetic exterior)
  - $m_l = 0, \pm1, \pm2, \ldots, \pm l$
- **numar cuantic de spin** m_s
  - determina valorile proiectiei momentului cinetic de spin si ale proiectiei momentului magnetic de spin pe o directie arbitrara (adesea directia campului magnetic exterior)
  - $m_s = \pm½$

2.3 Sisteme de particule. Numere cuantice

Numere cuantice

n, l, m_l - determina o *stare orbitala* a electronului

n, l, m_l, m_s - determina o *stare cuantica* a electronului

- **Principiul de excluziune al lui Pauli:**
  Intr-un sistem format din particule avand numarul cuantic de spin m_s semiintreg (electroni, protoni,neutroni),intr-o stare cuantica se poate gasi o singura particula componenta a sistemului.

2. Electroni in cristale

2.4 Starile electronilor in cristale

Ipoteze simplificatoare:

- *electroni indiscernabili*, functia de unda asociata unui electron descrie starile oricarui electron din cristal.
- *cristale unidimensionale*.
- *ioni imobili in noduri* (exista, insa, o interactiune electron-ion prin intermediul campului electric produs de ioni).
- exista o *interactiune* intre *electronii studiati* si campul electric produs de *alti electroni*.

$$-\frac{\hbar^2}{2m_0}\frac{d^2\psi_s}{dx^2} + U(x)\psi_s = w_s\psi_s$$

$$U(x) = U_0 + \sum_{n=1}^{\infty} U_n \cos\left(\frac{2nx\pi}{a}\right)$$

2.4 Starile electronilor in cristale

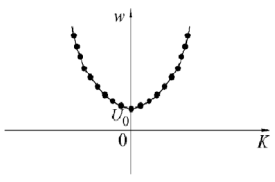
Aproximatia electronilor liberi:

- Ipoteze:
  - electronii nu interactioneaza cu ionii din nodurile retelei → $U = U_0$
  - conditie de ciclicitate (Born): $\psi(x) = \psi(x+L)$

$$\psi(x) = A\exp(jKx)$$

$$w = \frac{\hbar^2}{2m_0}K^2 + U_0$$

$$K = \frac{2n\pi}{L} \quad , n \in Z$$



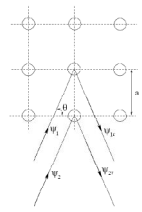
2.4 Starile electronilor in cristale

Aproximatia electronilor cvasiliberi:

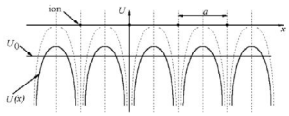
Ipoteze:

- electronii interactioneaza cu ionii din nodurile retelei → $U(x) = U_0 + \sum_{n=1}^{\infty} U_n \cos\left(\frac{2n\pi}{a}\right)$

reflexii Bragg cand $2a\sin\theta = n\lambda, \quad n = \pm 1, \pm 2, \ldots$



$K = \frac{n\pi}{a}$, pentru cristalul unidimensional



2.4 Starile electronilor in cristale

Aproximatia electronilor cvasiliberi:

$K = \pm\frac{\pi}{a}$ → unde stationare:

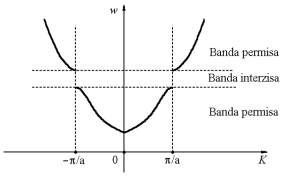
$$\psi(+) = A\exp\left(\frac{j\pi x}{a}\right) + A\exp\left(-\frac{j\pi x}{a}\right) 2A\cos\left(\frac{x\pi}{a}\right) \Rightarrow \mathcal{P}(+) = |\psi(+)|^2 \sim \cos^2\left(\frac{x\pi}{a}\right)$$

$$\psi(-) = A\exp\left(\frac{j\pi x}{a}\right) - A\exp\left(-\frac{j\pi x}{a}\right) 2Aj\sin\left(\frac{x\pi}{a}\right) \Rightarrow \mathcal{P}(-) = |\psi(-)|^2 \sim \sin^2\left(\frac{x\pi}{a}\right)$$

$$w(+) = \frac{\hbar^2 K^2}{2m_0} + U_0 - \frac{U_1}{2}$$

$$w(-) = \frac{\hbar^2 K^2}{2m_0} + U_0 + \frac{U_1}{2}$$

$$w_i = U_1 = w(-) - w(+)$$



2.4 Starile electronilor in cristale

Aproximatia electronilor cvasiliberi:

Masa efectiva a electronului:

$$\mathbf{F} = m_0\mathbf{a} \qquad \mathbf{F} = \mathbf{F}_{int} + \mathbf{F}_{ext}$$

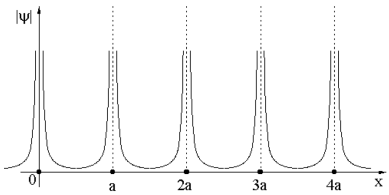
$$F_{ext} = m_0^* a \qquad \boxed{m_0^* = \hbar^2\left(\frac{\mathrm{d}^2 w}{\mathrm{d}K^2}\right)^{-1}}$$

2.4 Starile electronilor in cristale

Aproximatia electronilor puternic legati:

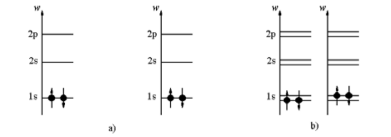
Ipoteze:

- functii de unda de tip Heitler-London

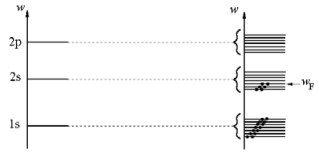


2.4 Starile electronilor in cristale

Aproximatia electronilor puternic legati:



Niveluri de energie pentru doi atomi de He: a) izolaţi, şi b) apropiaţi



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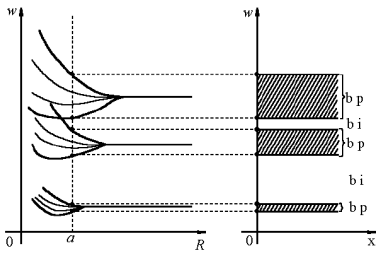
Aproximatia electronilor puternic legati:



2. Electroni in cristale

2.1. Modelul clasic al electronului

2.2 Modele cuantice. Unde asociate electronilor

2.3. Sisteme de particule. Numere cuantice

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2.5. Repartitia electronilor pe nivelurile benzilor permise

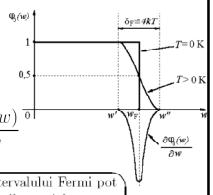
2.5 Repartitia electronilor pe nivelurile benzilor permise

Statistica Fermi-Dirac:

Repartitia electronilor pe nivelurile benzilor permise ➡ Statistica Fermi-Dirac

E = 0, echilibru termic: $\varphi_0(w) = \frac{1}{e^{\frac{w - w_F}{kT}} + 1}$

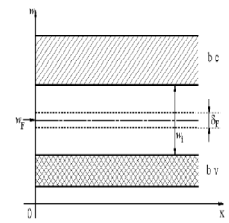
E ≠ 0, echilibru termic: $\varphi(w) = \varphi_0(w) + \tau q_0 \mathbf{v}\mathbf{E}\frac{\partial \varphi_0(w)}{\partial w}$



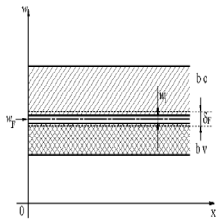
Concluzie: Numai electronii a căror energie aparţine intervalului Fermi pot fi electroni de conducţie, adică numai electronii de pe nivelurile parţial ocupate pot stabili un curent electric de conducţie în cristal.

2.5 Repartitia electronilor pe nivelurile benzilor permise

Conductori, semiconductori, izolatori:



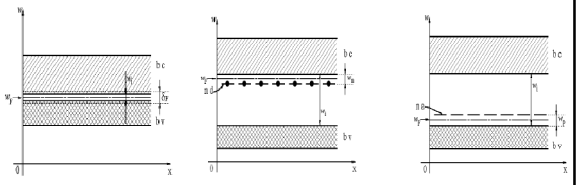
izolator
w_i = > 3 - 5 eV



semiconductor intrinsec
$w_i = 10^{-2} – 10^{-1}$ eV

2.5 Repartitia electronilor pe nivelurile benzilor permise

Conductori, semiconductori, izolatori:



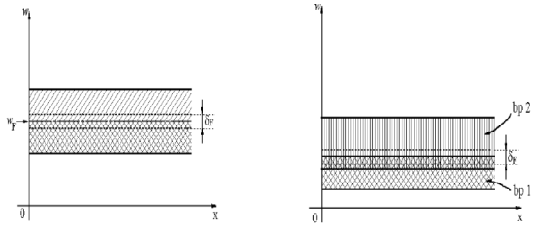
semiconductor intrinsec
$w_i = 10^{-2} – 10^{-1}$ eV

tip n
semiconductori extrinseci
$w_i = 0.5 – 1.5$ eV

tip p

2.5 Repartitia electronilor pe nivelurile benzilor permise

Conductori, semiconductori, izolatori:



metal monovalent

metal bivalent

2.5 Repartitia electronilor pe nivelurile benzilor permise

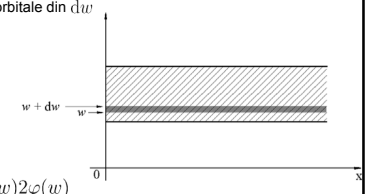
Concentratia electronilor dintr-o banda permisa:

$\mathrm{d}N_{niv}$ - concentratia nivelurilor orbitale din $\mathrm{d}w$

$g(w)$ - densitate de stari

$$\mathrm{d}N_{niv} = g(w)\mathrm{d}w$$

$$g(w) = \frac{(2m_0^*)^{\frac{3}{2}}}{4\pi^2\hbar^3} w^{\frac{1}{2}}$$



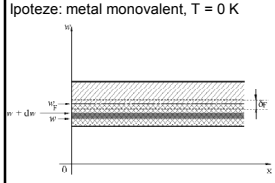
$$\mathrm{d}N_0 = \mathrm{d}N_{niv} 2\varphi(w) = g(w) 2\varphi(w)$$

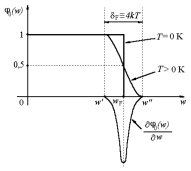
$$\mathrm{d}N_0 = \frac{(2m_0^*)^{\frac{3}{2}}}{2\pi^2\hbar^3} w^{\frac{1}{2}} \varphi(w)\mathrm{d}w \quad \Rightarrow \quad N_0 = \int_0^\infty \mathrm{d}N_0$$

2.5 Repartitia electronilor pe nivelurile benzilor permise

Concentratia electronilor dintr-o banda permisa:

Ipoteze: metal monovalent, T = 0 K





$$\left.\begin{aligned} dN_0 &= \frac{(2m_0^*)^{\frac{3}{2}}}{2\pi^2\hbar^3} w^{\frac{1}{2}} \varphi(w) dw \\ N_0 &= \int_0^{\infty} dN_0 \end{aligned}\right\} \Rightarrow \boxed{N_0 = \frac{(2m_0^*)^{\frac{3}{2}}}{3\pi^2\hbar^3} w_F(0)^{\frac{3}{2}}}$$

2.5 Repartitia electronilor pe nivelurile benzilor permise

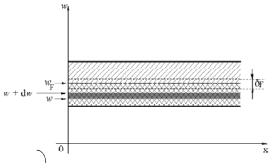
Concentratia electronilor dintr-o banda permisa:

Ipoteze: metal monovalent, T = 0 K

$$N_0 = \frac{(2m_0^*)^{\frac{3}{2}}}{3\pi^2\hbar^3} w_F(0)^{\frac{3}{2}}.$$

$$\Downarrow$$

$$\boxed{w_F(0) = \frac{\hbar^2}{2m_0^*}(3\pi^2 N_0)^{\frac{2}{3}}}$$



$$w_F(T) = w_F(0)\left[1 - \frac{\pi^2}{12}\left(\frac{kT}{w_F(0)}\right)^2\right]$$

La temperaturi uzuale (stare cristalina)

$$\boxed{w_F(T) \approx w_F(0)}$$