Kvadrupólus-felhasadás

$$\hat{\mathcal{H}}_Q = \frac{1}{5\varepsilon_0} \sum_{m=-2}^{2} (-1)^m \hat{T}_{2m} U_{2,-m} = \frac{e}{4} \sum_{m=-2}^{2} (-1)^m \hat{Q}_{2m} V_{2-m}$$

$$\langle I M' | \hat{Q}_{2m} | I M'' \rangle = (-1)^{I-M'} \begin{pmatrix} I & 2 & I \\ -M' & m & M'' \end{pmatrix} \langle I \| Q_2 \| I \rangle$$

$$Q := \langle I I | \hat{Q}_{20} | I I \rangle = \begin{pmatrix} I & 2 & I \\ -I & 0 & I \end{pmatrix} \langle I \| Q_2 \| I \rangle$$

$$\langle I M' | \hat{Q}_{2m} | I M'' \rangle = (-1)^{I-M'} \frac{\begin{pmatrix} I & 2 & I \\ -M' & m & M'' \end{pmatrix}}{\begin{pmatrix} I & 2 & I \\ -I & 0 & I \end{pmatrix}} Q$$

A 3j-szimbólumoktól is meg lehet szabadulni, ha ekvivalens operátorokat vezetünk be:

$$\hat{p}_{20} := \frac{1}{2}(3 I_z^2 - I^2)$$

$$\hat{p}_{2\pm1} := \mp\sqrt{\frac{3}{8}}\,(\hat{I}_z \hat{I}_\pm + \hat{I}_\pm \hat{I}_z)$$

$$\hat{p}_{2\pm2} := \sqrt{\frac{3}{8}}\,\hat{I}_\pm^2$$

$\hat{p}_{2m}$ másodrendű szférikus tenzor-operátor

$$\langle I M' | \hat{p}_{2m} | I M'' \rangle = (-1)^{I-M'} \begin{pmatrix} I & 2 & I \\ -M' & m & M'' \end{pmatrix} \langle I \| p_2 \| I \rangle$$

$$p := \langle I I | \hat{p}_{20} | I I \rangle = \begin{pmatrix} I & 2 & I \\ -I & 0 & I \end{pmatrix} \langle I \| p_2 \| I \rangle$$

$$\langle I M' | \hat{p}_{2m} | I M'' \rangle = (-1)^{I-M'} \frac{\begin{pmatrix} I & 2 & I \\ -M' & m & M'' \end{pmatrix}}{\begin{pmatrix} I & 2 & I \\ -I & 0 & I \end{pmatrix}} p$$

$$p \;\Downarrow\; \frac{1}{2}\left(3I^2 - I(I+1)\right)$$

$$\langle I M' | \hat{Q}_{2m} | I M'' \rangle = \frac{Q}{p} \langle I M' | \hat{p}_{2m} | I M'' \rangle$$

$$\Downarrow$$

$$\boxed{\hat{Q}_{2m} = \frac{2Q}{3I^2 - I(I+1)} \hat{p}_{2m}}$$

Az ETG-tenzor elemei:

$$V_{20} = V_{zz}$$

$$V_{2\pm1} = \mp\sqrt{\frac{2}{3}} \left(V_{xz} \pm i V_{yz} \right)$$

$$V_{2\pm2} = \frac{1}{\sqrt{6}} \left(V_{xx} - V_{yy} \pm 2i V_{xy} \right)$$

Az ETG-tenzor főtengely-rendszerében:

$$V_{20} = V_{zz}$$

$$V_{2\pm1} = 0$$

$$V_{2\pm2} = \frac{\eta}{\sqrt{6}} V_{zz}$$

$$\boxed{\hat{\mathcal{H}}_Q} = \frac{e}{4} \left(V_{20} Q_{20} + V_{2-2} Q_{22} + V_{22} Q_{2-2} \right) =$$

$$= \frac{e}{4} \underbrace{\frac{2 Q V_{zz}}{3I^2 - I(I+1)}}_{I(2I-1)} \Big[\underbrace{\hat{p}_{20}}_{\Downarrow\ \frac{1}{2}(3\hat{I}_z^2 - \hat{I}^2)} + \frac{\eta}{\sqrt{6}} \underbrace{(\hat{p}_{22} + \hat{p}_{2-2})}_{\Downarrow\ \sqrt{\frac{3}{8}}(\hat{I}_+^2 + \hat{I}_-^2)} \Big] =$$

$$\boxed{= \frac{e Q V_{zz}}{4I(2I-1)} \left[3\hat{I}_z^2 - I(I+1) + \frac{\eta}{2} (\hat{I}_+^2 + \hat{I}_-^2) \right]}$$

A vonalak helyzete

3/2 → 1/2 átmenet (pl. ^{57}Fe):

$I = 3/2$:

$$\mathcal{H}_{MM'} = \langle IM | \hat{\mathcal{H}}_Q | IM' \rangle = \underbrace{\hbar\omega_E(3/2)}_{\Downarrow \; \frac{eQV_{zz}}{\hbar} \frac{1}{4I(2I-1)}} \begin{pmatrix} 3 & 0 & \sqrt{3}\eta & 0 \\ 0 & -3 & 0 & \sqrt{3}\eta \\ \sqrt{3}\eta & 0 & -3 & 0 \\ 0 & \sqrt{3}\eta & 0 & 3 \end{pmatrix}$$

Sajátérték-egyenlet:

$$\sum_{M'} \mathcal{H}_{MM'} e_{\beta M'} = E_\beta e_{\beta M}$$

Sajátérték: $E_i = \hbar\omega_E \varepsilon_i$

$$\varepsilon_1 = \varepsilon_2 = 3\sqrt{1+\eta^2/3}$$

$$|e_1\rangle = e_+ \left|\tfrac{3}{2}\ \tfrac{3}{2}\right\rangle + e_- \left|\tfrac{3}{2}\ -\tfrac{1}{2}\right\rangle$$

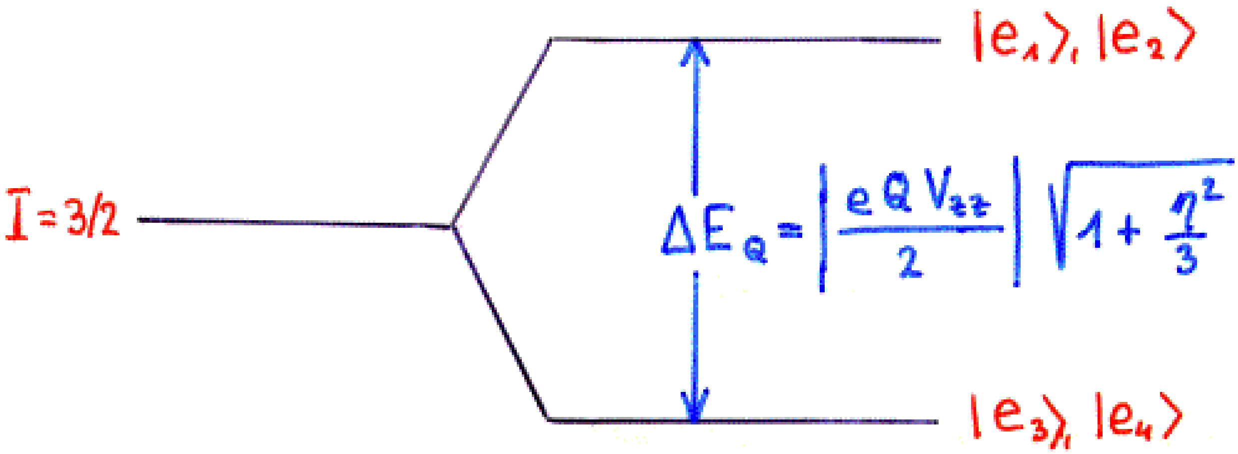
$$|e_2\rangle = e_+ \left|\tfrac{3}{2}\ -\tfrac{3}{2}\right\rangle + e_- \left|\tfrac{3}{2}\ \tfrac{1}{2}\right\rangle$$

$$\varepsilon_3 = \varepsilon_4 = -3\sqrt{1+\eta^2/3}$$

$$|e_3\rangle = e_- \left|\tfrac{3}{2}\ \tfrac{3}{2}\right\rangle - e_+ \left|\tfrac{3}{2}\ -\tfrac{1}{2}\right\rangle$$

$$|e_4\rangle = e_- \left|\tfrac{3}{2}\ -\tfrac{3}{2}\right\rangle - e_+ \left|\tfrac{3}{2}\ \tfrac{1}{2}\right\rangle$$

$$e_\pm = \frac{1}{\sqrt{2}} \sqrt{1 \pm \frac{1}{\sqrt{1+\frac{\eta^2}{3}}}}$$



A vonalhelyekből nyerhető információ

$$\Delta_{ik} = E_i(I_g) - E_k(I_a)$$

gerjesztett   alap-
állapot

$$\Delta_{ik} = \hbar\left[\omega_E(I_g)\varepsilon_i(I_g) - \omega_E(I_a)\varepsilon_k(I_a)\right] =$$

$$= \hbar\omega_E(I_a)\left[\frac{Q_g}{Q_a}\varepsilon_i(I_g) - \varepsilon_k(I_a)\right]$$

Teljes felhasadás (skálatényező) $\Rightarrow |V_{zz}|$

A spektrumot kell / nem kell tükrözni $\Rightarrow \mathrm{sign}(V_{zz})$

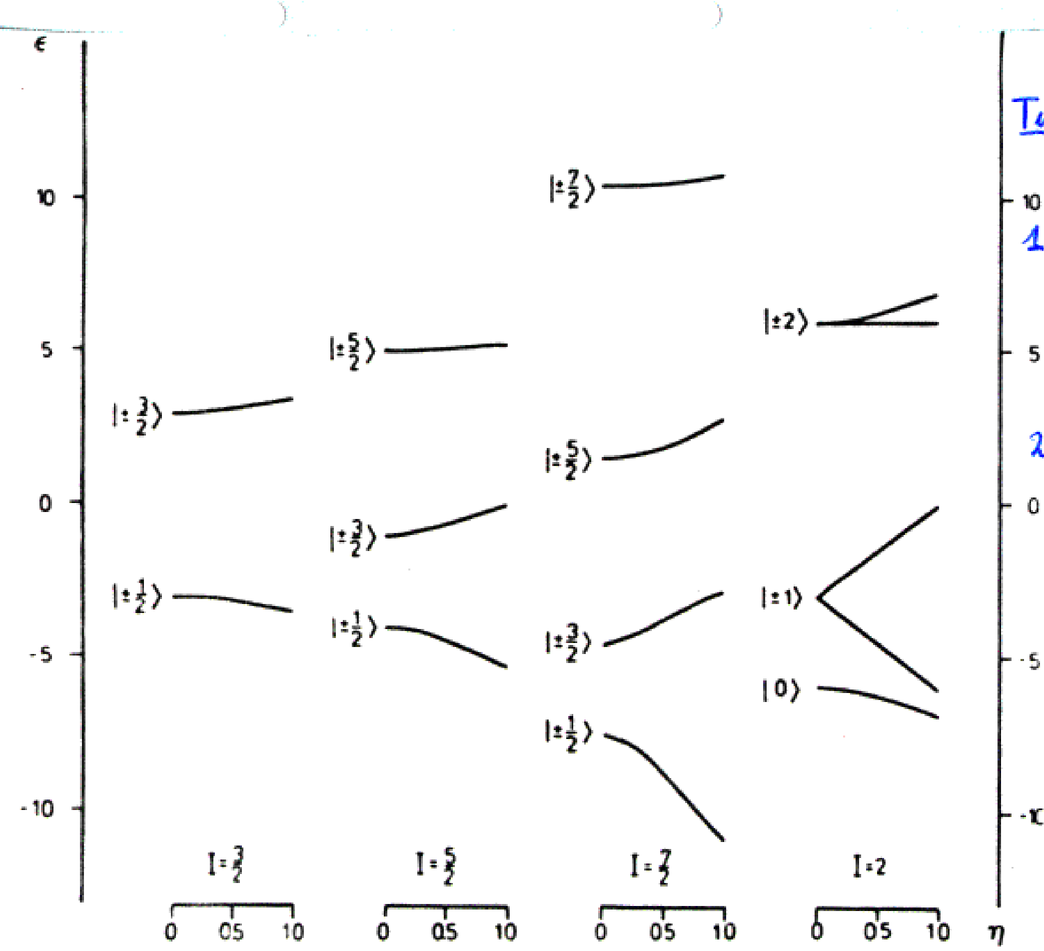
Vonalhelyek (ha kettőnél több vonal van) $\Rightarrow \eta$

Az ETG-tenzor iránya csak a vonalhelyekből nem határozható meg; ehhez a vonalintenzitások irányfüggését is mérni kell.

Eigenschaften:

1. $\frac{d\varepsilon_i}{d\eta} = 0$ bei $\eta = 0$ für I = halbzahlig

2. Symmetrische Aufspaltung bei $\eta = 1$



Tulajdonságok:

1. $\frac{d\varepsilon_i}{d\eta} = 0$ $\eta = 0$-nál, ha I = feles

2. A felhasadás szimmetrikus, ha $\eta = 1$

FIGURE 1. The energy splitting of the various spin states is plotted versus the asymmetry parameter η of the electric field gradient. The energies are given in units of $\mu_I = eQV_{zz}/4I(2I-1)$ for the I = 3/2, 2, and $2\mu_I$ for I = 5/2, 7/2.

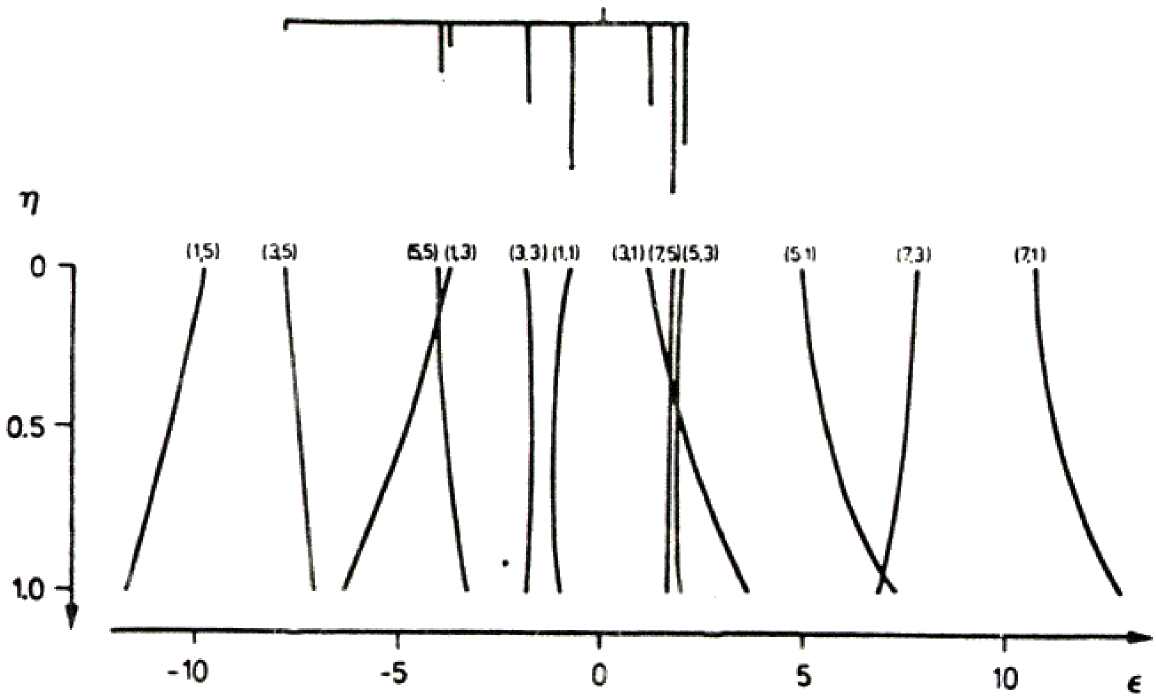


FIGURE 2. The dependence of the line positions δ_μ on the asymmetry parameter η is shown for an ($I_e = 7/2 \rightarrow I_g = 5/2$) transition. The ratio $\mu_{I_e}/\mu_{I_g} = 0.638$ corresponds to the ratio of the quadrupole moments $Q_e/Q_g = 1.34$ of the 21.6-keV transition of ^{151}Eu. The velocity is given in units of $\mu_{I_g}c/E_0$. The symbols (n,m) stand for the transition $(\pm n/2 \rightarrow \pm m/2)$, where the $|\pm m/2\rangle$ are the eigenstates of an axial EFG. On the top of the figure is the stick diagram of the spectrum at $\eta = 0$ with the intensities of a thin powder absorber in the case of a $M1$ transition.

Vonalintenzitások

M1 átmenetre:

$$I(M_a, m, M_g) \sim |\langle I_a, M_a | \hat{\mathcal{H}}(M1) | I_g, M_g \rangle|^2 F_{1m}(\theta)$$

$\Uparrow$ elsőrendű szférikus tenzoroperátor

$$I(M_a, m, M_g) \sim \begin{pmatrix} I_a & 1 & I_g \\ -M_a & m & M_g \end{pmatrix}^2 F_{1m}(\theta)$$

0, ha $M_a - M_g \neq m$

- $I_a = 1/2$, $I_g = 3/2$ (pl. ^{57}Fe):

$$\begin{pmatrix} 1/2 & 1 & 3/2 \\ \mp 1/2 & \mp 1 & \pm 3/2 \end{pmatrix}^2 = \frac{3}{12} \qquad \begin{pmatrix} 1/2 & 1 & 3/2 \\ \mp 1/2 & 0 & \pm 1/2 \end{pmatrix}^2 = \frac{2}{12}$$

$$\begin{pmatrix} 1/2 & 1 & 3/2 \\ \pm 1/2 & \mp 1 & \pm 1/2 \end{pmatrix}^2 = \frac{1}{12}$$

$$F_{1\pm1}(\theta) = \frac{1}{4}(1+\cos^2\theta) \qquad F_{10}(\theta) = \frac{1}{2}\sin^2\theta$$

- Tiszta kvadrupólus-kölcsönhatás, $\eta = 0$:

$$I_\pi(\theta) = \frac{3}{8}(1+\cos^2\theta) \qquad (M_g = \pm 3/2,\ M_a = \pm 1/2)$$

$$I_\sigma(\theta) = \frac{1}{8}(5 - 3\cos^2\theta) \qquad (M_g = \pm 1/2; \mp 1/2,\ M_a = \pm 1/2)$$

Textúra-mentes pormintára: $I_1 = I_2$

Anomáliák oka:

- textúra
- a Mössbauer-Lamb (Debye-Waller)-faktor anizotrópiája (Goldanszkij-Karjagin-effektus)

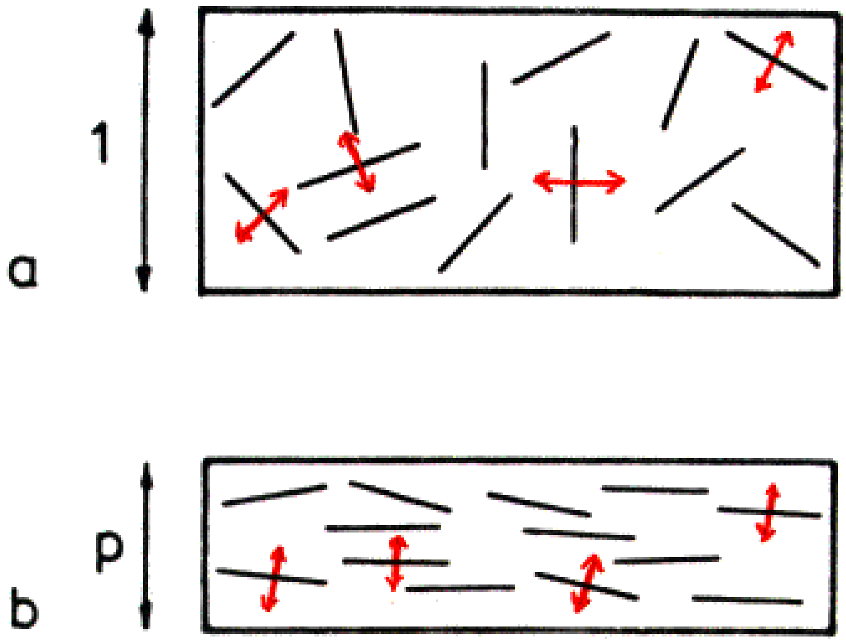


Fig. 1a and b. The appearance of texture in a non-oriented polycrystalline sample of height unity (a) after a compression to heigt p (b)

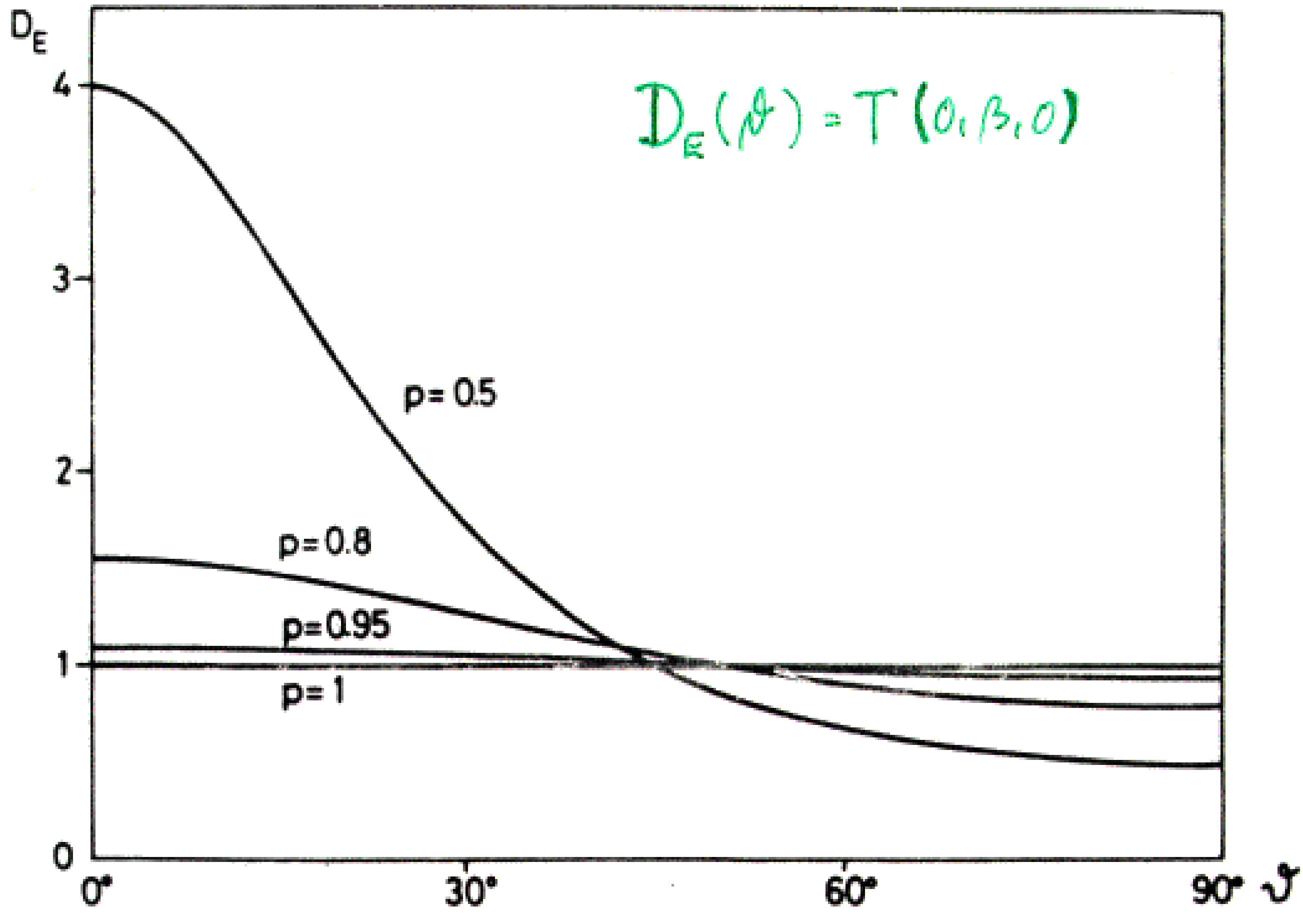


Fig. 5. The texture function $D_E(\vartheta)$ of planes after a compression from the original height of unity to p

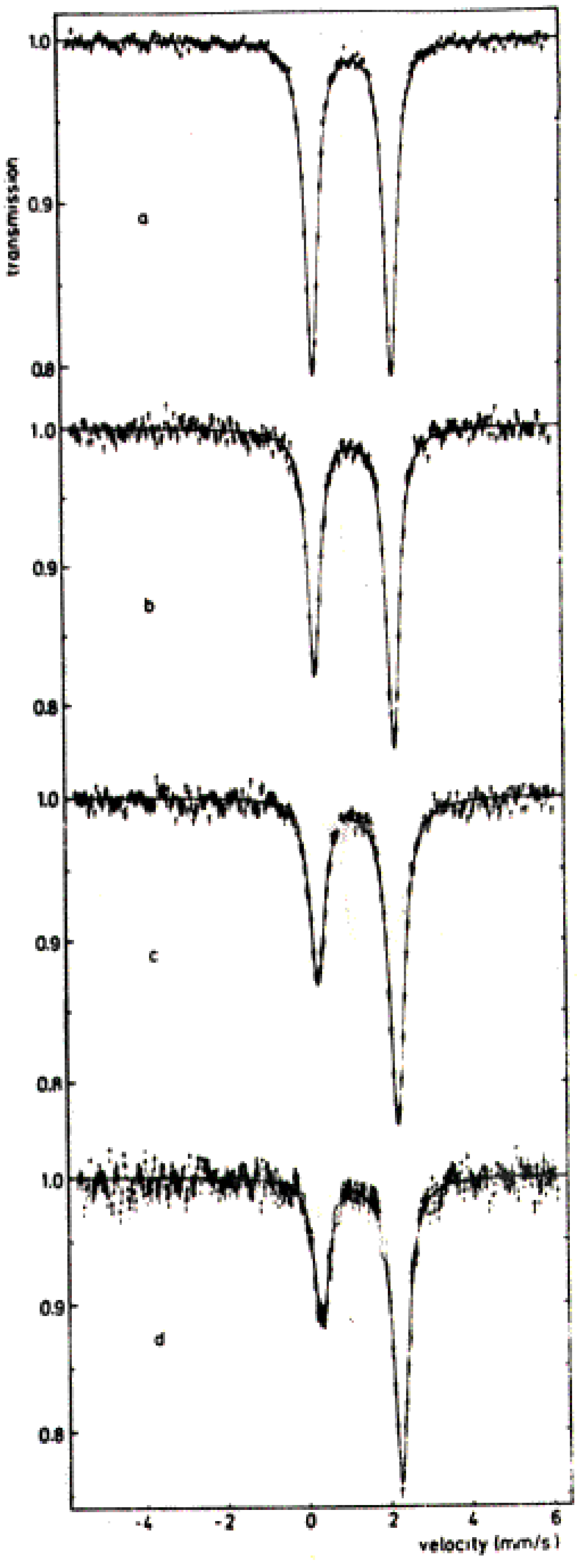


Fig. 2. Some typical Mössbauer spectra of polycrystalline $FeCO_3$ mixed with active carbon powder at 185 K after applying various longitudinal magnetic fields. (a) Original spectrum, (b) after 5 kG, (c) after 10 kG, (d) after 50 kG.

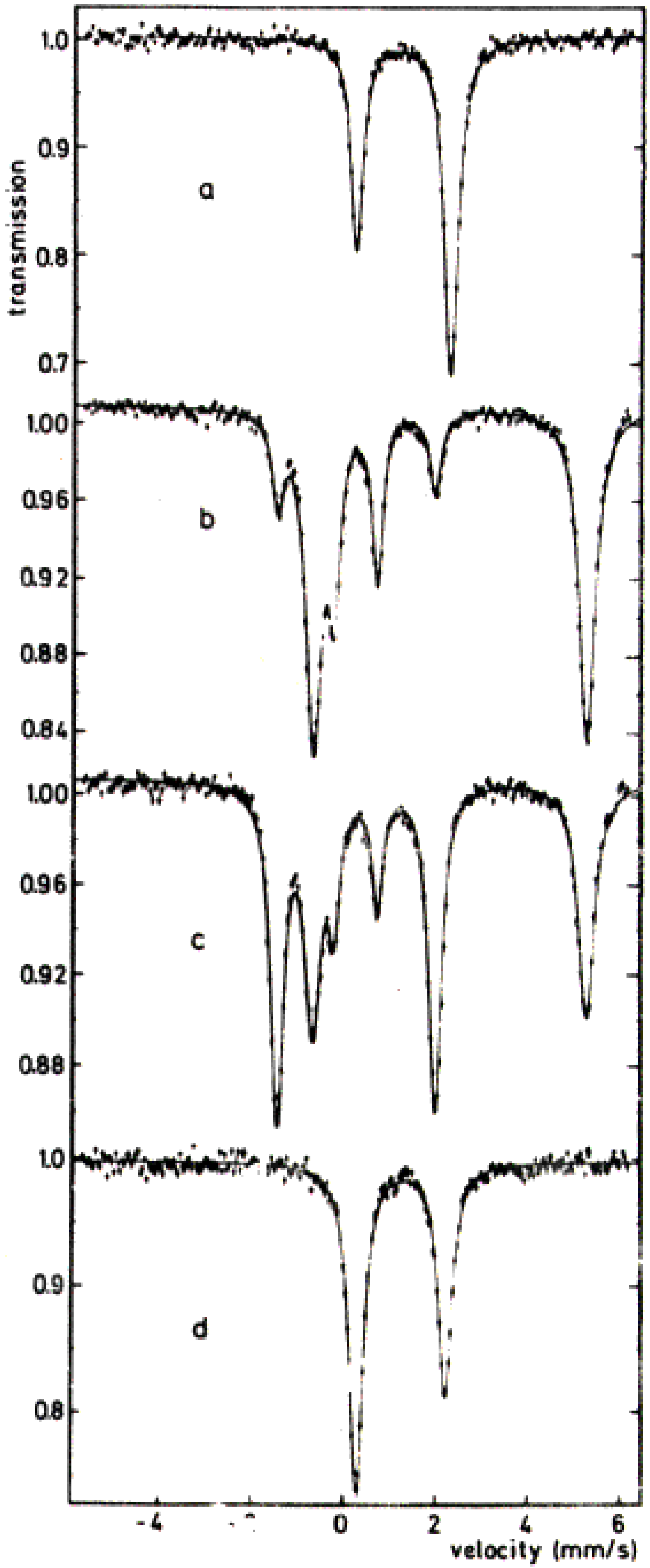


Fig. 4. The reversal of the induced texture: Mössbauer spectra of polycrystalline $FeCO_3$ mixed with active carbon powder. (a) Spectrum at 60 K after 7·5 kG at 60 K, (b) spectrum at 5 K after 7·5 kG at 60 K, (c) spectrum at 5 K after 50 kG at 5 K, (d) spectrum at 185 K after 50 kG at 5 K.

Az ETG eredete

$$q = \frac{V_{zz}}{e}$$

$$\eta q = \frac{V_{xx} - V_{yy}}{e}$$

$$q = (1 - R_s)\, q_{ion} + (1 - \gamma_\infty)\, q_{rács}$$

$$\eta q = \underbrace{(1 - R_s)\, \eta_{ion} q_{ion} + (1 - \gamma_\infty)}_{\text{Sternheimer-tényezők}}\, \eta_{rács}\, q_{rács}$$

$$0 \lesssim R_s \lesssim 1 \qquad -100 \lesssim \gamma_\infty \lesssim +100$$

Ponttöltés-modell:

$$q_{rács} = \frac{1}{e} \sum_i e_i \frac{3\cos^2\vartheta_i - 1}{r_i^3}$$

$$\eta_{rács}\, q_{rács} = \frac{1}{e} \sum_i e_i \frac{3\sin^2\vartheta_i \cos 2\varphi_i}{r_i^3}$$

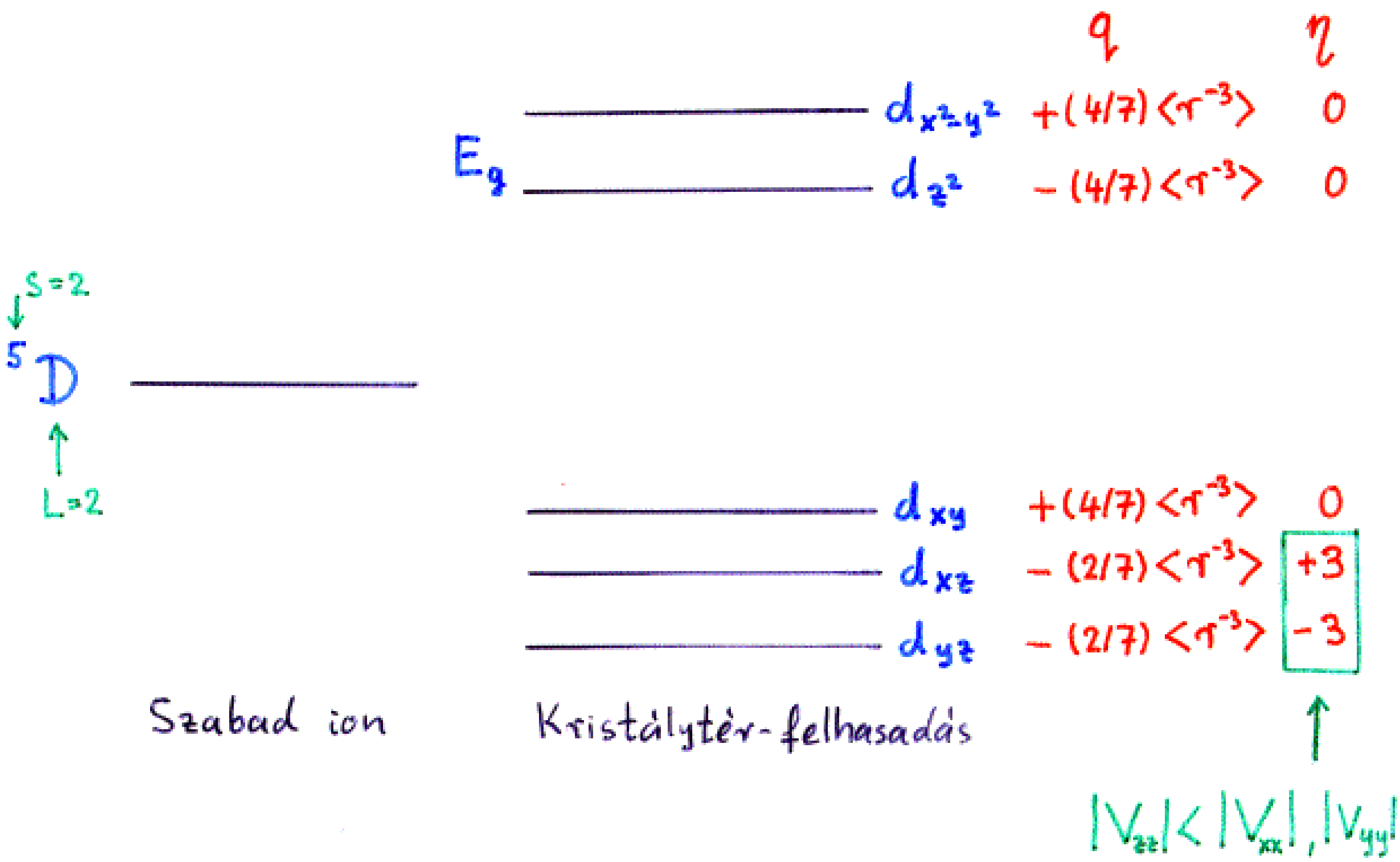
probléma: mekkorák az effektív töltések?

$$q_{ion} = -\sum_i \int \Psi^*(\underline{r}_1, \ldots \underline{r}_Z) \frac{3\cos^2\vartheta_i - 1}{r_i^3} \Psi(\underline{r}_1, \ldots \underline{r}_Z)\, d^3\underline{r}_1 \ldots d^3\underline{r}_Z$$

$$\eta_{ion}\, q_{ion} = -\sum_i \int \Psi^*(\underline{r}_1, \ldots \underline{r}_Z) \frac{3\sin^2\vartheta_i \cos 2\varphi_i}{r_i^3} \Psi(\underline{r}_1, \ldots \underline{r}_Z)\, d^3\underline{r}_1 \ldots d^3\underline{r}_Z$$

Elegendő az integrálokat a nem lezárt héjakra számolni.

Az egyes elektronállapotok járulékai (példa: Fe^{2+}):



- Gyors átmenet (relaxáció) az elektron-nívók között ($\tau \ll 1/\omega_E$): a mag az alnivók által keltett ETG termikus átlagát látja.

$\Downarrow$

a megfigyelt ETG hőmérsékletfüggő.

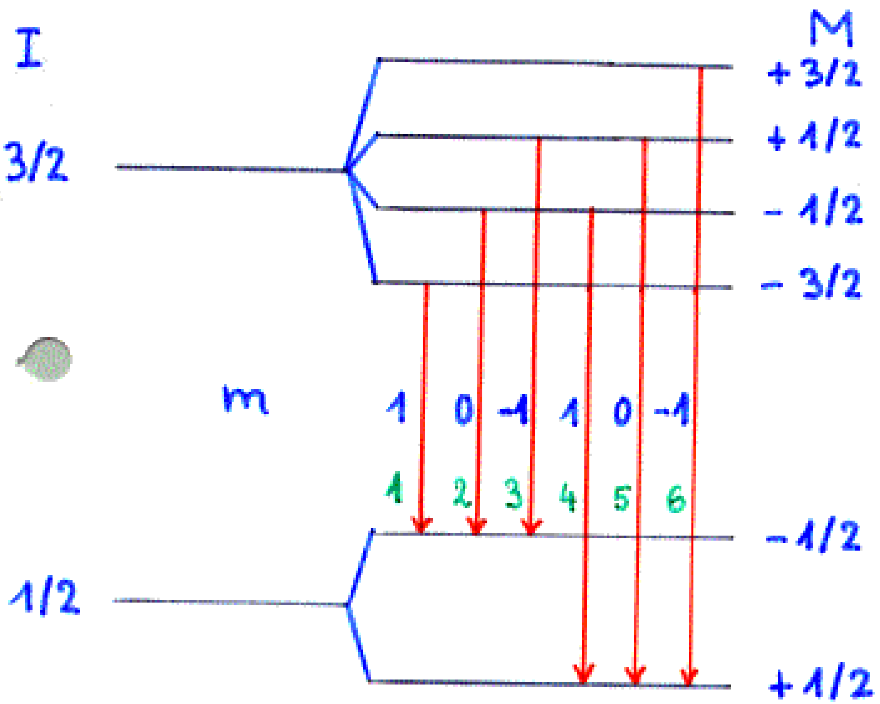
- Lassú átmenet ($\tau \gg 1/\omega_E$): a megfigyelt spektrum az egyes elektron-nivókhoz tartozó sztatikus alspektrumok Boltzmann-súlyozott átlaga.

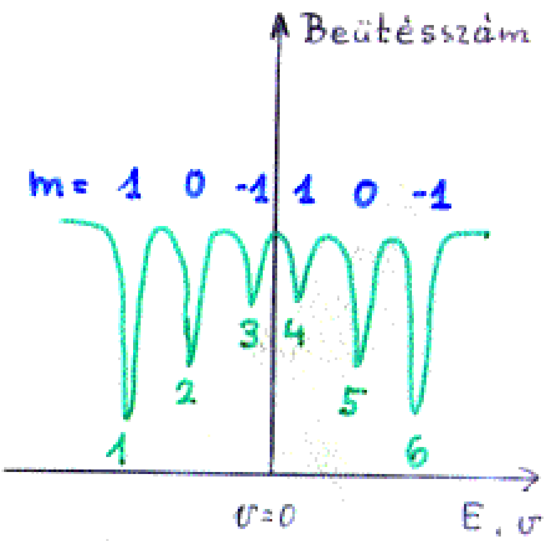
- Átmeneti tartomány ($\tau \approx 1/\omega_E$): "relaxációs" spektrumok

Mágneses felhasadás

$|I, M\rangle: \quad E_{mágn} = -g \mu_n B M$

Pl.: $I_g = 3/2$, $I_a = 1/2$, M1 átmenet (^{57}Fe)





$B \sim v_6 - v_1$

$$\underline{B} = \underline{B}_0 \boxed{- \frac{D\mu_0}{4\pi}\underline{M} + \frac{\mu_0}{3}\underline{M} + \underline{B}_d} + \underline{B}_s + \underline{B}_L + \underline{B}_D$$

külső tér

lemágnesezési tér (gömbre: $D = \frac{4\pi}{3}$)

Lorentz-tér

külső dipólusok tere

Fermi-féle kontakt-tér

pálya-impulzus-nyomaték-tér

spin-dipólus-tér

$\Downarrow$

spontán mágnesezettség hiányában elhanyagolható

$\underline{B}_s \sim \langle \underline{S} \rangle$

$\underline{B}_L \sim \langle \underline{L} \rangle$

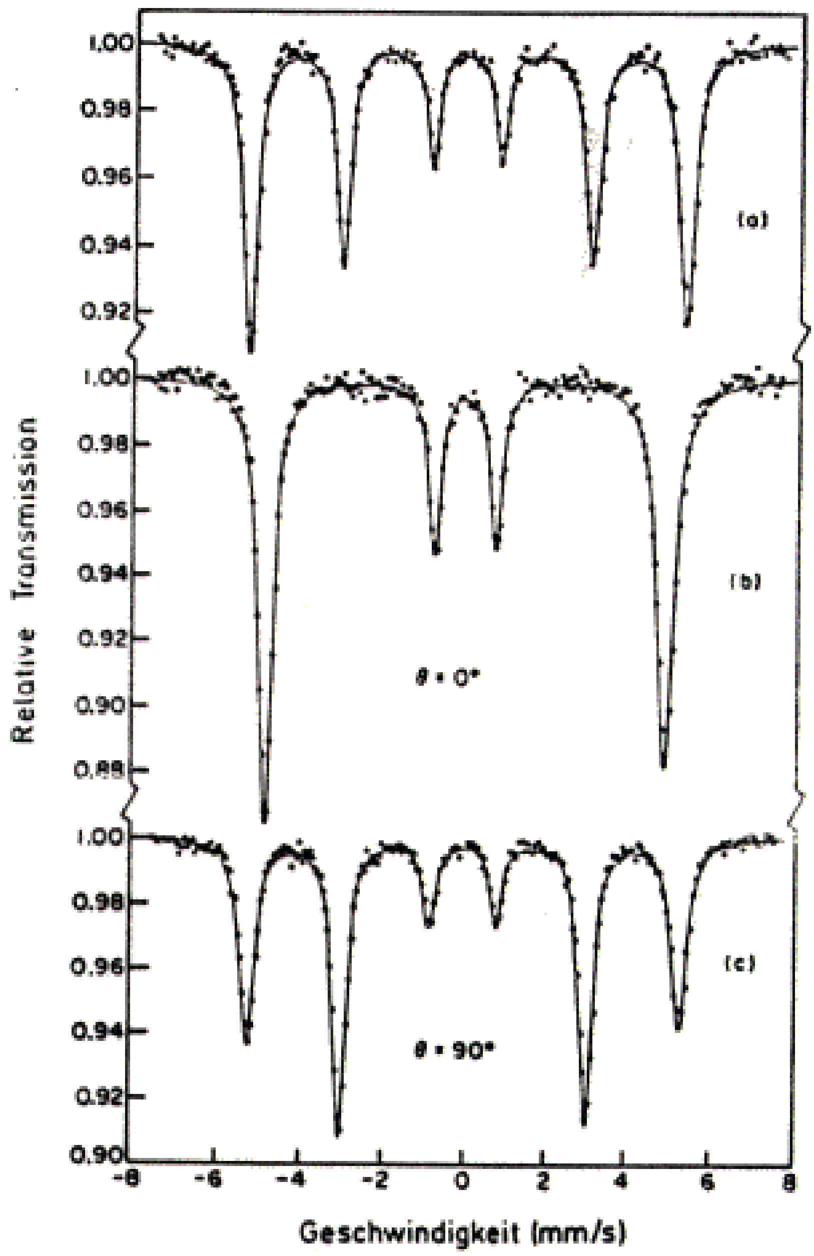
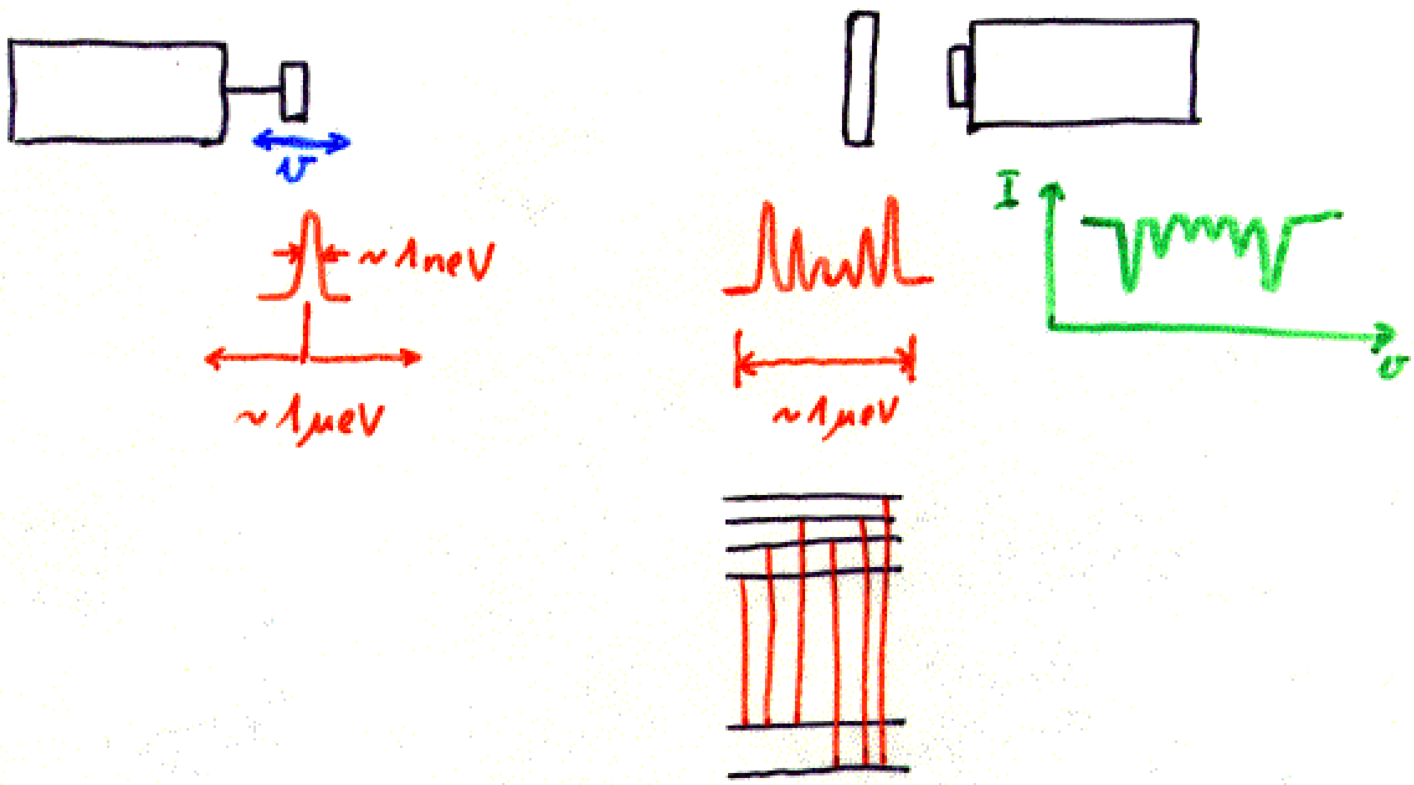


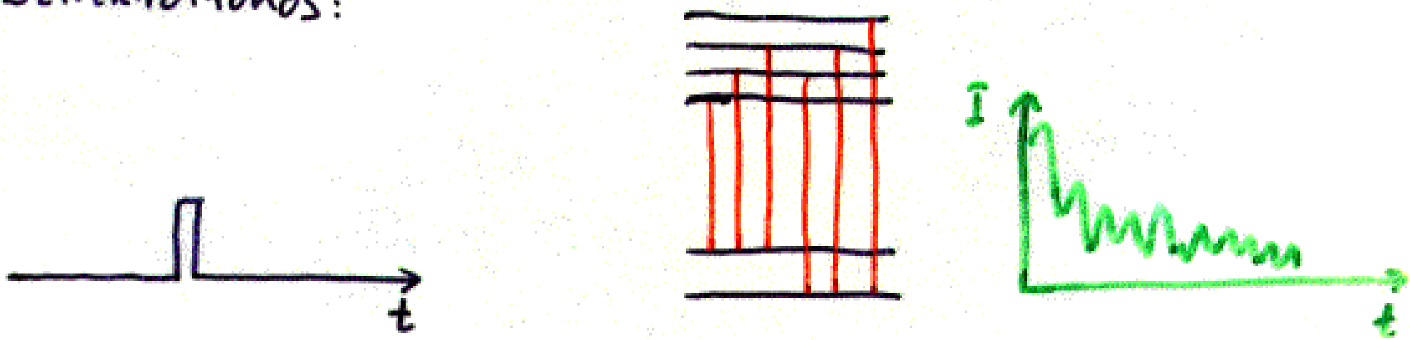
Abb. 4.23: ^{57}Fe Mößbauer-Spektrum für Eisen. Quelle: ^{57}Co in Pt.
a) Für Absorber aus unmagnetisiertem Eisen (die Richtungen des inneren $\vec{B}$-Felds sind statistisch verteilt).
b) Für Absorber aus magnetisiertem Eisen bei dem die Magnetisierung und damit das $\vec{B}$-Feld parallel zur Ausbreitungsrichtung $\vec{k}$ des γ-Quants steht.
c) Für Absorber aus magnetisiertem Eisem bei dem die Magnetisierung und damit das $\vec{B}$-Feld senkrecht auf der Ausbreitungsrichtung $\vec{k}$ des γ-Quants steht (GON 75)

Szinkrotronos vs. hagyományos Mössbauer-spektroszkópia

- Hagyományos:



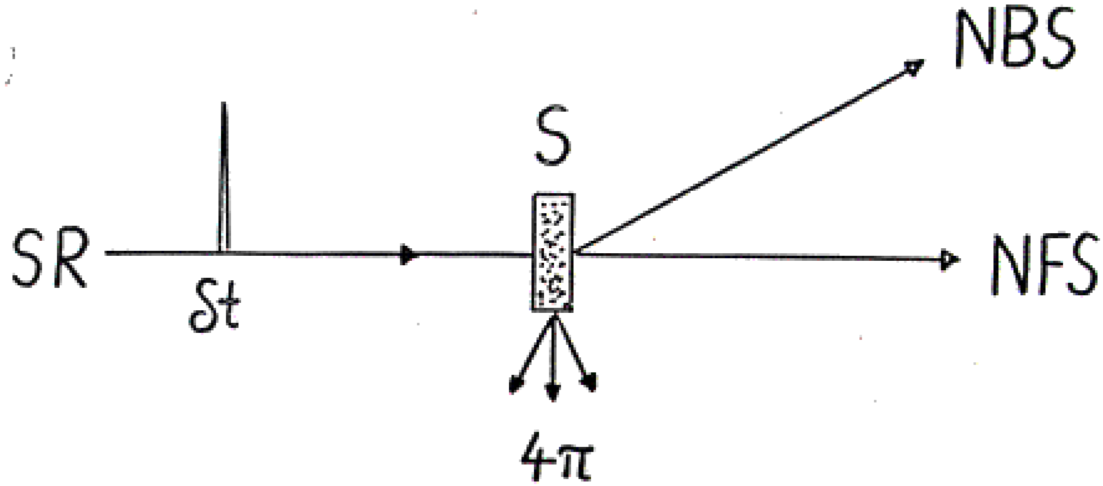
- Szinkrotronos:



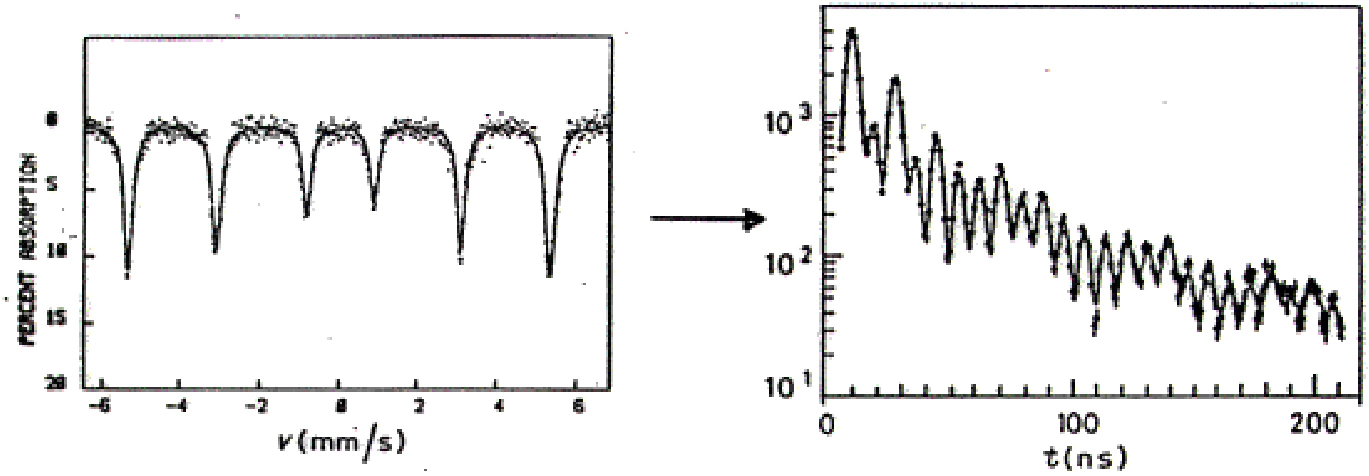
koherens gerjesztés, koherens bomlás

Interferencia a hiperfinom átmenetek között:
kvantum-beat szerkezet

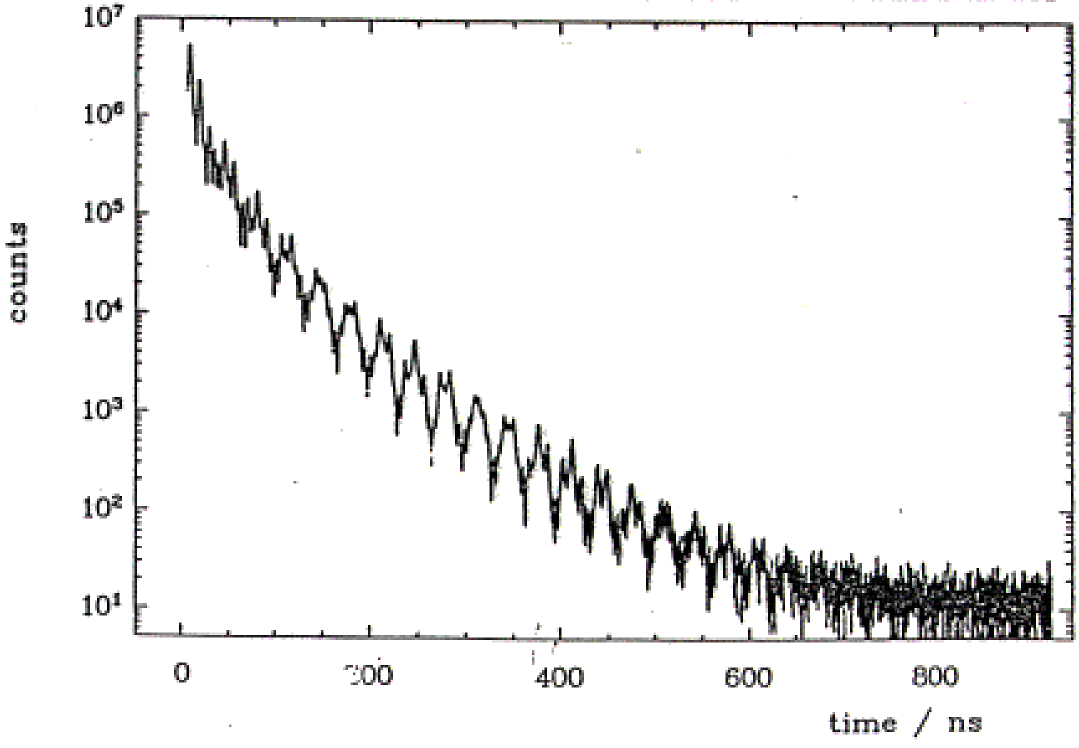
Célszerű a gerjesztő nyalábot ~1μeV-ra mono-
kromatizálni

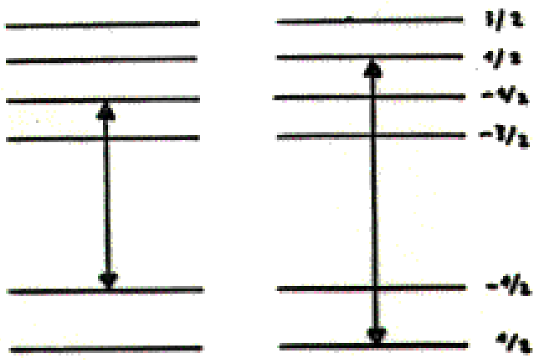


time dependence of response $\left\{ \begin{array}{l} \text{coh.} \\ \text{incoh.} \end{array} \right.$ of sample

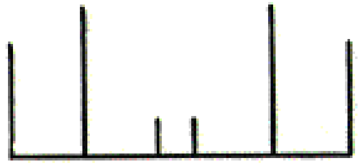


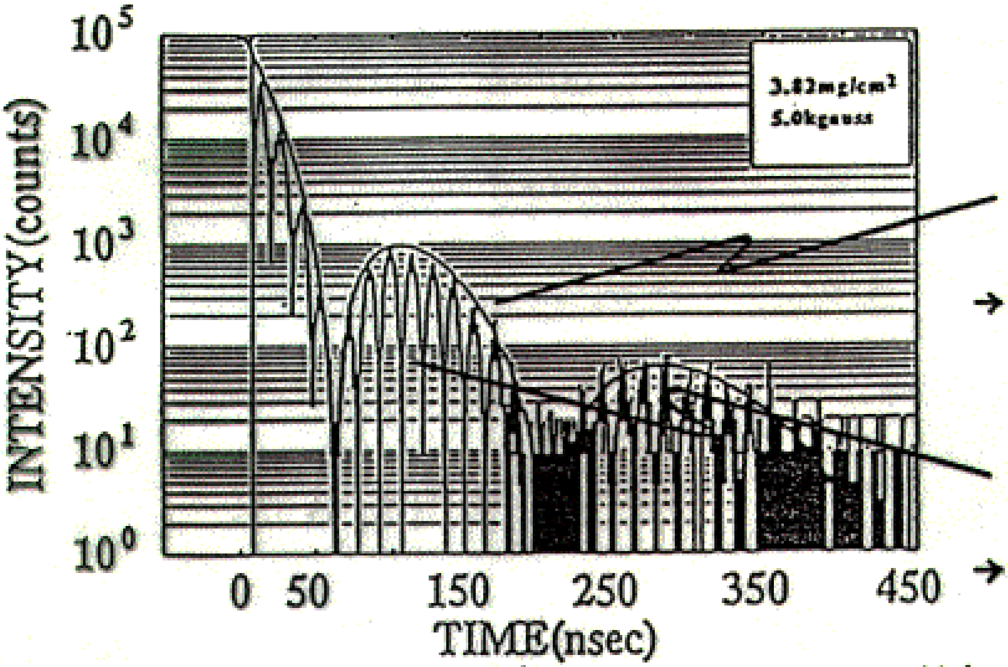
Quantum Beats





^{57}Fe : $\Delta m = 0$





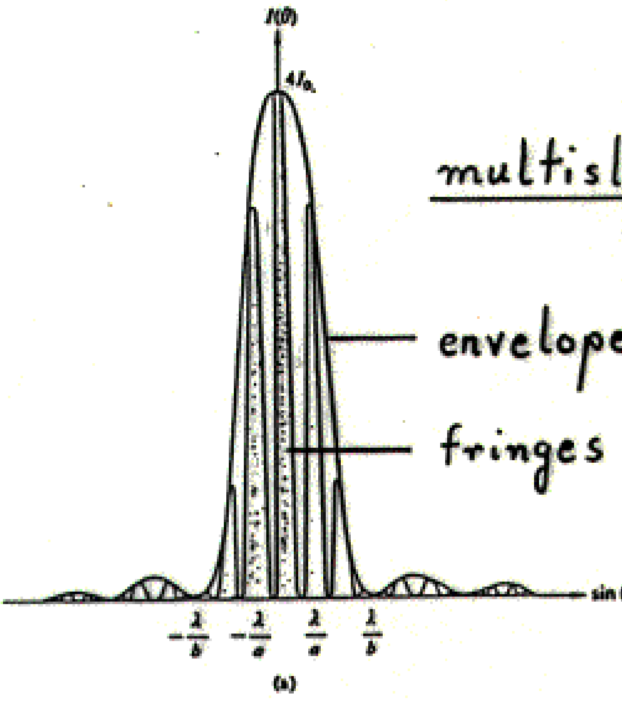
Dynamical Envelope

→ $d_{eff} \sim f_a$

Quantum Beats

→ hfi

Kikuta ... 93



multislit interference:

envelope (1 slit)

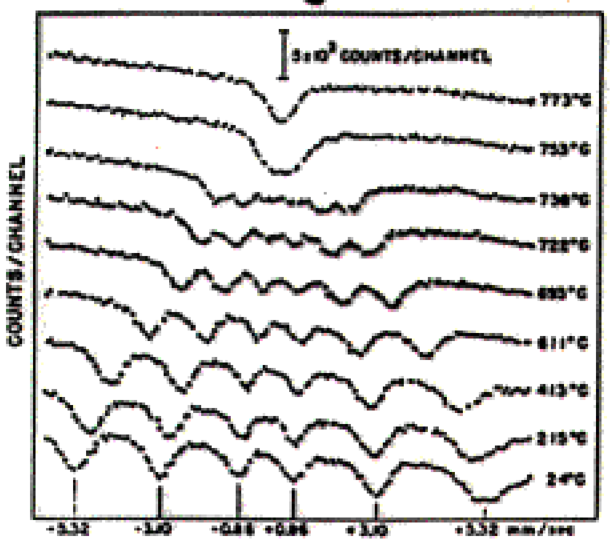
fringes (n slits)

reciprocal scales

MS	pMS
$\Gamma_0 = 5\,\mathrm{neV}$	$\tau_0 = 141\,\mathrm{ns}$
$\Delta_{hf} = 100\,\Gamma_0$	$T_{QB} = 8\,\mathrm{ns}$

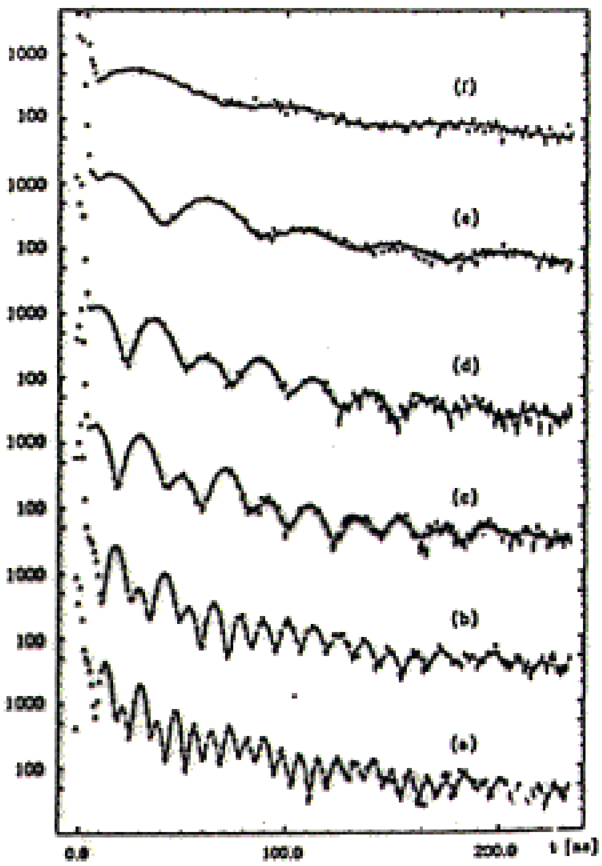
both scales accessible!

$^{57}Fe \rightarrow T_C$



Nagle ... 60

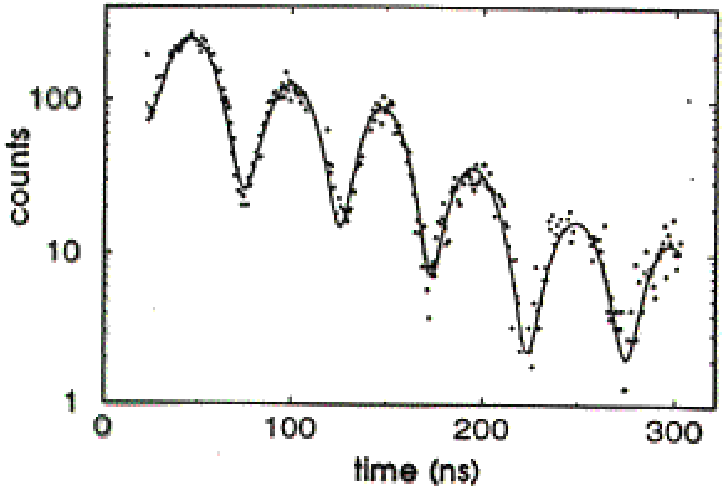
$^{57}FeBO_3\,(333) \rightarrow T_N$

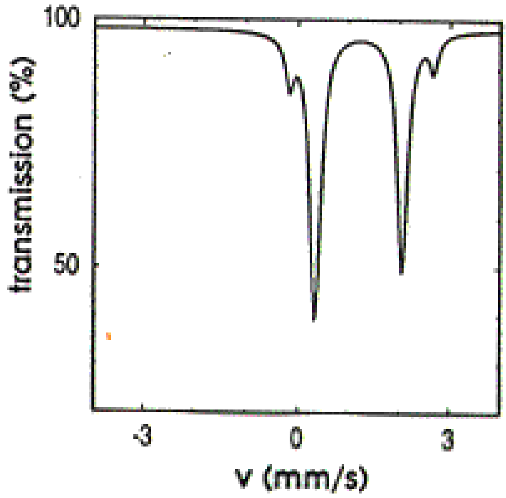


Rüter ... 90

Chumakov ... 90

Mohr's salt, $^{57}Fe\ (NH_4)_2\ (SO_4)_2 \cdot 6\ H_2O$ 1.1

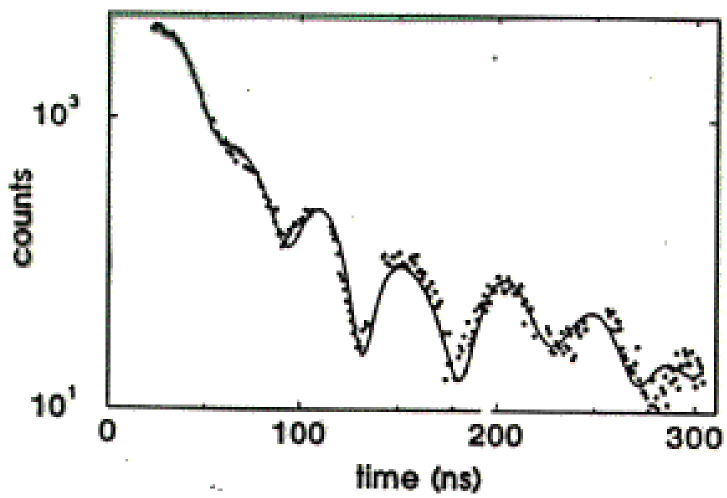


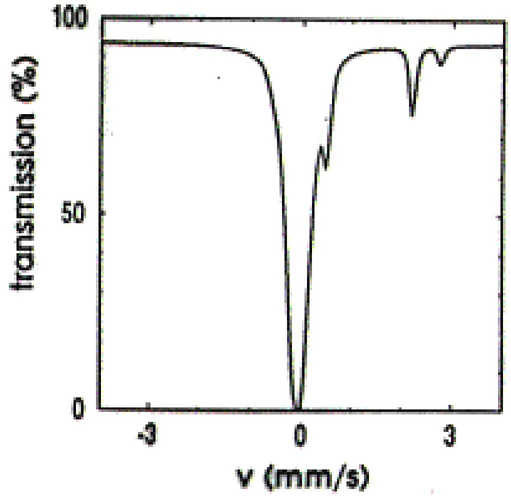


quadrupole splitting : 1.710(7) mm/s

data collection time : 1 hour

Mohr's salt + stainless steel





quadrupole splitting : 1.718(8) mm/s

isomer shift : 1.41(2) mm/s

data collection time : 2 hours