F7030 Rentgenový rozptyl na tenkých vrstvách

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Prezentace k přednášce
Numerické simulace
Příklady experimentů
Vybrané vztahy

Sylabus

1. Experimentální technika: zdroje, vznik rtg záření, goniometry, optické prvky (monochromátory, kolimátory, zrcadla, fokusační optika), detektory. Základní experimenty: polykrystalové a monokrystalové metody, mapování reciprokého prostoru

2. Kinematická teorie rozptylu: úvod do teorie rozptylu, rozptyl na elektronu, izolovaném atomu, krystal, strukturní a geometrický faktor, omezená velikost krystalu

3. Difrakce na polykrystalech I: strukturní faktor, velikost krystalitu (Scherrerova formule), vliv deformace na polohy a šířky difrakčních maxim, zbytková napětí, kvantifikace fázového složení (vnitřní normál)

4. Polykrystaly II: Full profile fitting; Textury, ODF (orientation distribution function); Debyeův vztah, PDF (pair distribution function).

5. SAXS: teoretický popis, řídké roztoky – Guinierův a Porodův vztah, uspořádané částice – long range a short-range order

6. Dokonalé, téměř dokonalé krystaly, epitaxní vrstvy: Kinematická teorie na monokrystalu a epitaxní vrstvě – polohy difrakcí, truncation rod, deformace v epitaxní vrstvě, relaxace. Mozaikový krystal

7. Dynamická teorie rtg reflexe: Jednovlnná aproximace – hloubka vniku, reflexe na hladkém rozhraní, multivrstvy (formalismus přenosové matice), TRXRF

8. Dynamická teorie rtg difrakce: Dvojvlnná aproximace: případ Bragg a Laue, Borrmannův jev, stojatá vlna, GID, epitaxní vrstvy

9. Semikinematická teorie I: DWBA, Rozptyl na drsných rozhraních – popis drsného rozhraní, příklady: fraktálové rozhraní, dvouúrovňové, vicinální, spekulární odraz a nespekulární rozptyl, drsné multivrstvy

10. Semikinematická teorie II: GISAXS na částicích na povrchu a uvnitř vzorku, Difuzní rozptyl na defektech v krystalu v okolí difrakce

11. Experimentální rozlišení Experimentální rozlišení v reciprokém prostoru: analyzer streak, detector streak, monochromator streak, DuMondovy grafy, disperzní a nedisperzní uspořádání, koherenční šířka a délka

12. Další rentgenové metody: Fluorescenční spektroskopie, absorpční spektroskopie – XAFS, XMCD.

Velký monokrystal

$$F^{crystal}(\mathbf{Q}) = \sum_{\ell}^{\text{All atoms}} f_\ell(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_\ell}$$

$$F^{crystal}(\mathbf{Q}) = \sum_{\mathbf{R}_n+\mathbf{r}_j}^{\text{All atoms}} f_j(\mathbf{Q}) e^{i\mathbf{Q}\cdot(\mathbf{R}_n+\mathbf{r}_j)} = \overbrace{\sum_{n} e^{i\mathbf{Q}\cdot\mathbf{R}_n}}^{\text{Lattice}} \overbrace{\sum_{j} f_j(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_j}}^{\text{Unit cell}}$$

$$F^{u.c.}(\mathbf{Q}) = \sum_{j} f_j(\mathbf{Q}) e^{i\mathbf{Q}\cdot\mathbf{r}_j}$$

One dimension

$$S_N(\mathrm{Q}) = \sum_{n=0}^{N-1} e^{i\mathrm{Q}n\mathrm{a}}$$

$$|S_N(\mathrm{Q})| = \frac{\sin(N\mathrm{Qa}/2)}{\sin(\mathrm{Qa}/2)}$$

$$\mathrm{Q} = (h+\xi)\mathrm{a}^*$$

$$|S_N(\xi)| = \frac{\sin(N\pi\xi)}{\sin(\pi\xi)} \rightarrow N \text{ as } \xi \rightarrow 0$$

Its width for large N may be estimated by setting $\xi = 1/(2N)$:

$$|S_N(\xi = \frac{1}{2N})| \approx \frac{1}{\pi/(2N)} = \left(\frac{2}{\pi}\right) N \approx \frac{N}{2}$$

$$N \rightarrow \infty$$

$$|S_N(\xi)| \rightarrow \delta(\xi)$$

$$|S_N(\mathrm{Q})| \rightarrow \mathrm{a}^* \sum_{\mathrm{G}_h} \delta(\mathrm{Q} - \mathrm{G}_h)$$

$$|S_N(\mathrm{Q})|^2 \rightarrow N\,\mathrm{a}^* \sum_{\mathrm{G}_h} \delta(\mathrm{Q} - \mathrm{G}_h)$$

Velký monokrystal

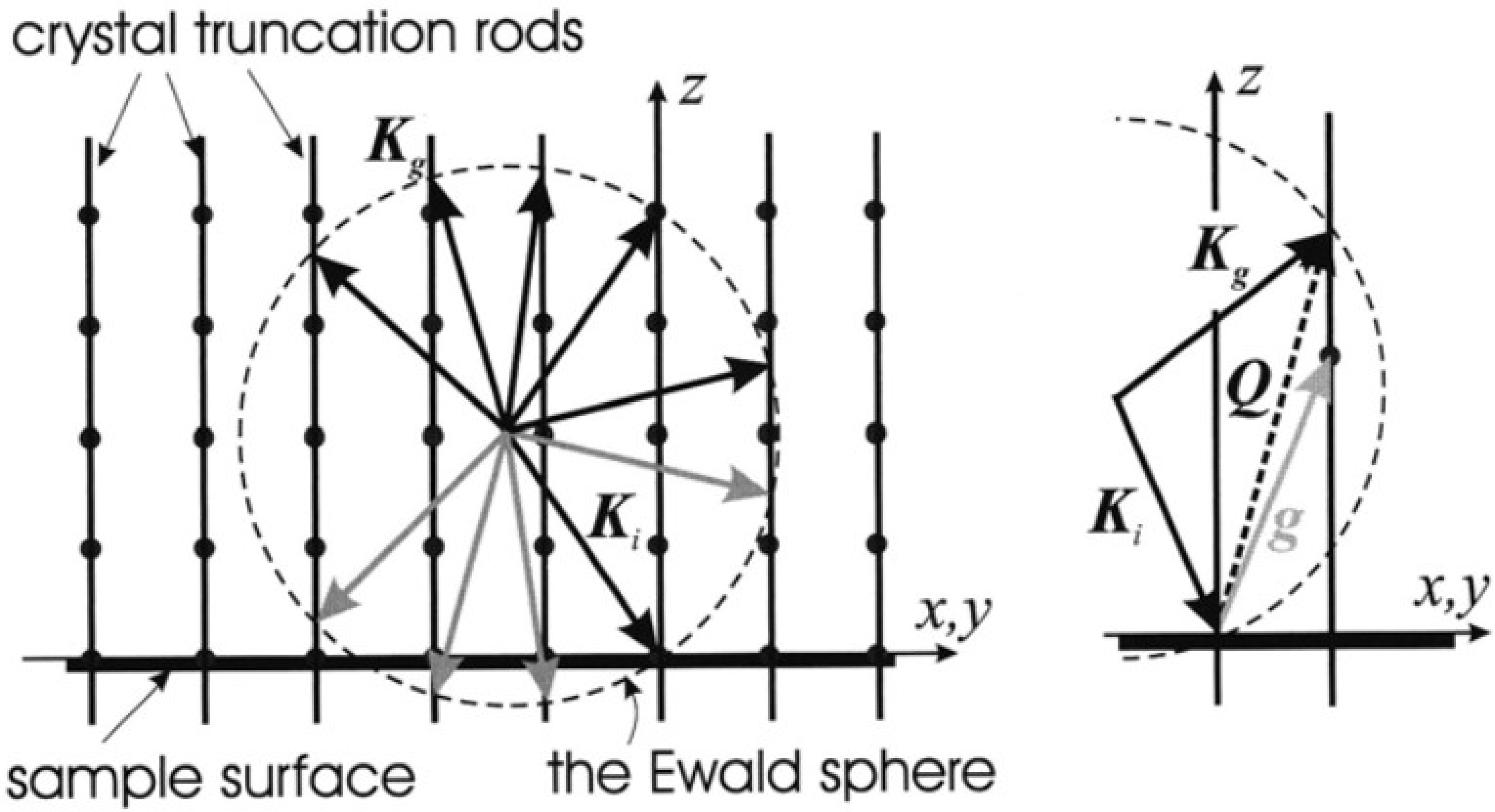
Two and three dimensions

$$|S_N(\xi_1, \xi_2)|^2 \to N_1 N_2 \, \delta(\xi_1)\, \delta(\xi_2)$$

$$|S_N(\mathbf{Q})|^2 \to (N_1 \mathrm{a}_1^*)(N_2 \mathrm{a}_2^*) \sum_{\mathbf{G}} \delta(\mathbf{Q} - \mathbf{G}) = N A^* \sum_{\mathbf{G}} \delta(\mathbf{Q} - \mathbf{G})$$

$$|S_N(\mathbf{Q})|^2 \to N \, v_c^* \sum_{\mathbf{G}} \delta(\mathbf{Q} - \mathbf{G})$$

Velký monokrystal



Velký monokrystal

$$F^{CTR} = A(\mathbf{Q}) \sum_{j=0}^{\infty} e^{i Q_z a_3 j} e^{-\beta j} = \frac{A(\mathbf{Q})}{1 - e^{i Q_z a_3} e^{-\beta}}$$

$A(\mathbf{Q})$ is the scattering amplitude from a layer of atoms

$$\delta(Q_x - h a_1^*)\, \delta(Q_y - k a_2^*)$$

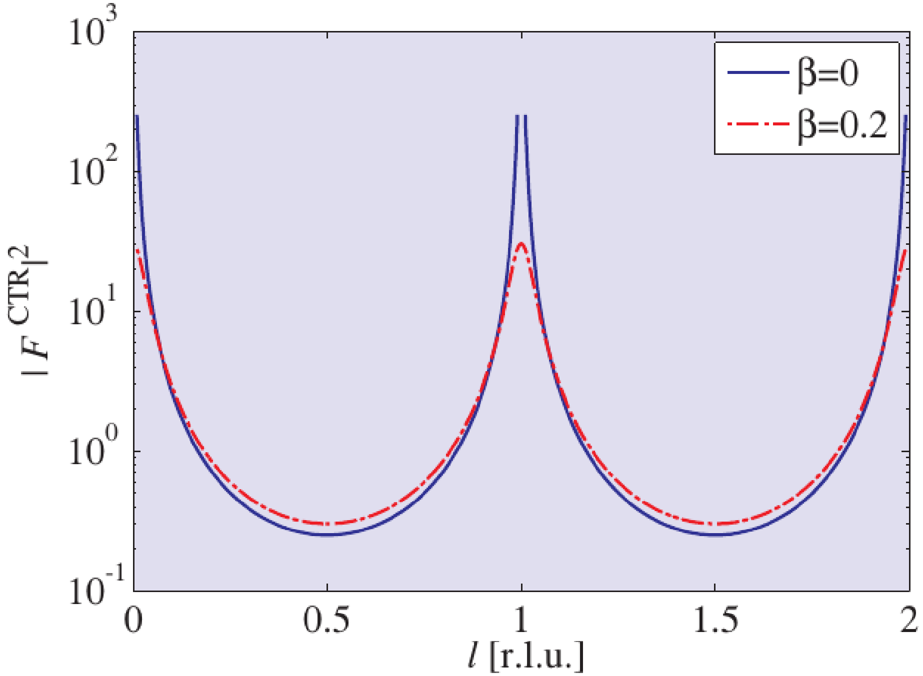
$\beta = a_3 \mu / \sin\theta$ is the absorption parameter per layer.

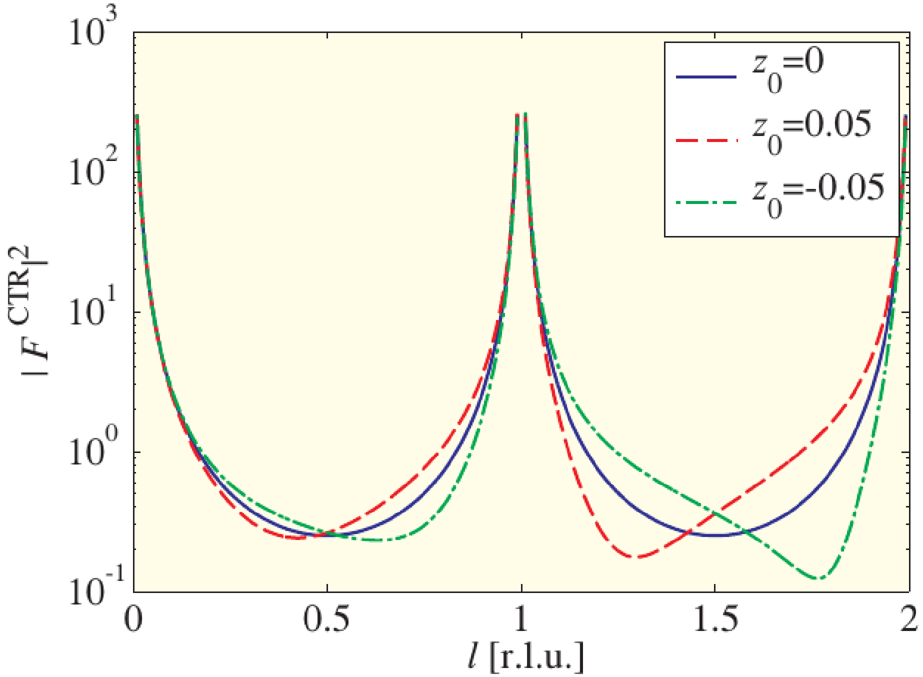
$$I^{CTR} = |F^{CTR}|^2 = \frac{|A(\mathbf{Q})|^2}{(1 - e^{i Q_z a_3} e^{-\beta})(1 - e^{-i Q_z a_3} e^{-\beta})}$$

$$Q_z = q_z + 2\pi l / a_3$$

$$I^{CTR} \approx \frac{|A(\mathbf{Q})|^2}{q_z^2 a_3^2 + \beta^2}$$

Velký monokrystal





z_0 posun horní atomové vrstvy

Epitaxní vrstvy

$$J(\boldsymbol{Q}) = I_i K^2 \frac{4(\pi r_{\mathrm{el}} C)^2}{V_{\mathrm{cell}}^2} \sum_{\boldsymbol{g}_\parallel} \delta^{(2)}(\boldsymbol{Q}_\parallel - \boldsymbol{g}_\parallel) \times$$

$$\times \left| F_{\mathrm{cell}}(\boldsymbol{Q}) \sum_{g_z} G_{\mathrm{cryst}}(Q_z - g_z) \right|^2 .$$

$$G_{\mathrm{cryst}}(q_z) = \int_{-T}^{0} \mathrm{d}z \mathrm{e}^{-\mathrm{i}q_z z} = \frac{\mathrm{i}}{q_z} \left(1 - \mathrm{e}^{-\mathrm{i}q_z T}\right) \equiv$$

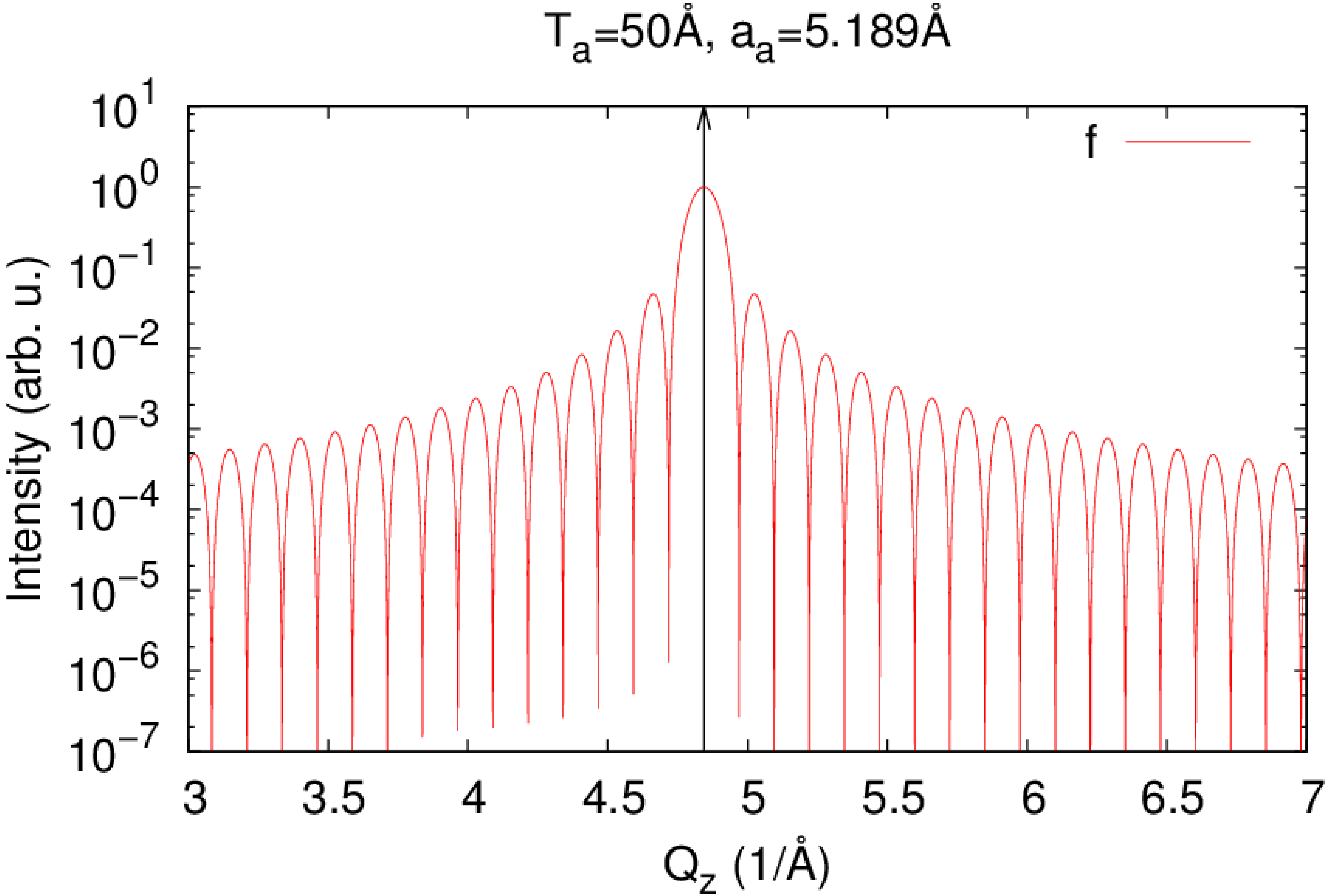
$$\mathrm{e}^{-\mathrm{i}q_z T/2} T \mathrm{sinc}\left(\frac{q_z T}{2}\right),$$

$$J(\boldsymbol{Q}) = I_i K^2 \frac{4(\pi r_{\mathrm{el}} C)^2}{V_{\mathrm{cell}}^2} \delta^{(2)}(\boldsymbol{Q}_\parallel - \boldsymbol{h}_\parallel) \left| F_{\mathrm{cell}}(\boldsymbol{h}) G_{\mathrm{cryst}}(Q_z - h_z) \right|^2$$

$$\chi(\boldsymbol{r}) = \sum_{\boldsymbol{g}} \chi_{\boldsymbol{g}} \mathrm{e}^{\mathrm{i}\boldsymbol{g}.\boldsymbol{r}} \qquad \chi_{\boldsymbol{g}} = -\frac{r_{\mathrm{el}} C \lambda^2}{\pi V_{\mathrm{cell}}} \sum_s f_s(\boldsymbol{g}) \mathrm{e}^{-\mathrm{i}\boldsymbol{g}.\boldsymbol{r}_s}$$

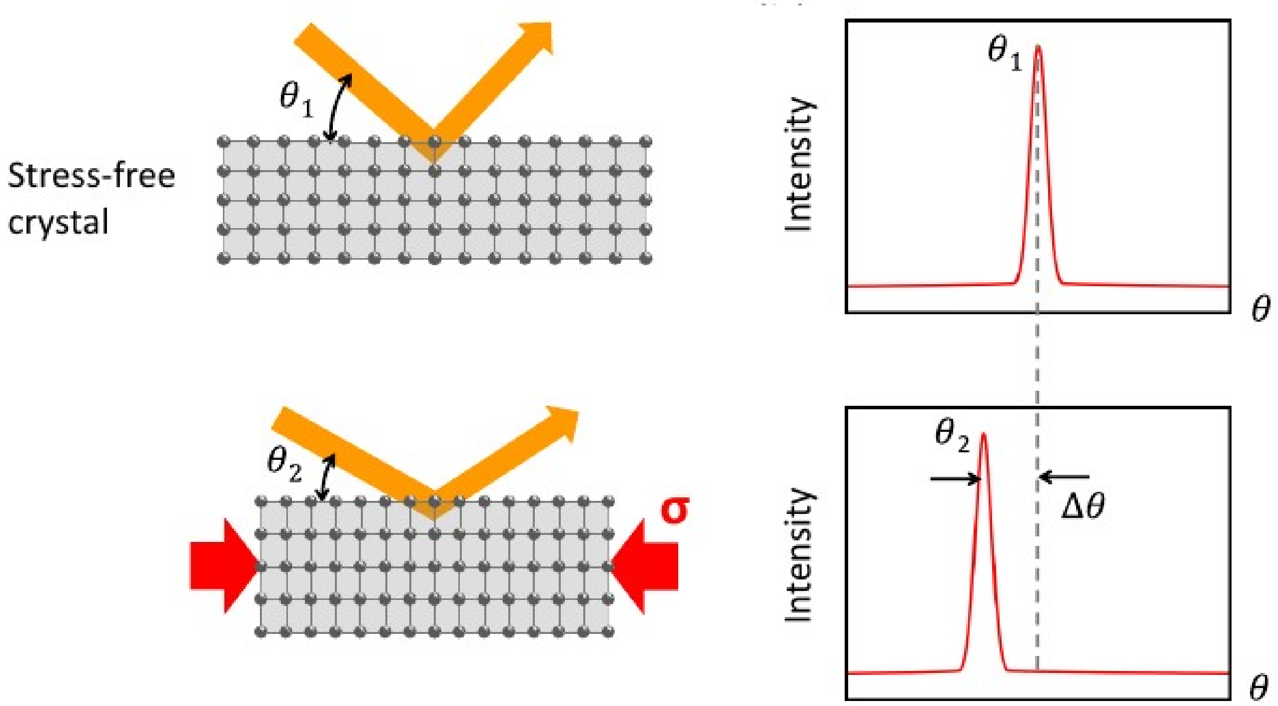
Epitaxní vrstvy

Jednoduchá vrstva, šipka poloha 2pi/a



Epitaxní vrstvy

Principle of X-ray diffraction based stress/strain analysis



- X-ray diffraction uses the crystal lattice as a "strain gauge"
- The relation between the lattice parameter and diffraction angle is defined by Bragg's law, $2d \sin \theta_B = n\lambda$
- Most sensitive stress/strain analysis method for semi. (ITRS 2011)

Epitaxní vrstvy

$$\Delta Q_z = \frac{2\pi}{T}$$

$$\Delta\eta_i = \lambda\frac{\gamma_{\boldsymbol{h}}}{\sin(2\Theta_B)T}$$

$$\Delta\eta_i = \frac{\lambda}{2T\cos\Theta_B}$$

Epitaxní vrstvy

Example: Fully strained SiGe epilayer

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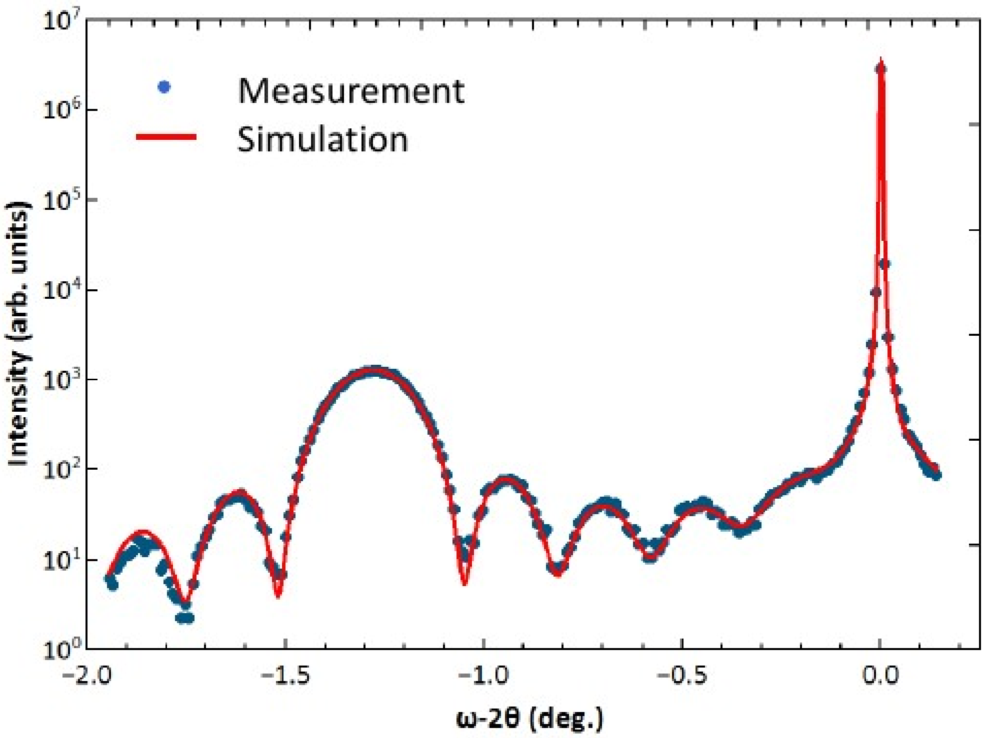


Symmetric 004 reflection from 22.5 nm epitaxial film of $Si_{1-x}Ge_x$ with x = 49% on a Si(001) substrate

- Composition / strain determined from measured lattice misfit
- Misfit normal to surface from layer peak position

$$\Delta d/d = -\Delta\omega \cot \theta_B$$

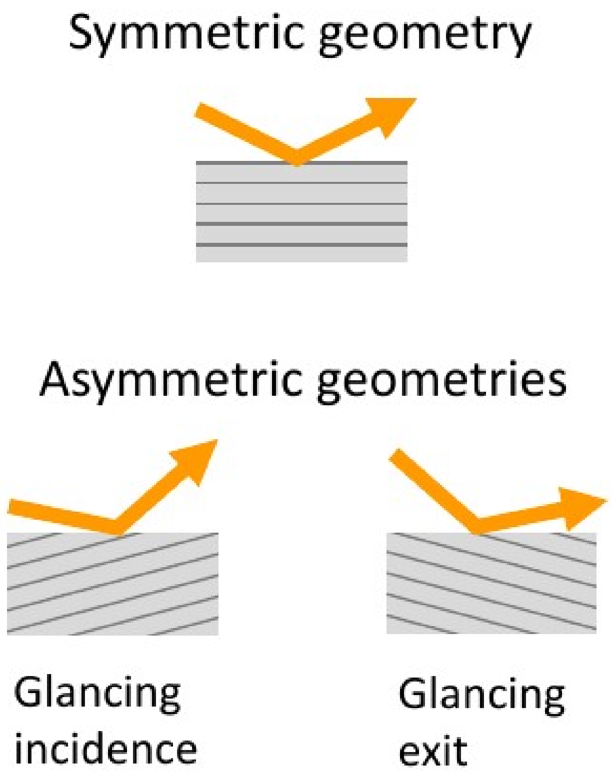
- Thickness from interference fringe period

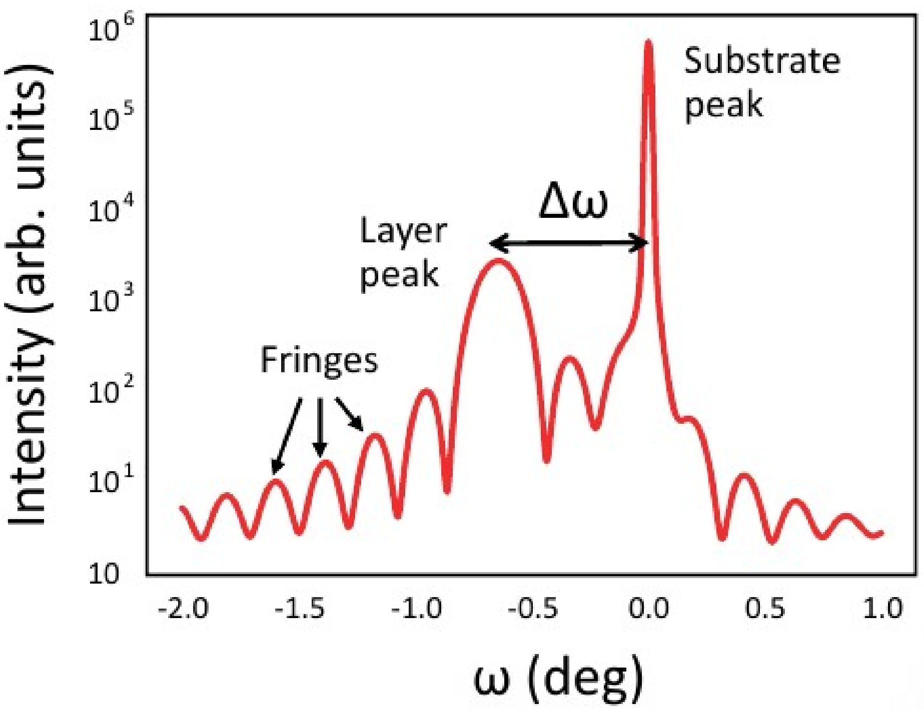
$$t = \lambda/(2\Delta\omega_f \cos \theta_B)$$

- No dependence on uncertain materials parameters

Epitaxní vrstvy

Common Bragg diffraction geometries and anatomy of a HRXRD curve





- Symmetric Bragg geometry is sensitive to lattice parameter perpendicular to the surface
- Asymmetric geometries are also sensitive to the lattice parameters both parallel and perpendicular to the surface

Epitaxní vrstvy

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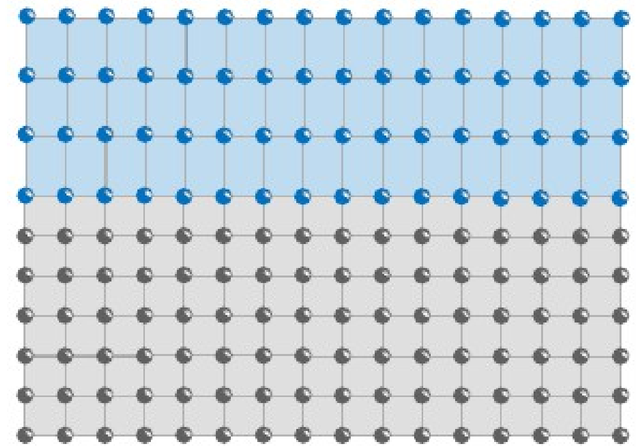
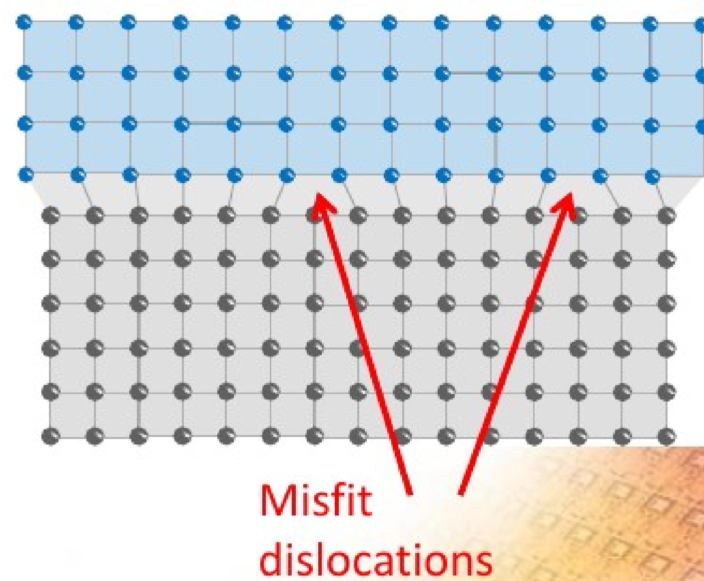
Lattice deformation in epitaxial thin-films

- If the lattice mismatch to the substrate and/or thickness is small, then an epilayer can be strained so that the in-plane lattice parameter is equal to that of the substrate (fully strained)
  - Tetragonal distortion of the unit cell
- For large mismatch or thickness, it may become energetically favorable to relax
  - Creation of dislocations and/or roughening

… more on this later





Epitaxní vrstvy

$$\varepsilon_{\|} = \frac{a_{\|} - a_0}{a_0}, \quad \varepsilon_{\perp} = \frac{a_{\perp} - a_0}{a_0}.$$

$$\varepsilon_{\perp} = -2\frac{\nu}{1-\nu}\varepsilon_{\|}.$$

$$a_0 = \frac{(1-\nu)a_{\perp} + 2\nu a_{\|}}{1+\nu}.$$

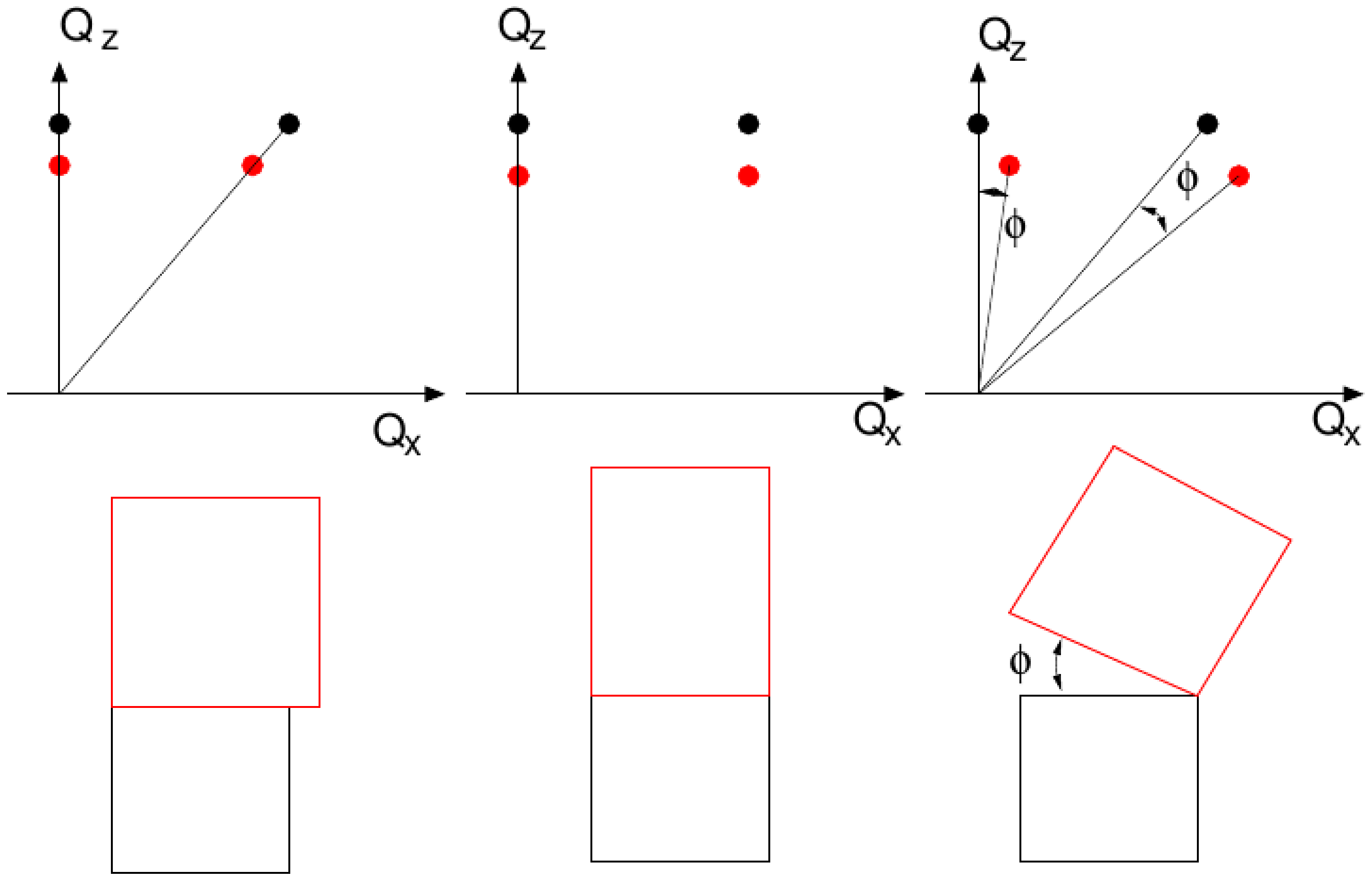
$$\nu_{001} = \frac{C_{12}}{C_{11} + C_{12}}, \quad \nu_{111} = \frac{1}{2}\frac{C_{11} + 2C_{12} - 2C_{44}}{C_{11} + 2C_{12} + C_{44}}$$

$$R = \frac{a_{L\|} - a_S}{a_{L\infty} - a_S}$$

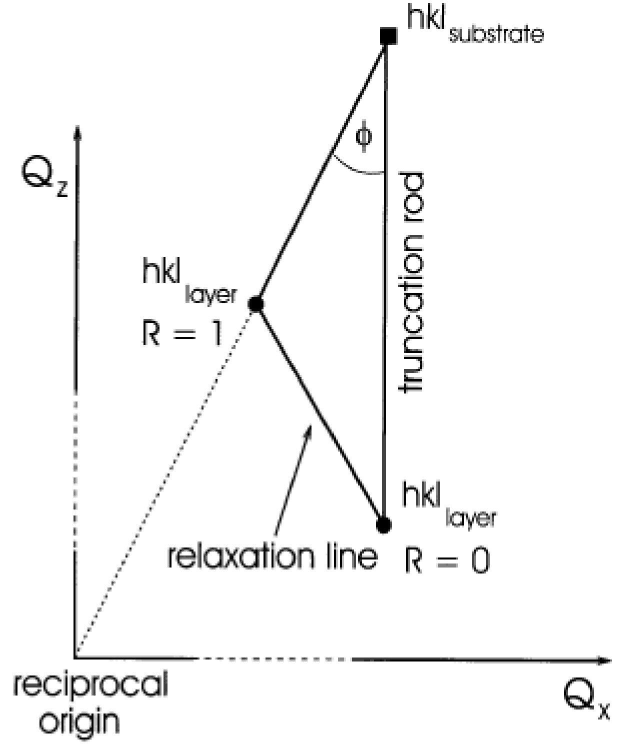
$$a_r = \sqrt{\frac{a_{\perp}^2 + 2a_{\|}^2}{3}}, \quad \cos\alpha_r = \frac{a_{\perp}^2 - a_{\|}^2}{a_{\perp}^2 + 2a_{\|}^2}$$

Epitaxní vrstvy

Polohy difrakčních maxim pro různé vzájemné polohy mříží vrstvy a substrátu



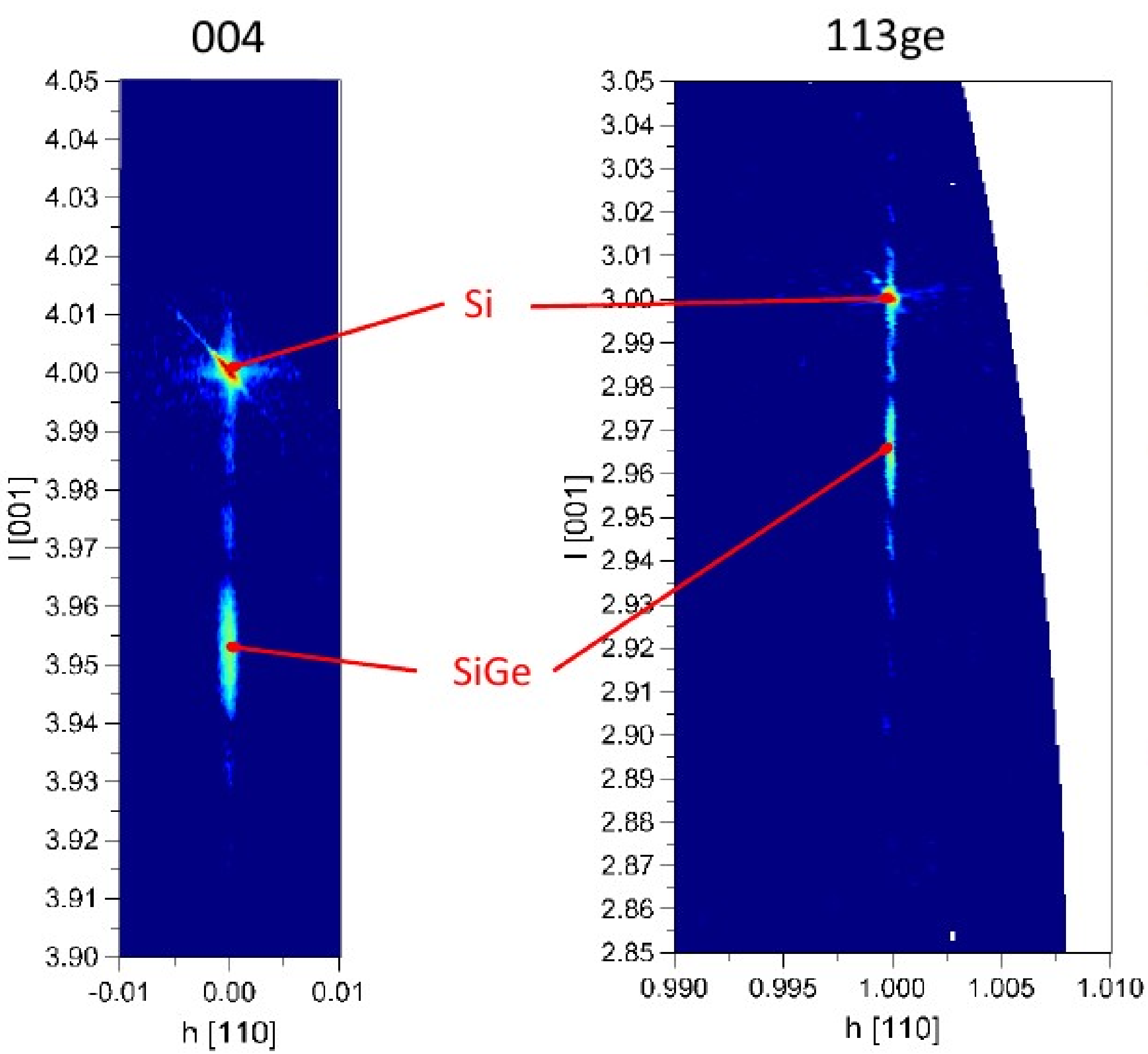
Epitaxní vrstvy



Epitaxní vrstvy

RSMs from fully strained epitaxial thin-films

37.6 nm $Si_{0.81}Ge_{0.19}$ on Si(001)

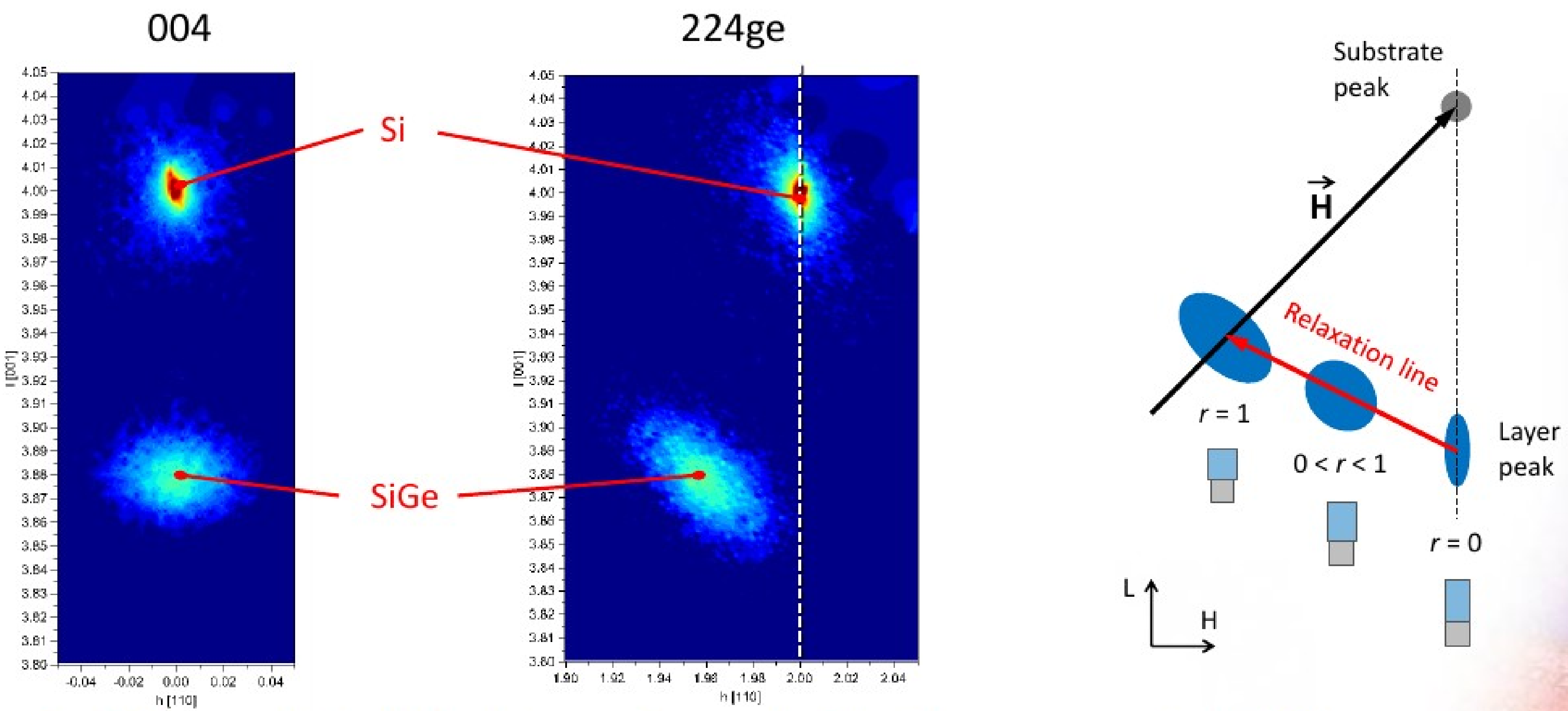


- Layer peak position gives the lattice parameters
  $$\Delta a_{\perp}/a = \Delta L/L$$
  $$\Delta a_{||}/a = \Delta H/H$$
- Composition and relaxation can be obtained
- Peak in the asymmetric RSM is located at H = 1 indicating the layer is fully strained ($a_{SiGe,||} = a_{Si}$)
- Thickness fringes are visible in the L direction
  $$t \propto 1/\Delta L_{fringes}$$

Epitaxní vrstvy

RSMs from relaxed epitaxial thin-films

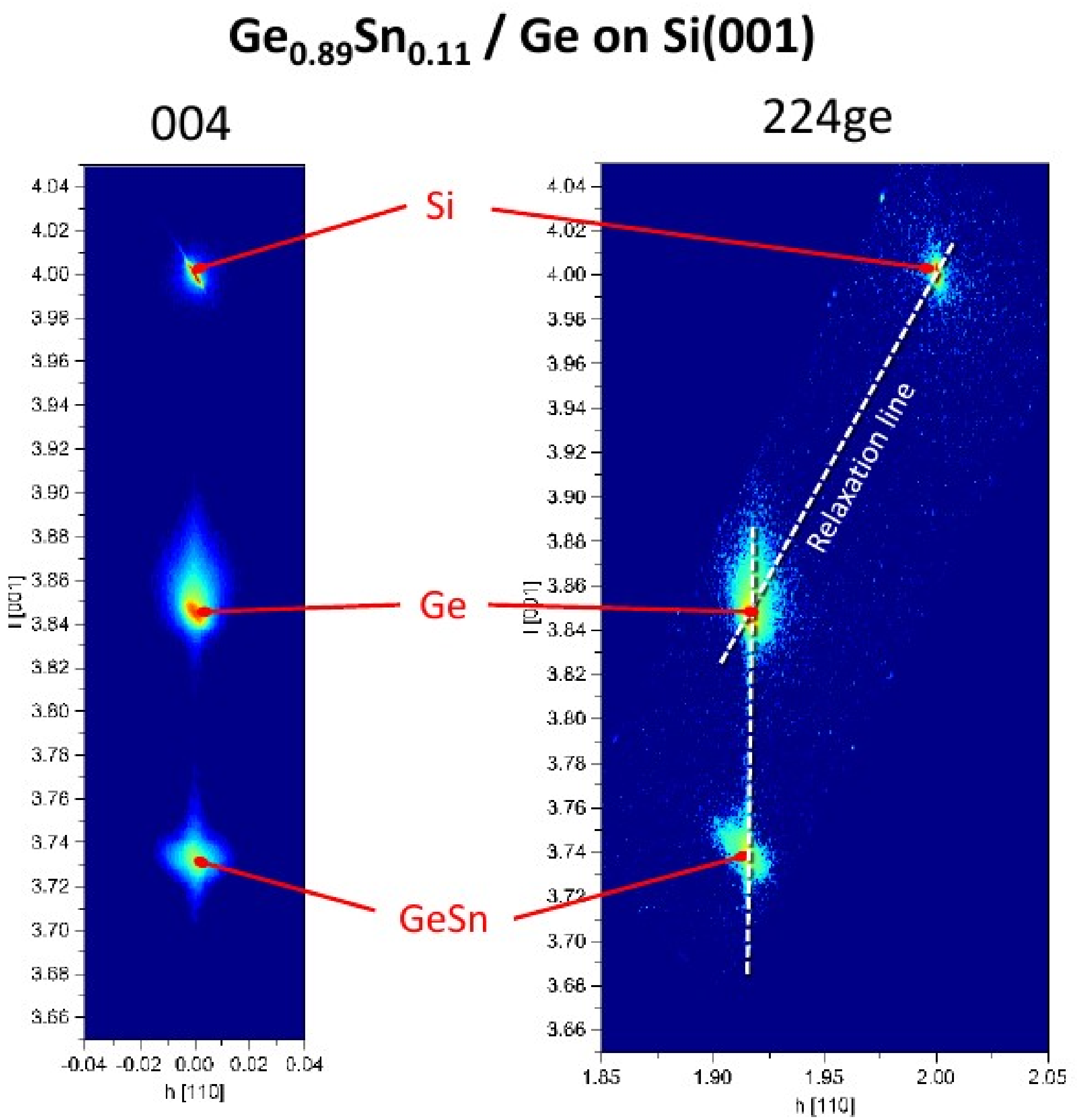
~35 nm $Si_{0.33}Ge_{0.67}$ (R = 70%) on Si(001)



- SiGe peak is shifted away from H=2 in the asymmetric 224ge map indicating relaxation ($a_{SiGe,||} > a_{Si}$)
- Peak is broadened due to dislocations, $w(H)/H \propto 1/\sqrt{\rho}$

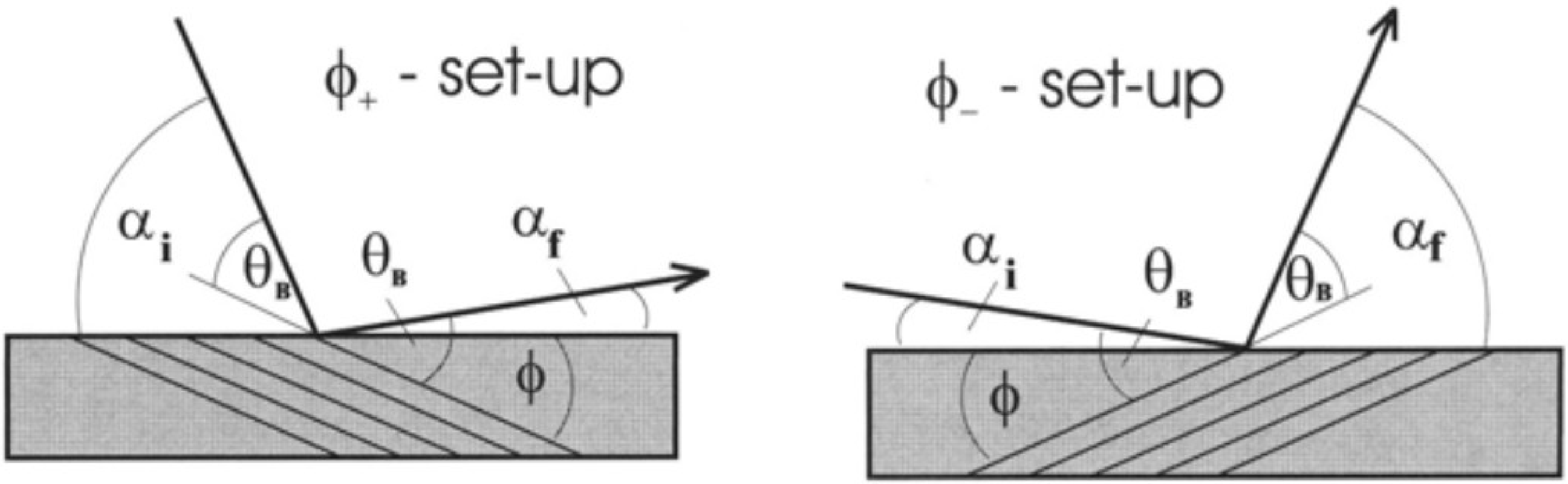
Epitaxní vrstvy

RSMs from strained thin-films on strain relaxed buffers (SRBs)



- Ge peak is shifted away from H < 2 in the asymmetric 224ge map indicating relaxation ($a_{Ge,||} > a_{Si}$)
- GeSn peak is not shifted in H wrt to Ge peak ($a_{GeSn,||} = a_{Si}$)
- Composition and relaxation of each layer can be obtained

Epitaxní vrstvy



$$\delta_{L\perp} = \Delta\phi \tan\phi - \Delta\Theta_B \cot\Theta_B,$$

$$\delta_{L||} = -\Delta\phi \ \cot\phi - \Delta\Theta_B \cot\Theta_B.$$

Epitaxní vrstvy

Comparison of HRXRD data from strained and relaxed SiGe epilayers

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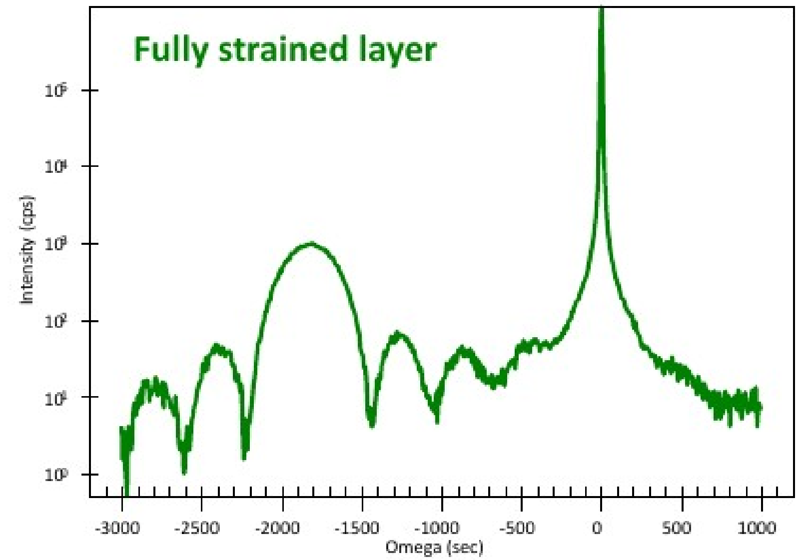
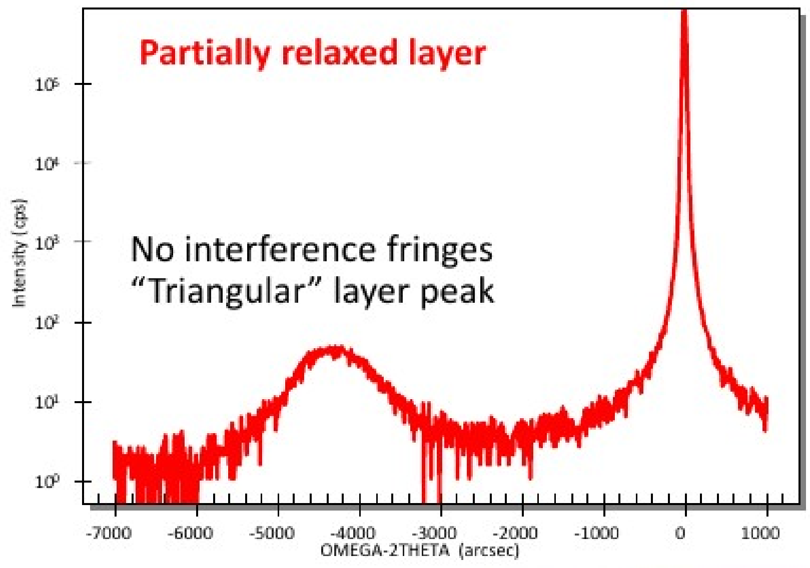
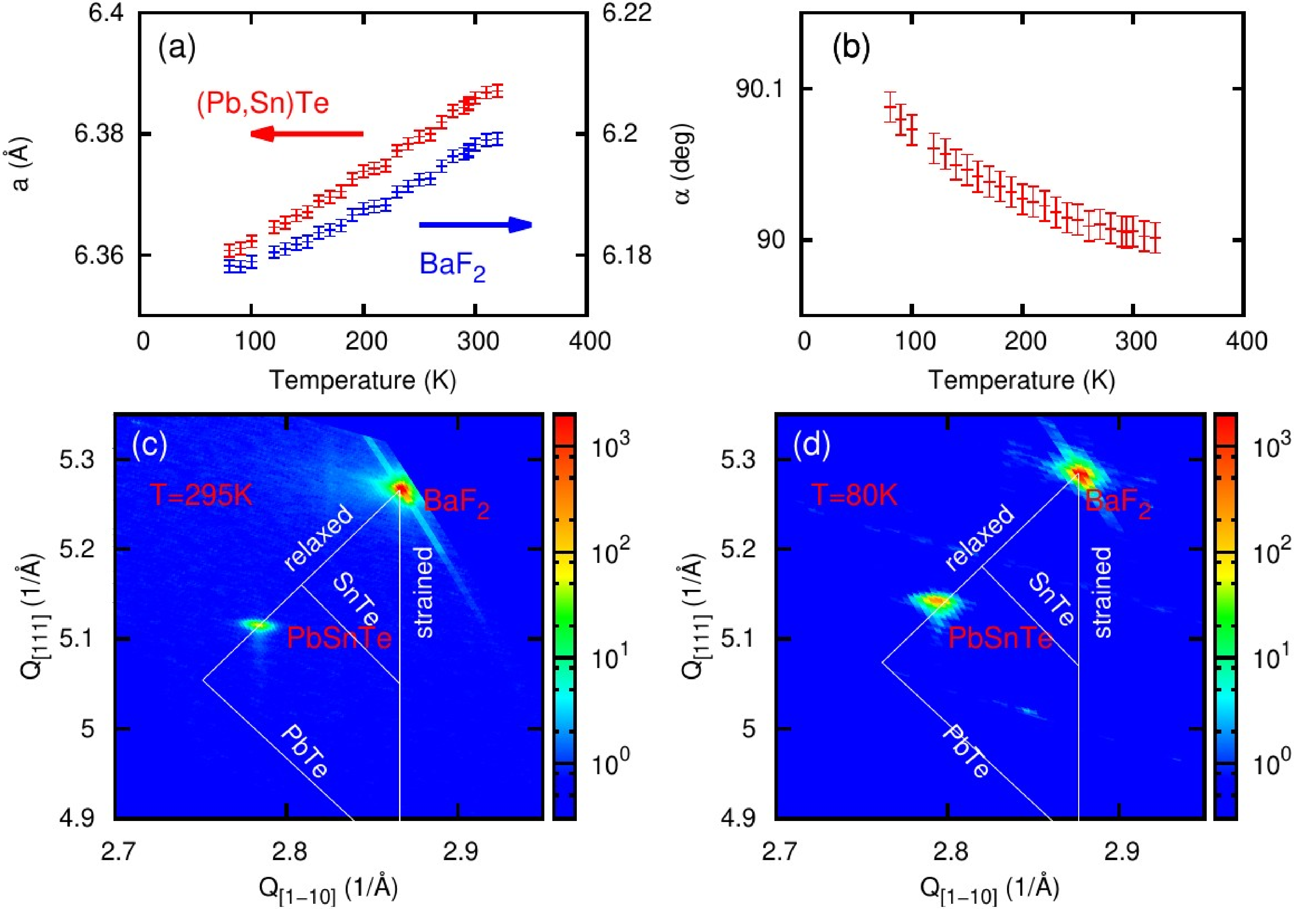
- Degradation of device performance and yield loss
  - Relaxed material has about 50% less strain than a pseudomorphic layer
  - Relaxed material will contain dislocations at the interface and in the layer - increased leakage?
- HRXRD provides a unique, automated solution for strain metrology and assessment of lattice defectivity





Epitaxní vrstvy



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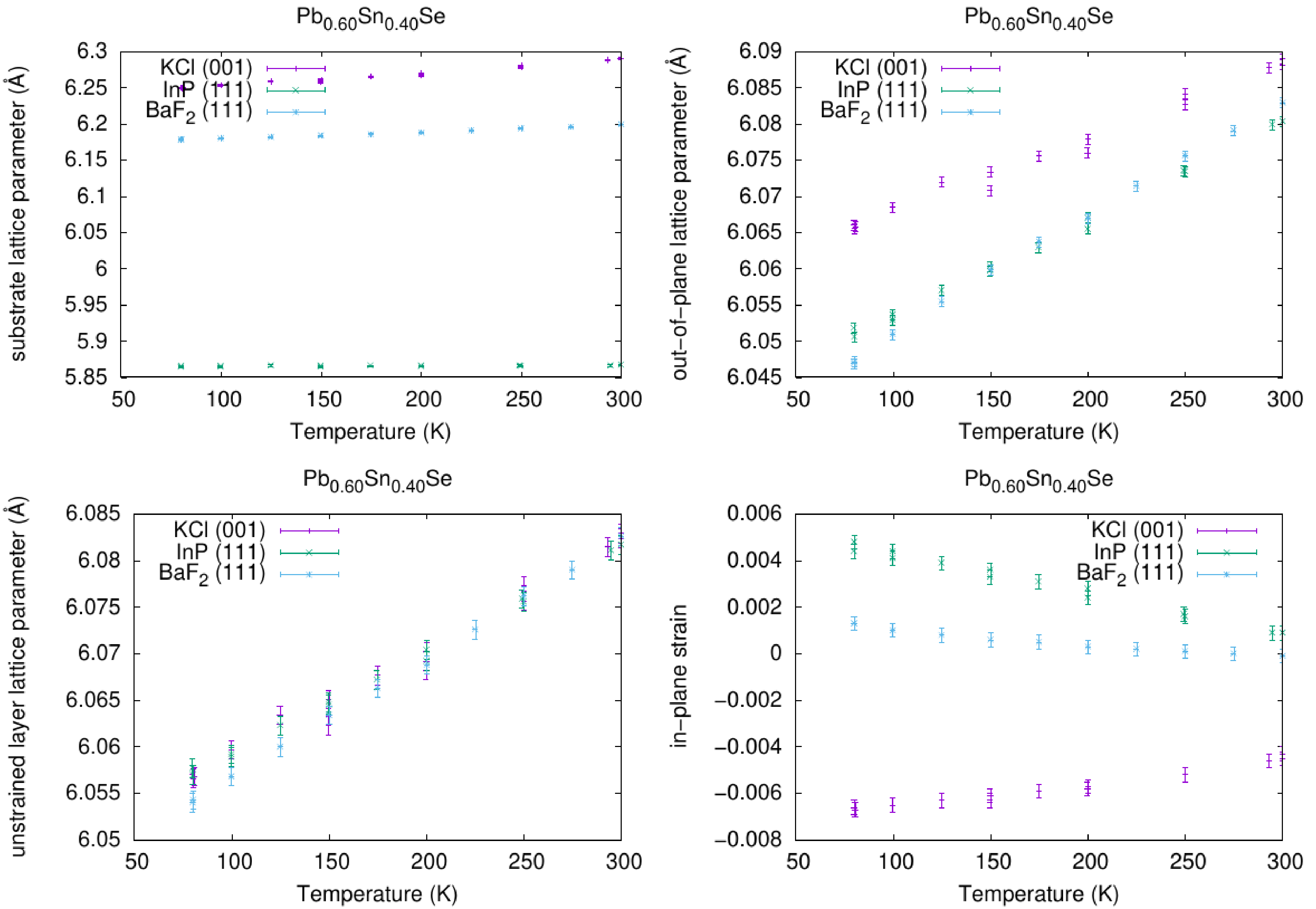

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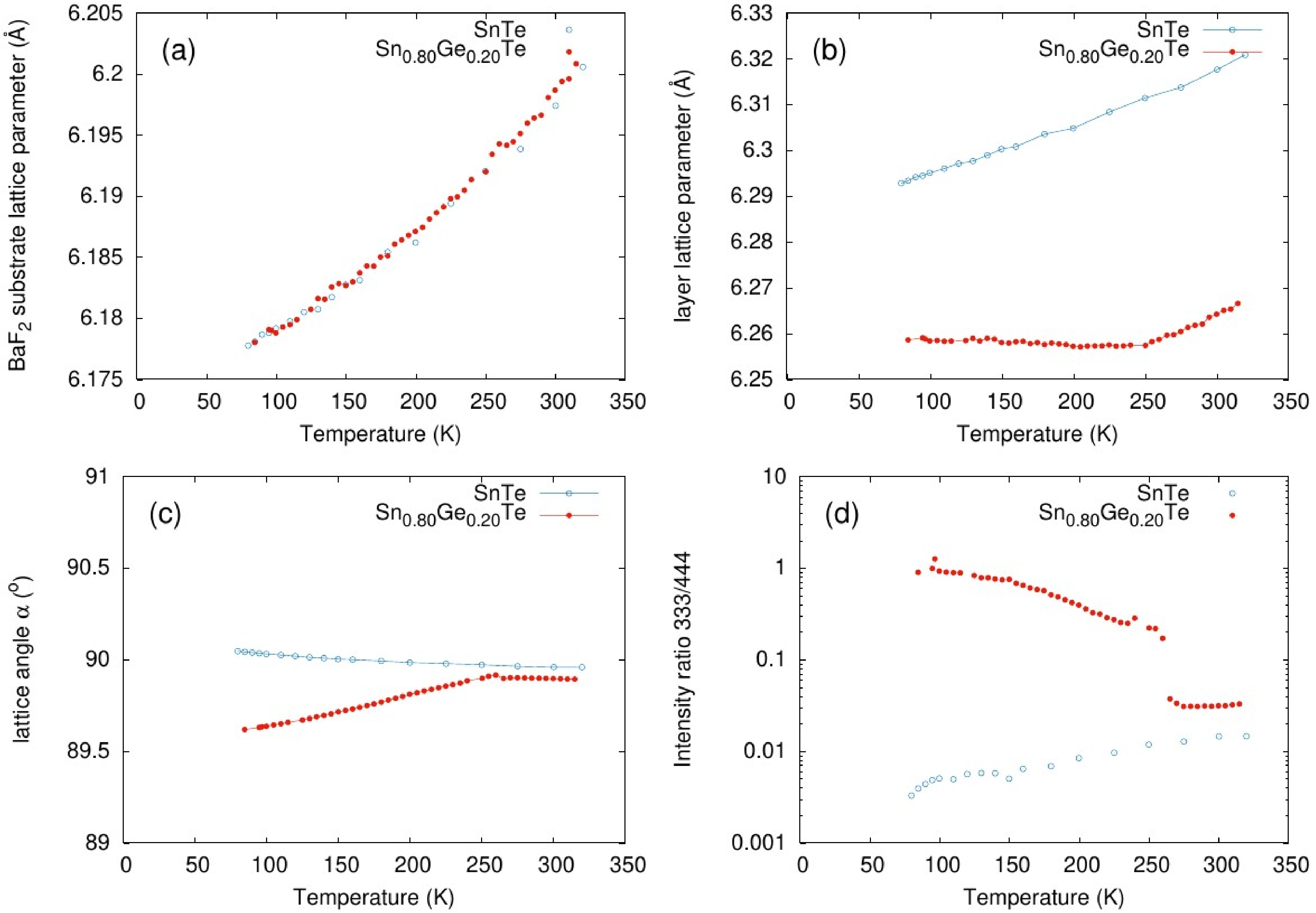


Epitaxní vrstvy

$$F_{n,\mathrm{cell}}(\boldsymbol{Q}) = \mathrm{e}^{-\mathrm{i}\boldsymbol{Q}.\boldsymbol{u}_n} \sum_s f_s(\boldsymbol{Q}) \mathrm{e}^{-\mathrm{i}\boldsymbol{Q}.(\boldsymbol{r}_s + \boldsymbol{u}_{ns})}$$

$$F_{n,\mathrm{cell}}(\boldsymbol{Q}) = \mathrm{e}^{-\mathrm{i}\boldsymbol{Q}.\boldsymbol{u}_n} F_{\mathrm{cell}}(\boldsymbol{Q})$$

$$E(\boldsymbol{r}) = -\mathrm{i}E_i \frac{r_{\mathrm{el}}C}{2\pi V_{\mathrm{cell}}} \int \frac{\mathrm{d}^2\boldsymbol{K}_\parallel}{K_z} \mathrm{e}^{\mathrm{i}\boldsymbol{K}.\boldsymbol{r}} F_{\mathrm{cell}}(\boldsymbol{Q}) \times$$

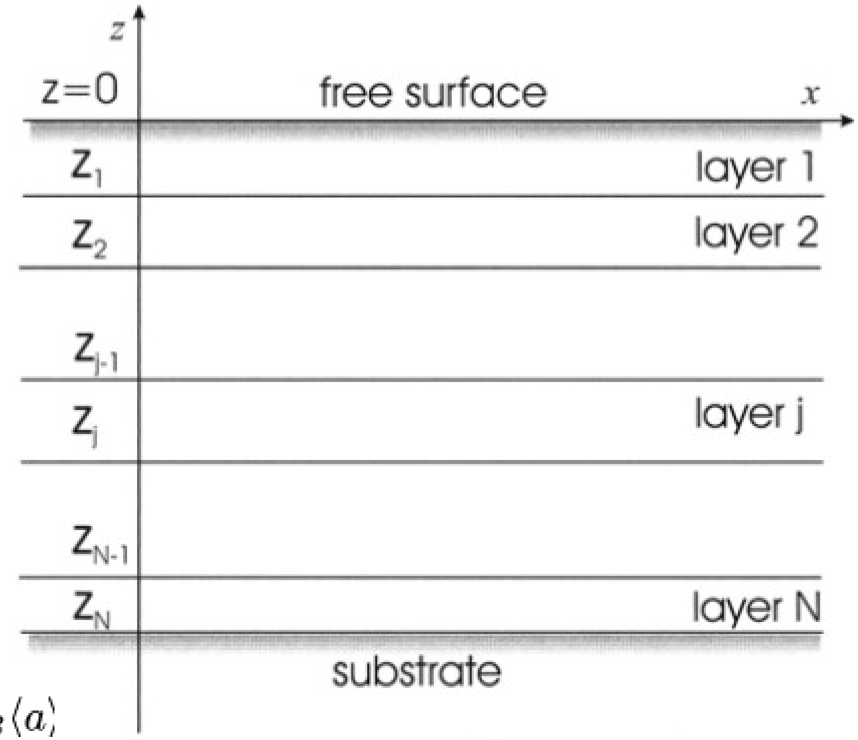
$$\times \sum_{\boldsymbol{g}} \int_{V_{\mathrm{cryst}}} \mathrm{d}^3\boldsymbol{r'} \mathrm{e}^{-\mathrm{i}(\boldsymbol{Q}-\boldsymbol{g}).\boldsymbol{r'}} \mathrm{e}^{-\mathrm{i}\boldsymbol{Q}.\boldsymbol{u}(\boldsymbol{r'})}, \ \boldsymbol{Q} = \boldsymbol{K} - \boldsymbol{K}_i$$

Epitaxní vrstvy

$$I = I_i \frac{4(\pi r_{\mathrm{el}} C)^2}{V_{\mathrm{cell}}^2} \sum_{\boldsymbol{g}_\parallel} \left| \frac{1}{K_{\boldsymbol{g}z}} \sum_{g_z} \sum_{n=1}^{N} F_{\mathrm{cell}}^{(n)}(\boldsymbol{g}_\parallel, K_{\boldsymbol{g}z} - K_{iz}) \times \right.$$

$$\left. \times\, G_{\mathrm{layer}}^{(n)}(K_{\boldsymbol{g}z} - \tilde{K}_{\boldsymbol{g}z}) \right|^2$$

$$G_{\mathrm{layer}}^{(n)}(Q_z) = \int_{z_{n+1}}^{z_n} \mathrm{d}z \mathrm{e}^{-\mathrm{i}Q_z(z+u(z))}$$



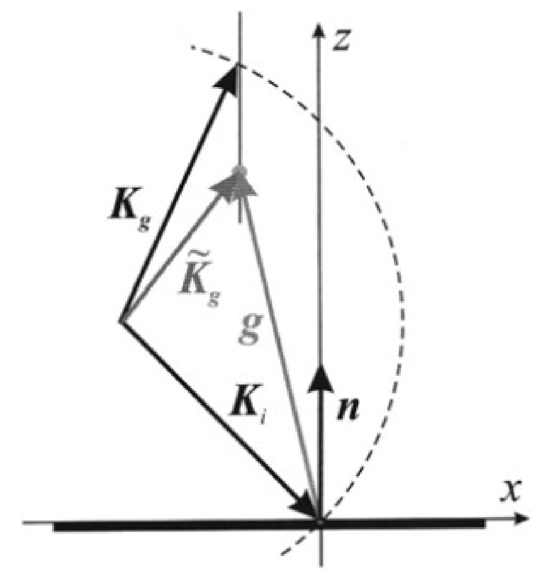
$$\langle a \rangle = \frac{n_A a_A + n_B a_B}{n_A + n_B}$$

$$u_B(z) = \delta_B \Delta z$$

$$\delta_{A,B} = (a_{A,B} - \langle a \rangle)/\langle a \rangle$$

$$u_A(z) = \delta_A \Delta z + (\delta_B - \delta_A) n_B \langle a \rangle$$

$$\Delta z = z - z_m$$



$$I = I_i \frac{4(\pi r_{\mathrm{el}} C)^2}{V_{\mathrm{cell}}^2} \sum_{\boldsymbol{g}_\parallel} \left| \frac{1}{K_{\boldsymbol{g}z}} \sum_{g_z} F_{\mathrm{period}}(\boldsymbol{g}_\parallel, K_{\boldsymbol{g}z} - K_{iz}) \times \right.$$

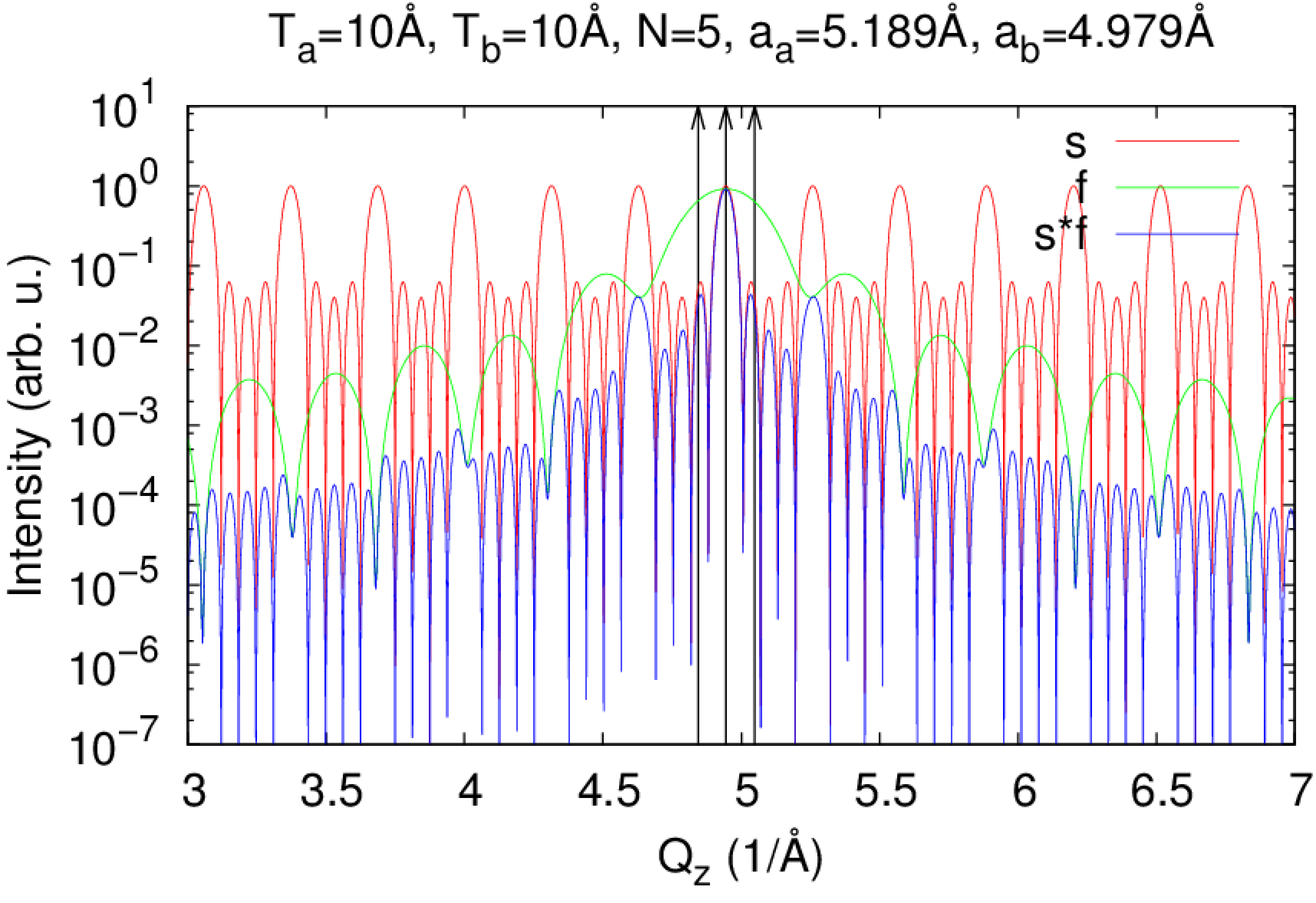
$$\left. \times G_{\mathrm{multilayer}}(K_{\boldsymbol{g}z} - \tilde{K}_{\boldsymbol{g}z}) \right|^2,$$

$$F_{\mathrm{period}}(\boldsymbol{Q}) = F_{\mathrm{cell}}^{(B)}(\boldsymbol{Q}) \frac{\mathrm{e}^{-\mathrm{i}q_B T_B} - 1}{-\mathrm{i}q_B} + F_{\mathrm{cell}}^{(A)}(\boldsymbol{Q}) \mathrm{e}^{-\mathrm{i}q_B T_B} \frac{\mathrm{e}^{-\mathrm{i}q_A T_A} - 1}{-\mathrm{i}q_A}$$

$$q_{A,B} = Q_z - g_z + Q_z \delta_{A,B} \qquad G_{\mathrm{multilayer}}(q) = \mathrm{e}^{\mathrm{i}qD} \frac{\mathrm{e}^{\mathrm{i}qT} - 1}{\mathrm{e}^{\mathrm{i}qD} - 1}, \; q = K_{\boldsymbol{g}z} - \tilde{K}_{\boldsymbol{g}z}$$

Epitaxní vrstvy

Multivrstva s – geometrický faktor, f – strukturní faktor, sf – celková intenzita



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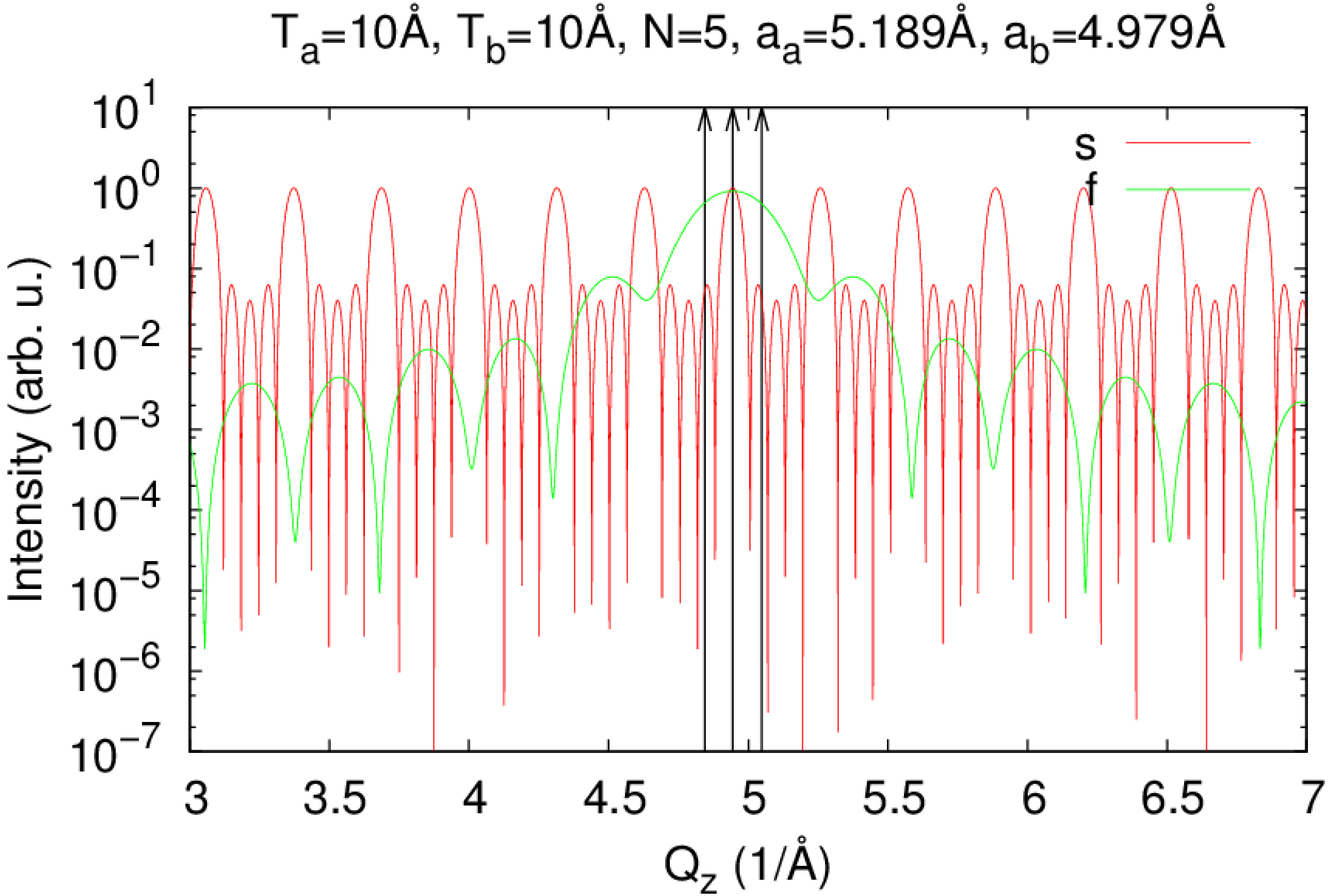

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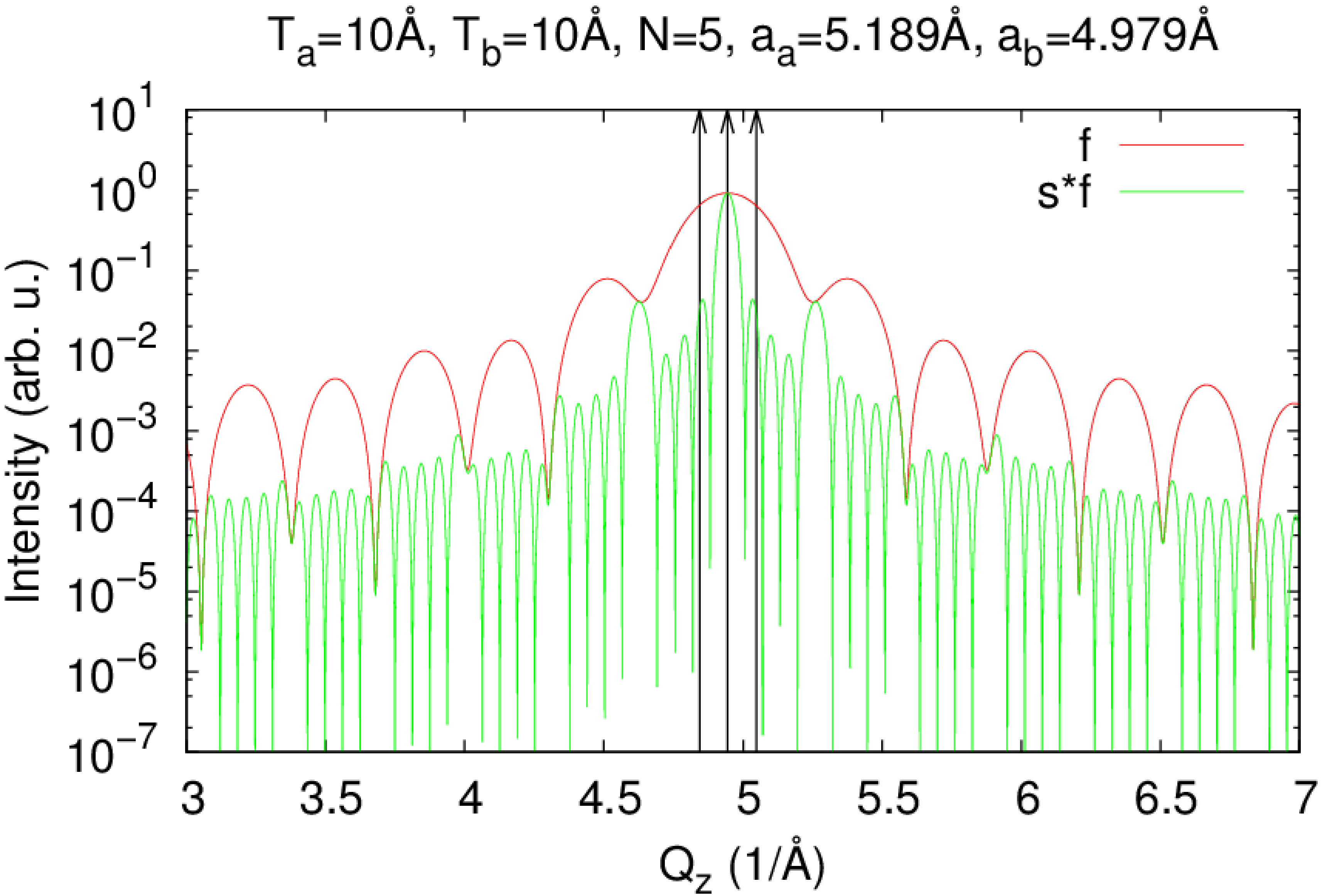

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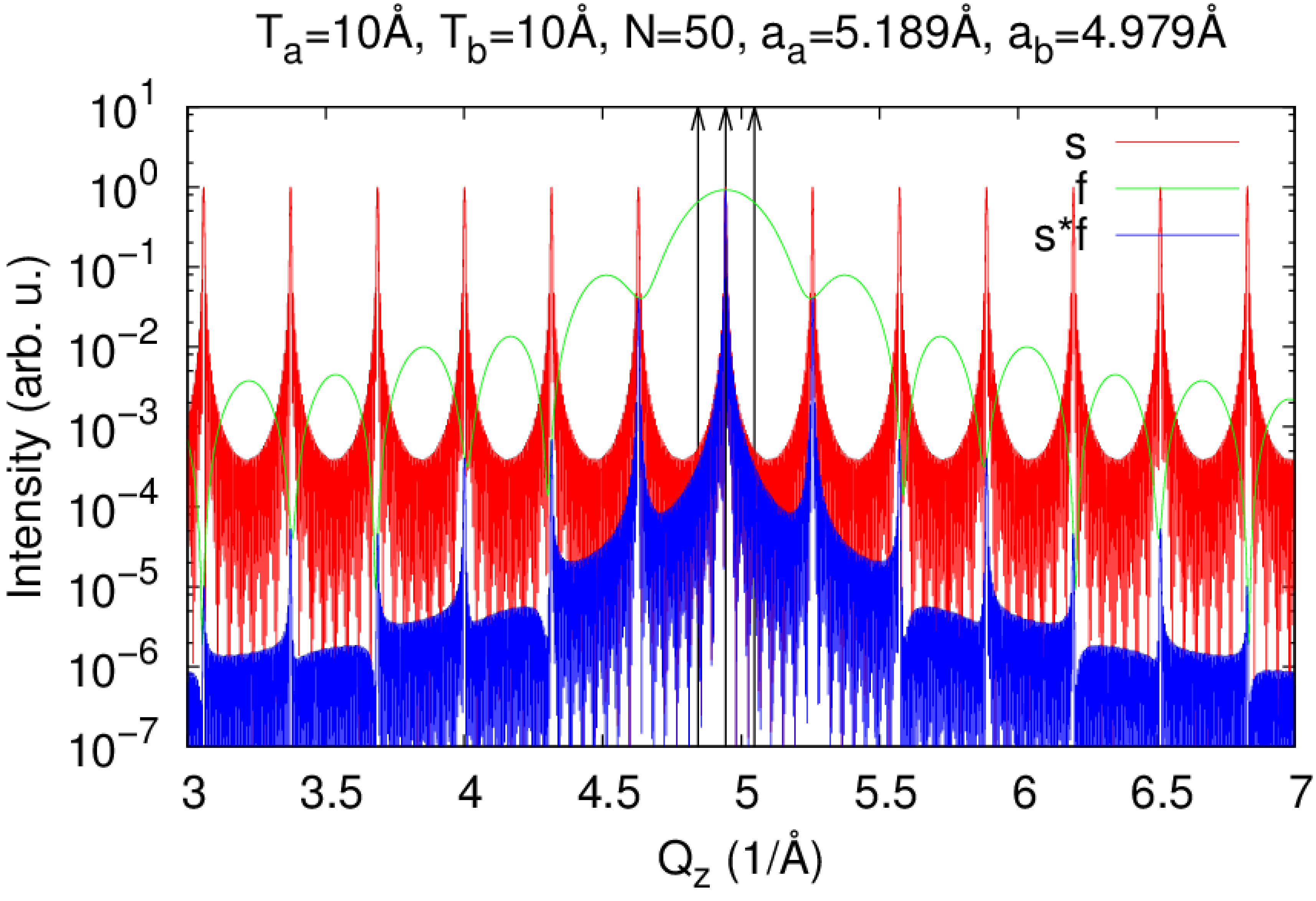

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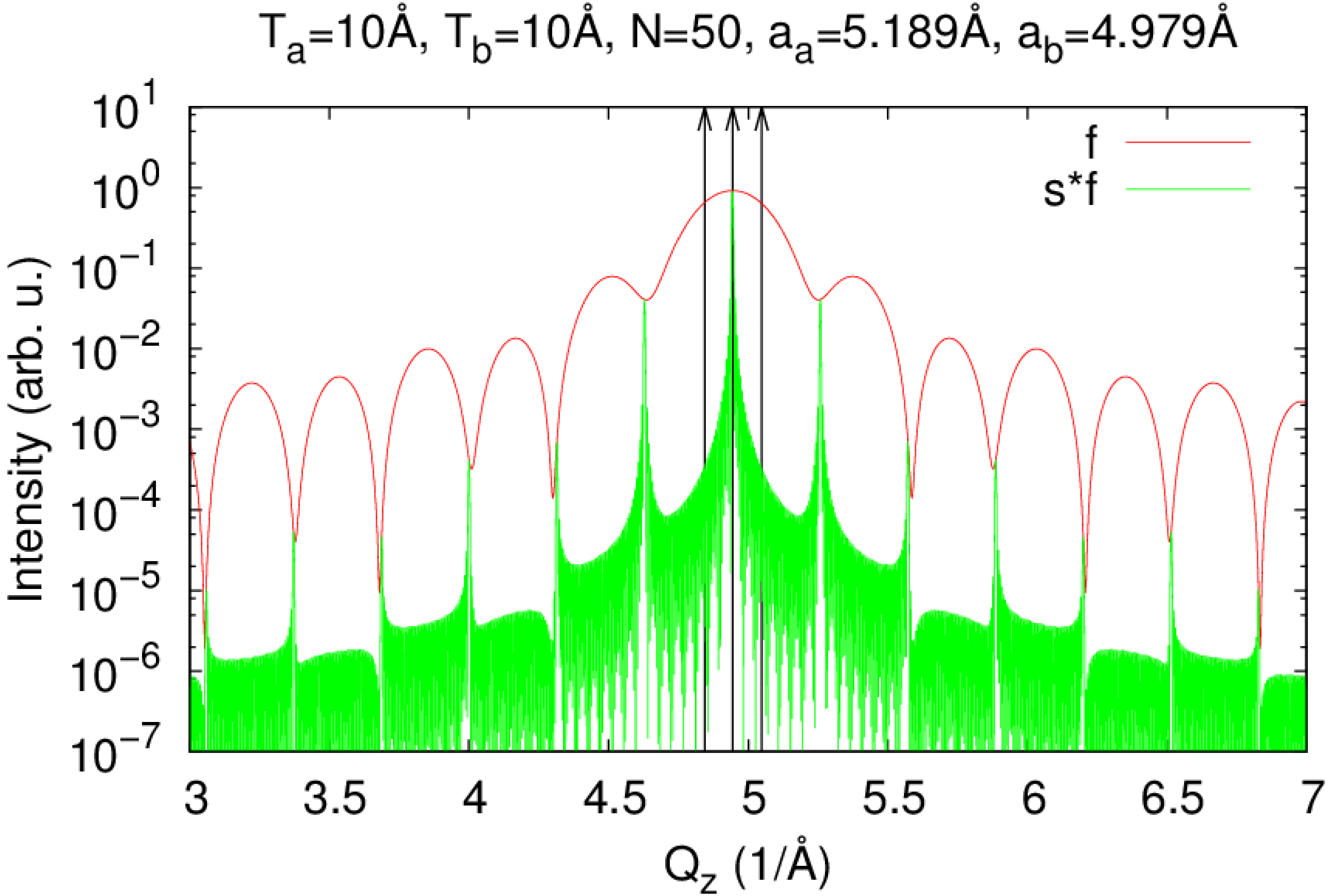

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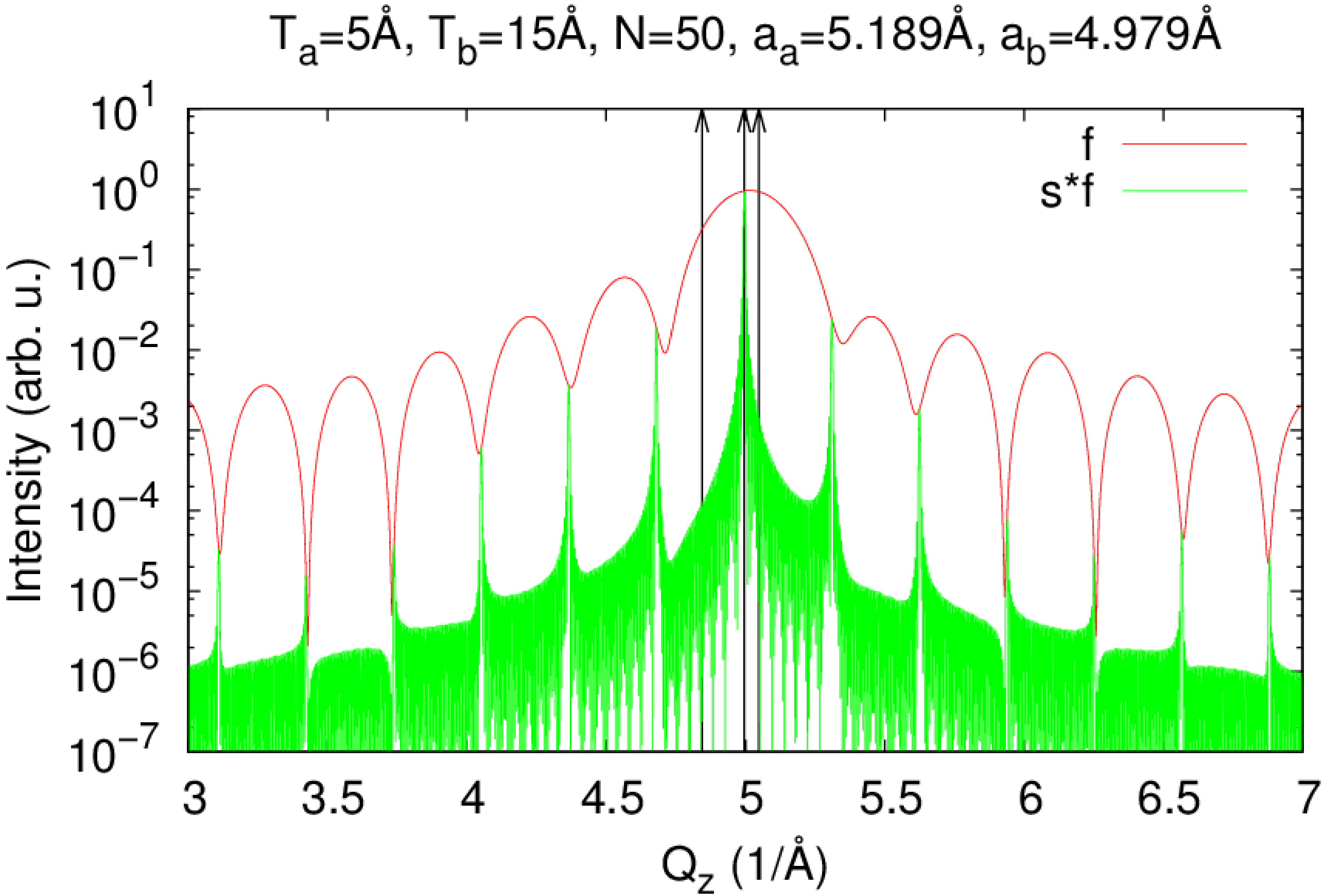
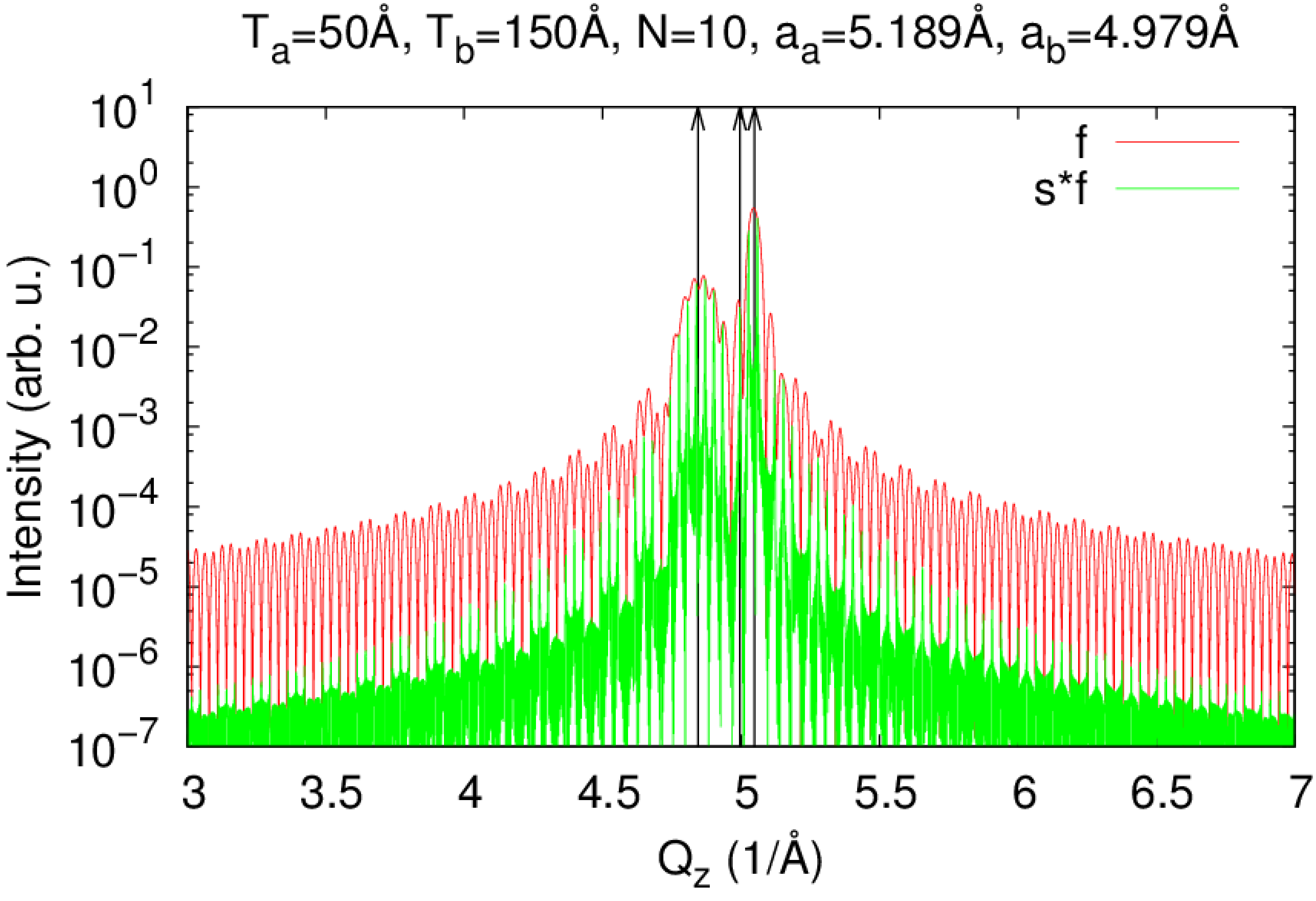


Epitaxní vrstvy

Multivrstva s – geometrický faktor, f – strukturní faktor, sf – celková intenzita



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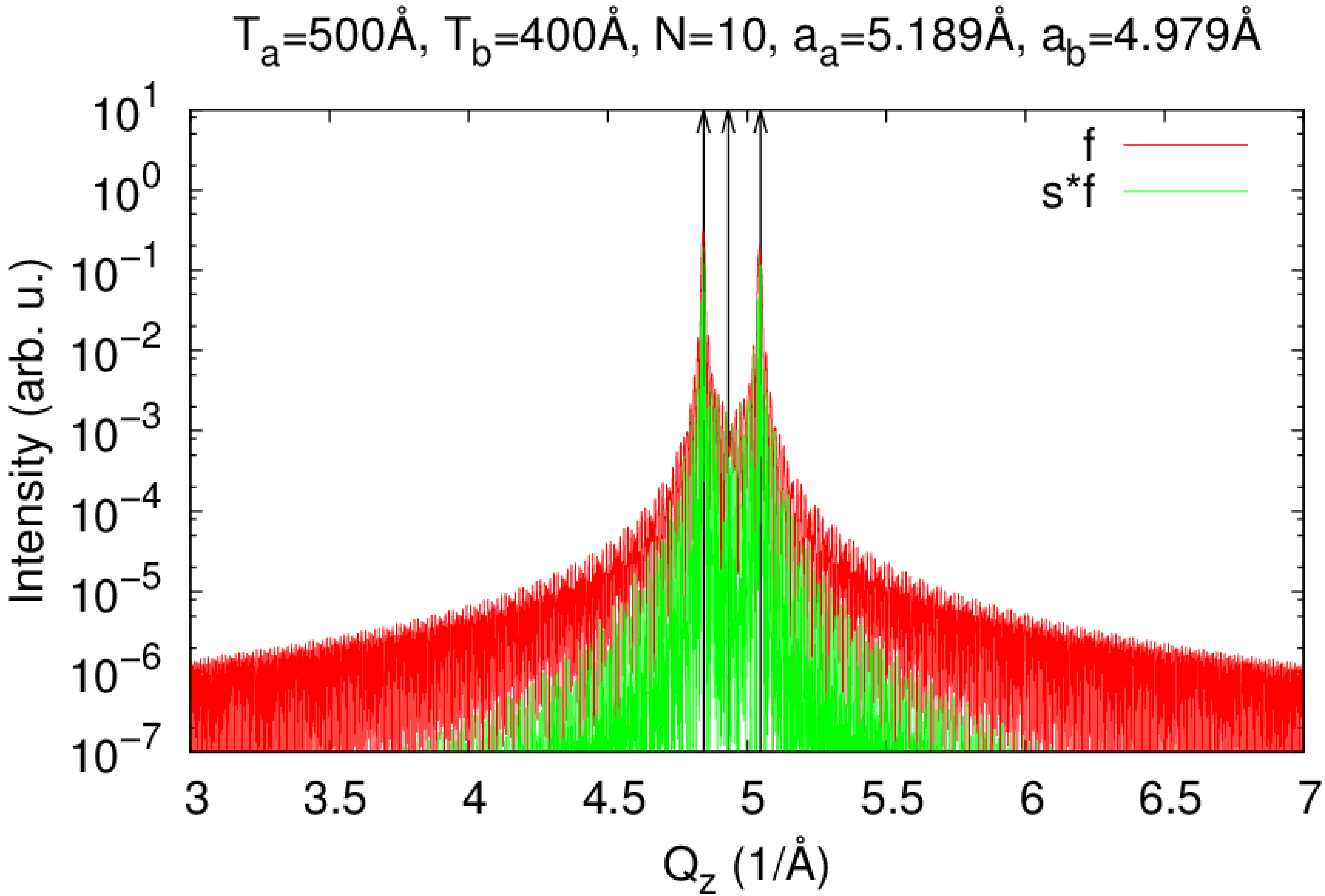


Epitaxní vrstvy

$$\chi^{\mathrm{def}}(\boldsymbol{r}) = \sum_{\boldsymbol{g}} [\chi_{\boldsymbol{g}} + \delta\chi_{\boldsymbol{g}}(\boldsymbol{r})] \mathrm{e}^{\mathrm{i}\boldsymbol{g}.(\boldsymbol{r}-\boldsymbol{u}(\boldsymbol{r}))} \equiv \sum_{\boldsymbol{g}} \chi_{\boldsymbol{g}}^{\mathrm{def}}(\boldsymbol{r}) \mathrm{e}^{\mathrm{i}\boldsymbol{g}.(\boldsymbol{r}-\boldsymbol{u}(\boldsymbol{r}))}$$

$$J_{\mathrm{coh}}(\boldsymbol{Q}) = I_i \frac{K^6}{4} \left| \left\langle \chi_{\boldsymbol{h}}^{\mathrm{def}} \mathrm{e}^{-\mathrm{i}\boldsymbol{h}.\delta\boldsymbol{u}} \right\rangle \right|^2 \delta^{(2)}(\boldsymbol{Q}_\parallel - \boldsymbol{h}_\parallel^{\mathrm{def}}) \times$$

$$\times \left| G_{\mathrm{cryst}}(Q_z - h_z^{\mathrm{def}}) \right|^2,$$

$$I_{\mathrm{coh}} = I_i \frac{K^4}{4(K_{\boldsymbol{h}z}^{\mathrm{def}})^2} \left| \left\langle \chi_{\boldsymbol{h}}^{\mathrm{def}} \mathrm{e}^{-\mathrm{i}\boldsymbol{h}.\delta\boldsymbol{u}} \right\rangle \right|^2 \left| G_{\mathrm{cryst}}(K_{\boldsymbol{h}z}^{\mathrm{def}} - \tilde{K}_{\boldsymbol{h}z}^{\mathrm{def}}) \right|^2$$

$$I_{\mathrm{incoh}} = I_i \frac{K^4}{16\pi^2} \int \frac{\mathrm{d}^2\boldsymbol{K}_\parallel}{K_z^2} \int \mathrm{d}^2(\boldsymbol{r}_\parallel - \boldsymbol{r'}_\parallel) \int_{-T}^{0} \mathrm{d}z \times$$

$$\times \int_{-T}^{0} \mathrm{d}z' \mathrm{e}^{-\mathrm{i}(\boldsymbol{K} - \tilde{\boldsymbol{K}}_{\boldsymbol{h}}^{\mathrm{def}}).(\boldsymbol{r}-\boldsymbol{r'})} M(\boldsymbol{r} - \boldsymbol{r'}).$$

$$M(\boldsymbol{r''} - \boldsymbol{r'''}) = \mathrm{Cov}\left(\chi_{\boldsymbol{h}}^{\mathrm{def}}(\boldsymbol{r''}) \mathrm{e}^{-\mathrm{i}\boldsymbol{h}.\delta\boldsymbol{u}(\boldsymbol{r''})}, \chi_{\boldsymbol{h}}^{\mathrm{def}}(\boldsymbol{r'''}) \mathrm{e}^{-\mathrm{i}\boldsymbol{h}.\delta\boldsymbol{u}(\boldsymbol{r'''})} \right)$$

$$\mathrm{Cov}(a,b) = \langle ab^* \rangle - \langle a \rangle \langle b \rangle^*$$

Epitaxní vrstvy

$$C(\boldsymbol{r}'', \boldsymbol{r}''') \equiv C(\boldsymbol{r}'' - \boldsymbol{r}''') =$$

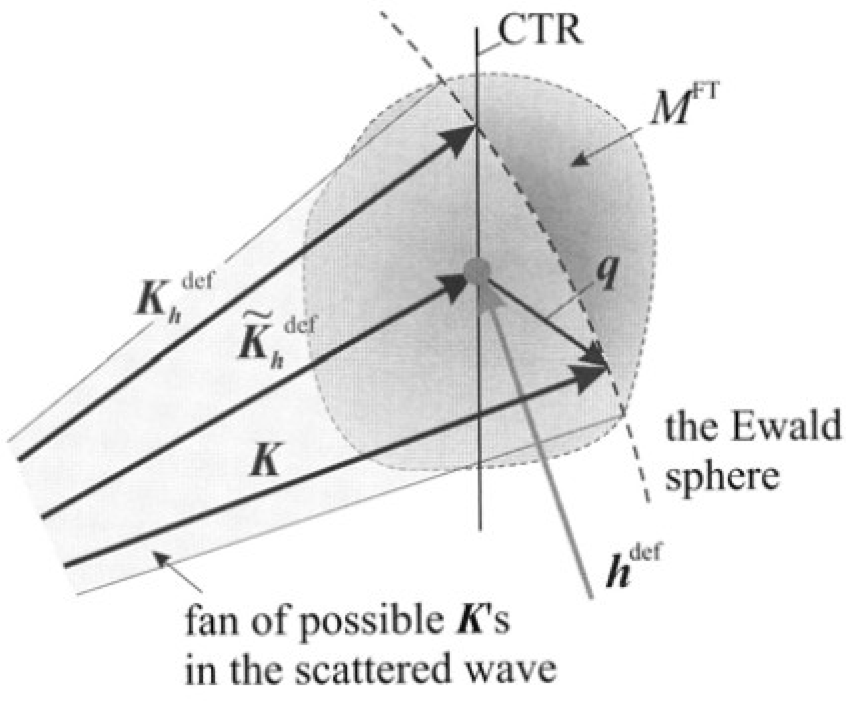
$$= \left\langle \chi_{\boldsymbol{h}}^{\mathrm{def}}(\boldsymbol{r}'')(\chi_{\boldsymbol{h}}^{\mathrm{def}}(\boldsymbol{r}'''))^{*} \mathrm{e}^{-\mathrm{i}\boldsymbol{h}.(\delta\boldsymbol{u}(\boldsymbol{r}'')-\delta\boldsymbol{u}(\boldsymbol{r}'''))} \right\rangle$$

correlation function of the crystal deformation

$$C(\boldsymbol{r}'' - \boldsymbol{r}''') = \left\langle \chi_{\boldsymbol{h}}^{\mathrm{def}}(\boldsymbol{r}'') \mathrm{e}^{-\mathrm{i}\boldsymbol{h}.\delta\boldsymbol{u}(\boldsymbol{r}'')} \right\rangle \left\langle \chi_{\boldsymbol{h}}^{\mathrm{def}}(\boldsymbol{r}''') \mathrm{e}^{-\mathrm{i}\boldsymbol{h}.\delta\boldsymbol{u}(\boldsymbol{r}''')} \right\rangle^{*} +$$

$$+M(\boldsymbol{r}'' - \boldsymbol{r}''').$$

Epitaxní vrstvy



Epitaxní vrstvy

$$\Psi^{\alpha}(\boldsymbol{r}) = \chi_{\boldsymbol{h}} \left(1 - \mathrm{e}^{-\mathrm{i}\boldsymbol{h}.\boldsymbol{v}^{\alpha}(\boldsymbol{r})}\right) + \Delta\chi_{\boldsymbol{h}} \Omega^{\alpha}(\boldsymbol{r}) \mathrm{e}^{-\mathrm{i}\boldsymbol{h}.\boldsymbol{v}^{\alpha}(\boldsymbol{r})}$$

$$M(\boldsymbol{r}, \boldsymbol{r}') = \int \mathrm{d}^3\boldsymbol{r}'' \sum_{\alpha} n^{\alpha}(\boldsymbol{r}'') \Psi^{\alpha}(\boldsymbol{r} - \boldsymbol{r}'') \Psi^{\alpha *}(\boldsymbol{r}' - \boldsymbol{r}'')$$

$$J_{\mathrm{incoh}}(\boldsymbol{Q}) = I_i \frac{K^6 T}{16\pi^2} \sum_{\alpha} n^{\alpha} \left|\Psi^{\alpha \mathrm{FT}}(\boldsymbol{q})\right|^2$$

$$\Psi^{\alpha}_{\mathrm{Huang}}(\boldsymbol{r}) = \chi_{\boldsymbol{h}} \left(1 - \mathrm{e}^{-\mathrm{i}\boldsymbol{h}.\boldsymbol{v}^{\alpha}(\boldsymbol{r})}\right)$$

$$\Psi^{\alpha}_{\mathrm{Huang}}(\boldsymbol{r}) \approx \mathrm{i}\chi_{\boldsymbol{h}} \boldsymbol{h}.\boldsymbol{v}^{\alpha}(\boldsymbol{r})$$

$$\boldsymbol{v}(\boldsymbol{r}) = \begin{cases} P\boldsymbol{r}/r^3 & \text{for } r > R \\ P\boldsymbol{r}/R^3 & \text{for } r \leq R \end{cases}$$

$$J_{\mathrm{Huang}}(\boldsymbol{Q}) = I_i \frac{K^6 T}{16\pi^2} |\chi_{\boldsymbol{h}}|^2 \sum_{\alpha} n^{\alpha} \left|\boldsymbol{h}.\boldsymbol{v}^{\alpha \mathrm{FT}}(\boldsymbol{q})\right|^2$$

Epitaxní vrstvy

$$\Psi^{\alpha}_{\mathrm{core}}(\boldsymbol{r}) = \Delta\chi_{\boldsymbol{h}}\Omega^{\alpha}(\boldsymbol{r})\mathrm{e}^{-\mathrm{i}\boldsymbol{h}.\boldsymbol{v}^{\alpha}(\boldsymbol{r})}$$

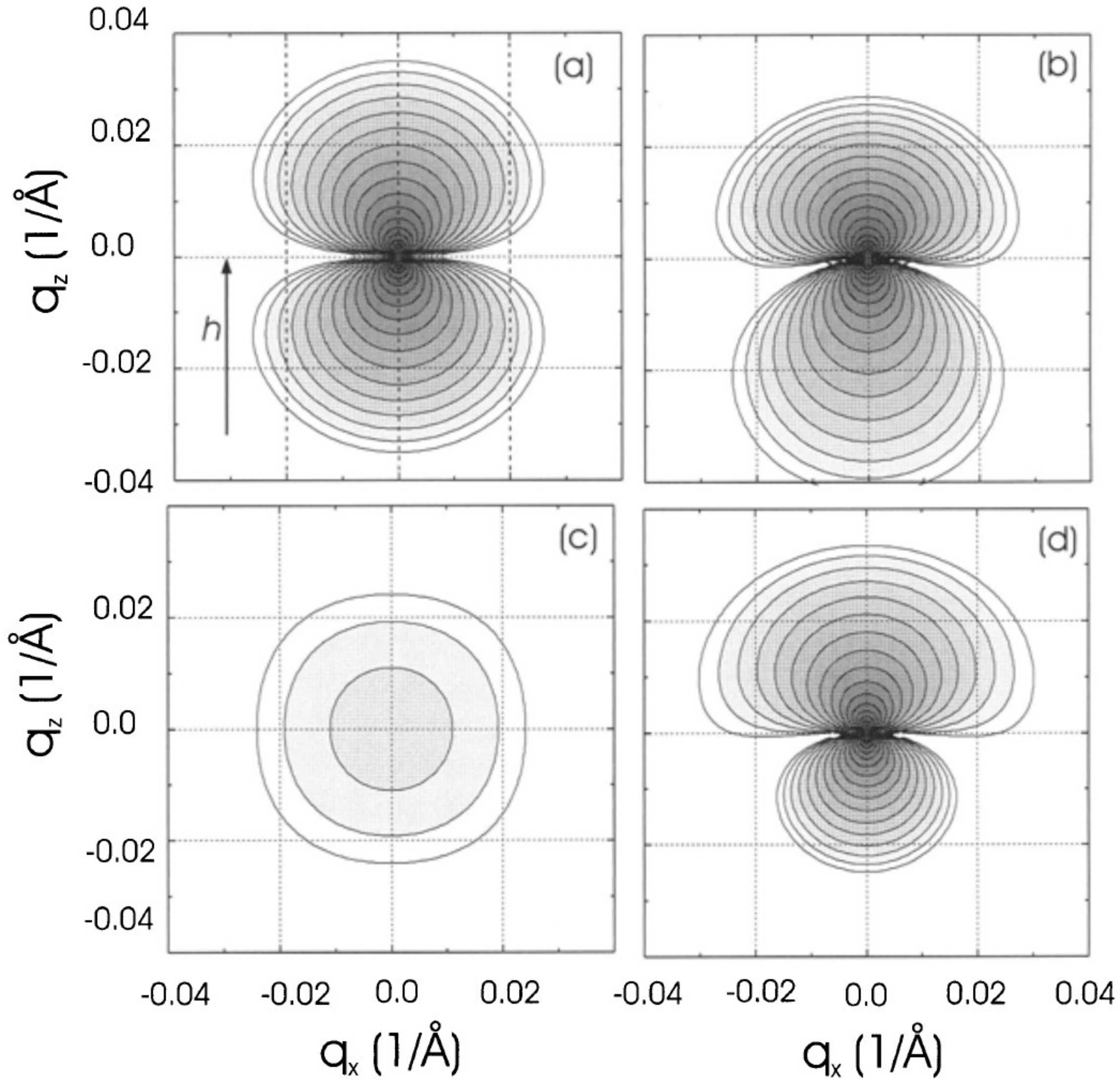
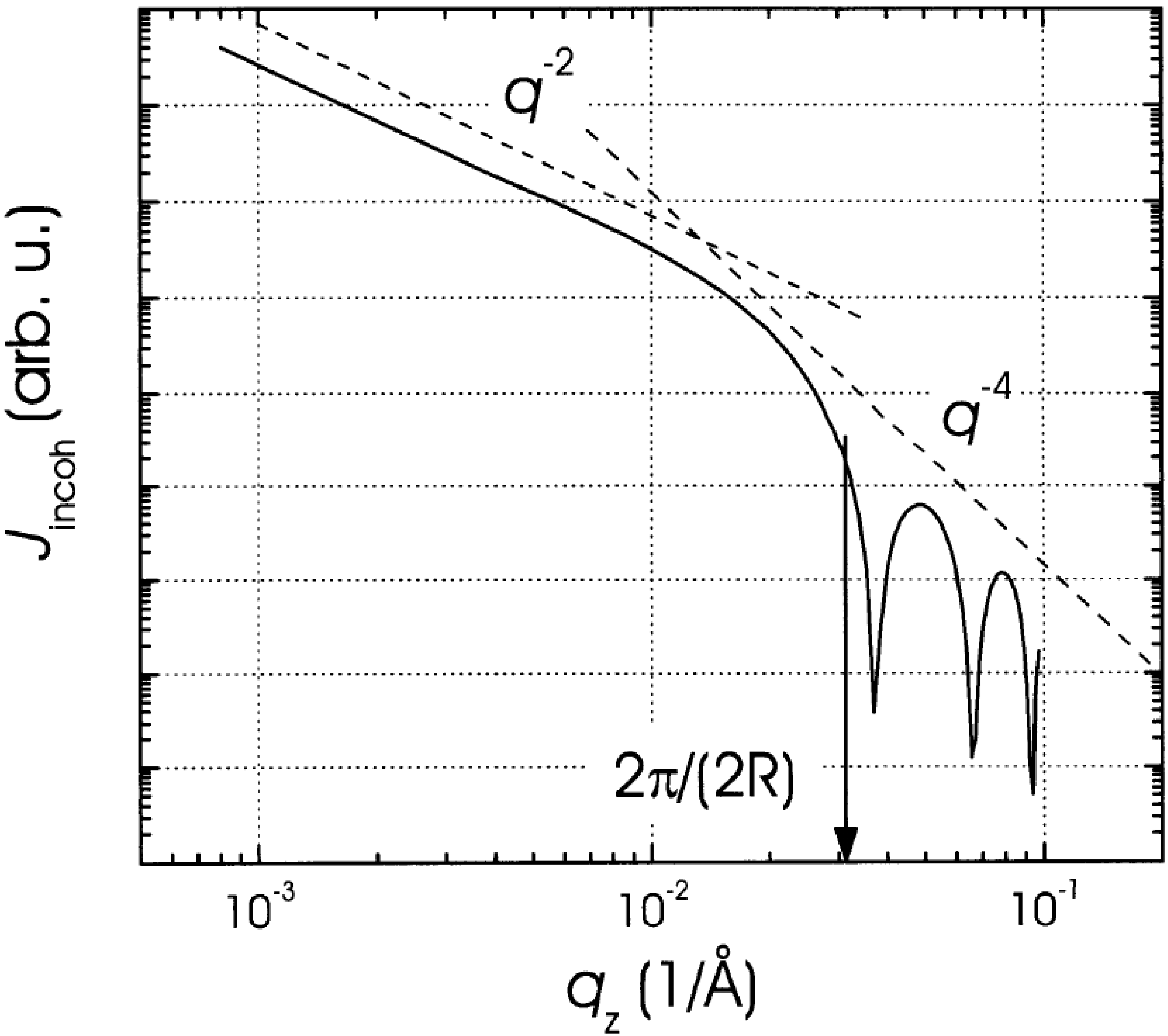
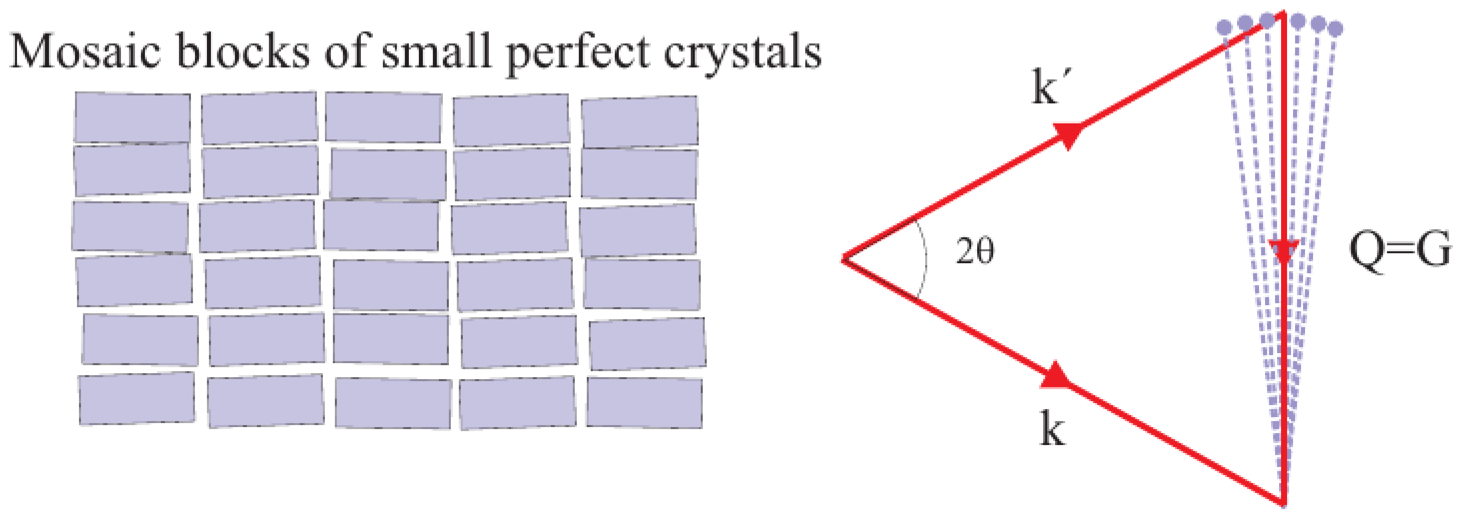


Fig. 10.1. Diffuse intensity distribution in reciprocal space calculated for spherical inclusions with radius 10 nm and the lattice mismatch 0.5%. Panel (a) shows the Huang scattering using the approximation $\exp(-\mathrm{i}\boldsymbol{h}.\boldsymbol{v}) - 1 \approx -\mathrm{i}\boldsymbol{h}.\boldsymbol{v}$; in (b) the Huang scattering is presented without this approximation. Panel (c) represents the core scattering; in (d) the total scattered intensity is depicted. The contour step is $10^{0.25}$.

Epitaxní vrstvy



Epitaxní vrstvy



Epitaxní vrstvy

$$C(\boldsymbol{r}-\boldsymbol{r}') = |\chi_{\boldsymbol{h}}|^2 \left\langle \mathrm{e}^{-\mathrm{i}\boldsymbol{h}.(\boldsymbol{u}(\boldsymbol{r})-\boldsymbol{u}(\boldsymbol{r}'))} \right\rangle =$$

$$= |\chi_{\boldsymbol{h}}|^2 P(\boldsymbol{r}-\boldsymbol{r}') \left\langle \mathrm{e}^{-\mathrm{i}\boldsymbol{h}.(\boldsymbol{u}(\boldsymbol{r})-\boldsymbol{u}(\boldsymbol{r}'))} \right\rangle_{\mathrm{rot}},$$

$$P(\boldsymbol{\varrho}) = \frac{\int \mathrm{d}^3\boldsymbol{r}'' \Omega(\boldsymbol{r}'')\Omega(\boldsymbol{\varrho}+\boldsymbol{r}'')}{\int \mathrm{d}^3\boldsymbol{r}'' \Omega(\boldsymbol{r}'')}, \;\; \boldsymbol{\varrho} = \boldsymbol{r}-\boldsymbol{r}'$$

$$P(\boldsymbol{\varrho}) = \begin{cases} 1 - \frac{3}{4}\frac{|\boldsymbol{\varrho}|}{R} + \frac{1}{16}\left(\frac{|\boldsymbol{\varrho}|}{R}\right)^3 & \text{for } |\boldsymbol{\varrho}| \le 2R \\ 0 & \text{for } |\boldsymbol{\varrho}| > 2R \end{cases}$$

$$\left\langle \mathrm{e}^{-\mathrm{i}\boldsymbol{h}.(\boldsymbol{u}(\boldsymbol{r})-\boldsymbol{u}(\boldsymbol{r}'))} \right\rangle_{\mathrm{rot}} = \exp\left[-\frac{1}{6}\Delta^2 |\boldsymbol{h} \times (\boldsymbol{r}-\boldsymbol{r}')|^2\right]$$

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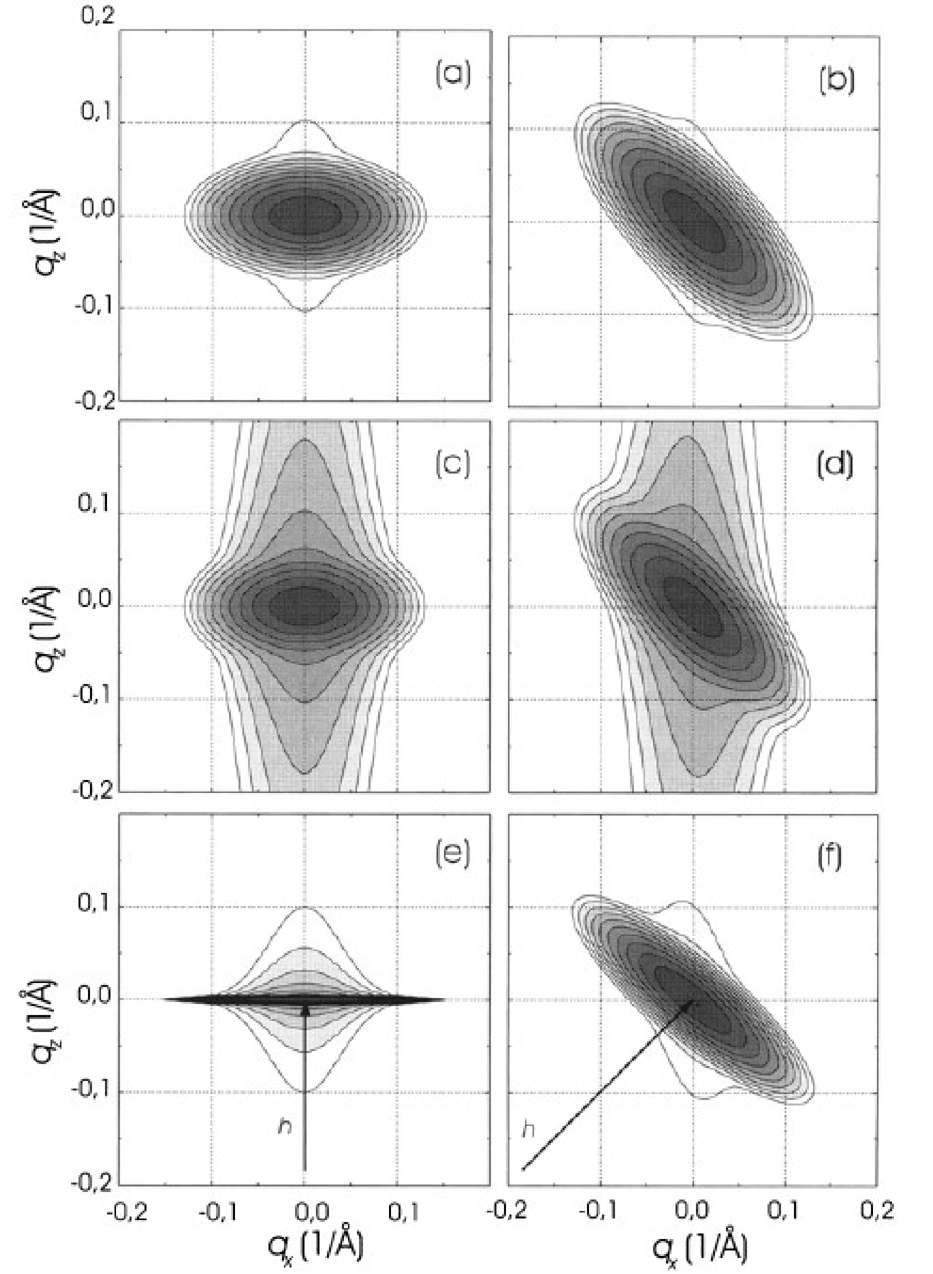

Fig. 10.15. The intensity maps of a mosaic layer calculated in symmetric 004 diffraction (a,c,e) and asymmetric 404 diffraction (b,d,f). The layer thickness was 10 μm (a,b,e,f) and 100 nm (c,d). In all panels, the root mean square misorientation of the blocks was 0.5°. In (a-d) the blocks were spherical with radius 10 nm; in (e,f) they were columnar with the horizontal radius 10 nm and height 2 μm. In (e) and (f) the directions of the diffraction vectors are denoted by arrows; the step of the intensity contours was $\sqrt{10}$.