Intensity measurement of equal thickness fringes in wedge-shaped crystal images and estimation of crystal potential

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Introduction

Analysis of Equal Thickness Fringes

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Improvement of dynamical electron diffraction theory
and
Evaluation of structure factor of crystals

- Two beam excited Bragg condition
- Multi beam excited zone-axis condition

1) **GaAs** and **InP**

K. Nishio, H. Kakibayashi, T. Isshiki, H. Saijo and M. Shiojiri,
J. Electron Microscopy **43** (1994) 198–202.

2) **Si** and **MgO**

K. Nishio, T. Isshiki and M. Shiojiri,
J. Electron Microscopy **49** (2000) in print.

Computer simulation

Crystal potential
⇓
Scattering process
⇓
Imaging process

⟸ Reliable experimental data

Objective inspection of the simulation program
is indispensable for its accuracy

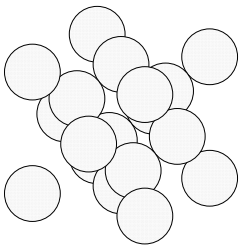
Experimental

Specimen

Si

Diamond-type

$a = 0.54307$ nm

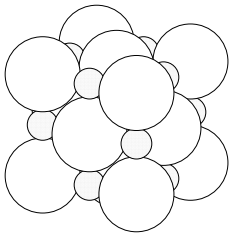


prepared by cleaving a Si (001) wafer along the $\{110\}$.

MgO

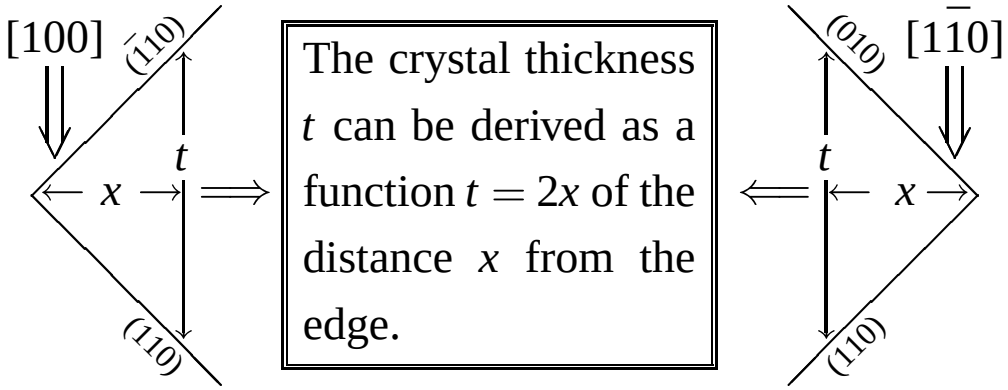
NaCl-type

$a = 0.42112$ nm



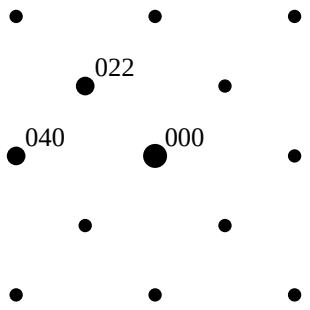
prepared by burning Mg in air.

Observed direction

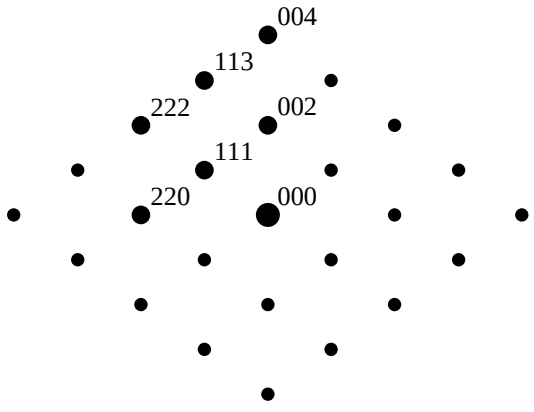


The crystal orientations were exactly adjusted by Kikuchi lines.

Observed diffraction spots



000, 022, 040



000, 002, 111, 220, 004, 113, 222

Equipment

TEM	
JEM-2010FEF JEM-2010EF	Equipped with an Ω-type energy filter
Recording media	
Imaging Plate	Pixel size: 25 μm, Dynamic range: 14 bits

Observed conditions

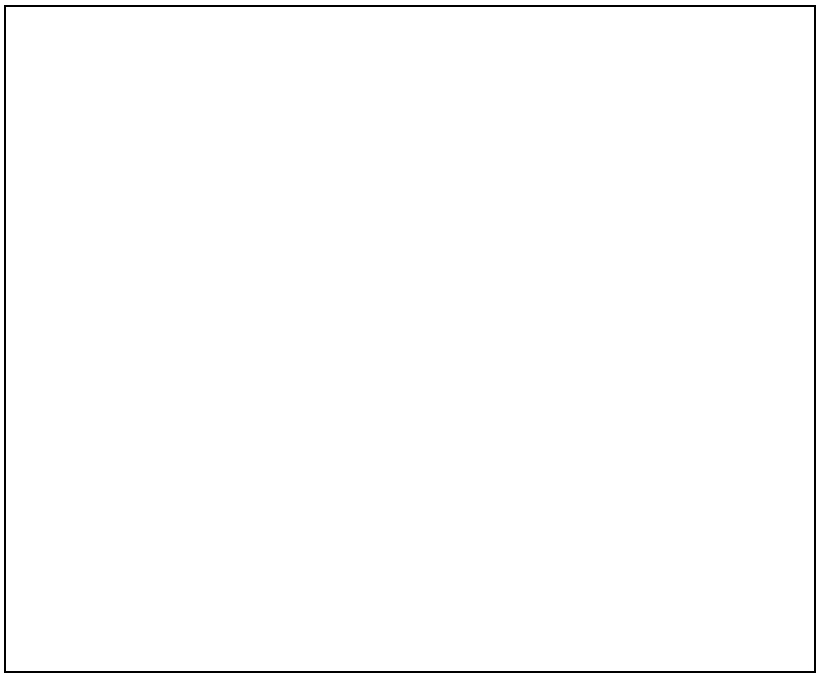
Specimen	Si	MgO
Orientation	[100]	[$1\bar{1}0$]
Dif. spot	000, 022, 040	000, 111, 002, 220, 113, 222, 004
Accel. volt.	200 kV	
Energy filter	Zero-loss filter ($\pm$5 eV), unfilter	
Mag.	$\geq$ 200,000	

Computer simulation

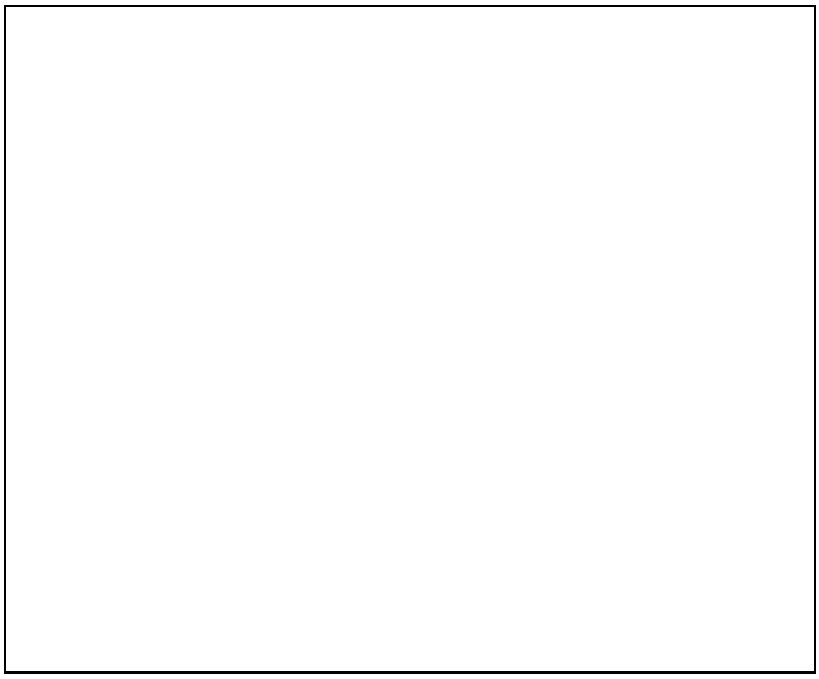
Dynamical calculation	Multi-slice method	
Atomic scattering factor	Si, Mg, O	**DT**
	Mg^{2+}	**DT, Peng**
	O^{2-}	**TMI, Peng**
Temperature factor	Mg, O	**ZORS**

DT: Doyle and Turner, *Acta Cryst.* **A24** (1968) 390
TMI: Tanji, Masaoka and Ito, *J. Elec. Microsc.* **38** (1989) 409
Peng: Peng, *Acta Cryst.* **A54** (1998) 481
ZORS: Zuo, O'Keeffe, Rez and Spence, *Phys. Rev. Lett.* **78** (1997) 4777

Example of bright field images



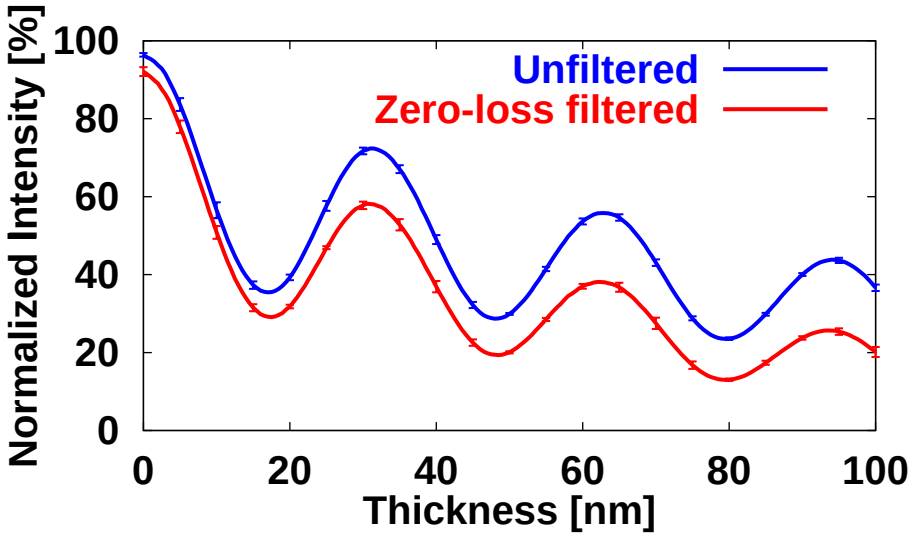
Zero-loss filtered ($-5 \sim +5$ eV) TEM image



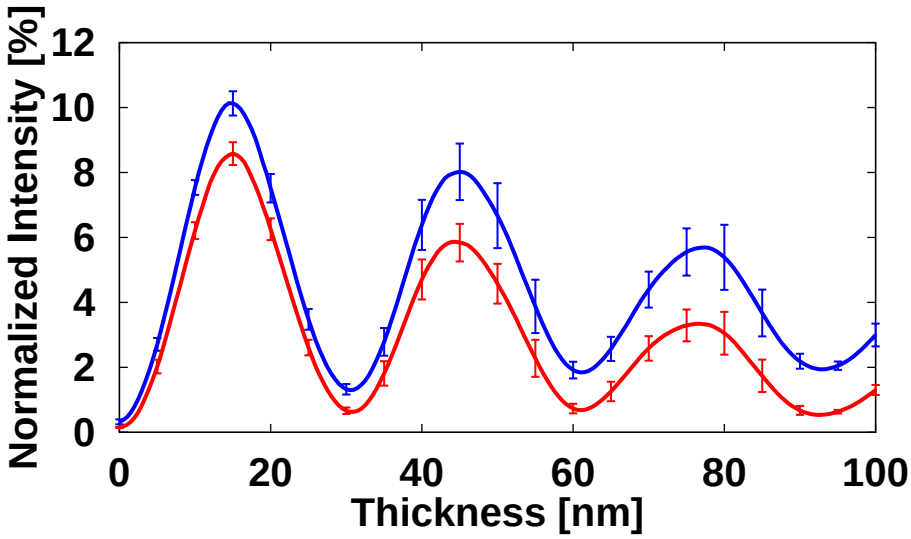
Unfiltered TEM image

Intensity profiles of [100] Si

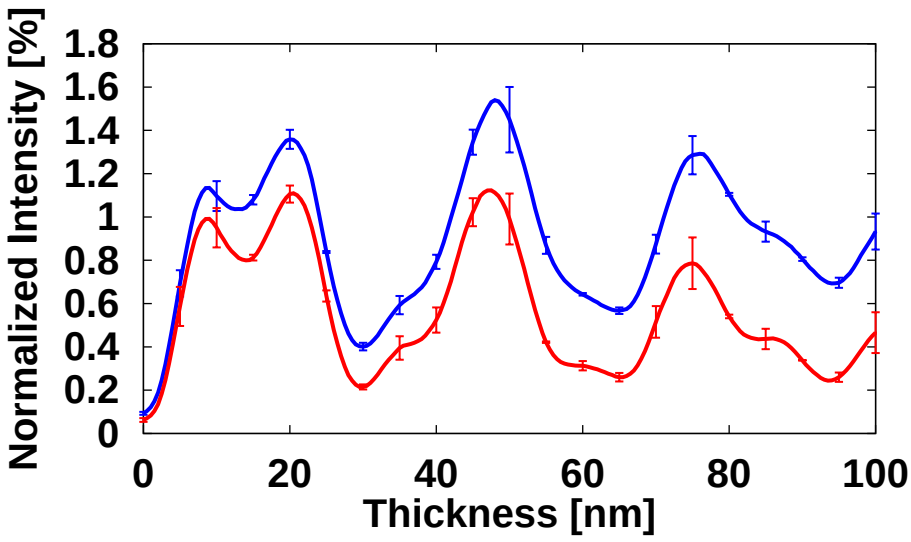
000



022



040



Fitting procedure for Si

- **Correlation coefficient**

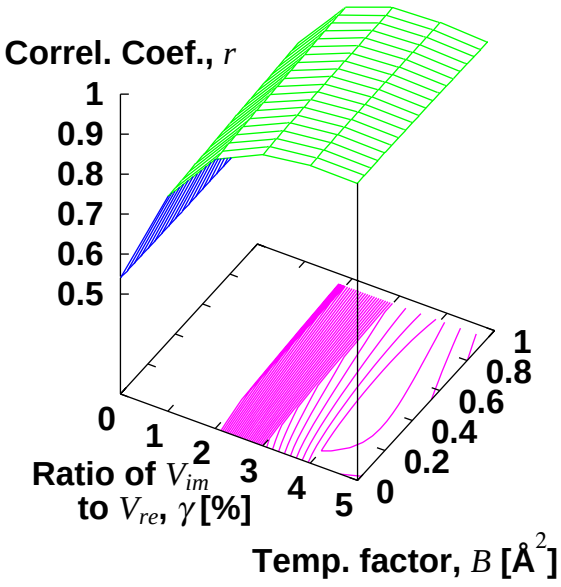
$$r = \frac{\sum \{I_{exp}(t) - \bar{I}_{exp}\}\{I_{cal}(t) - \bar{I}_{cal}\}}{\sqrt{\sum \{I_{exp}(t) - \bar{I}_{exp}\}^2 \sum \{I_{cal}(t) - \bar{I}_{cal}\}^2}}$$

- **Fitting parameters**
  - B: Temperature factor ($B = 0, 0.05, 0.10, \cdots, 1$ Å^2)

    Temperature factor is in Debye-Waller factor, $\exp\left(-Bs^2\right)$

  - γ: Absorption coefficient ($\gamma = 0, 1, \cdots, 10$ %)

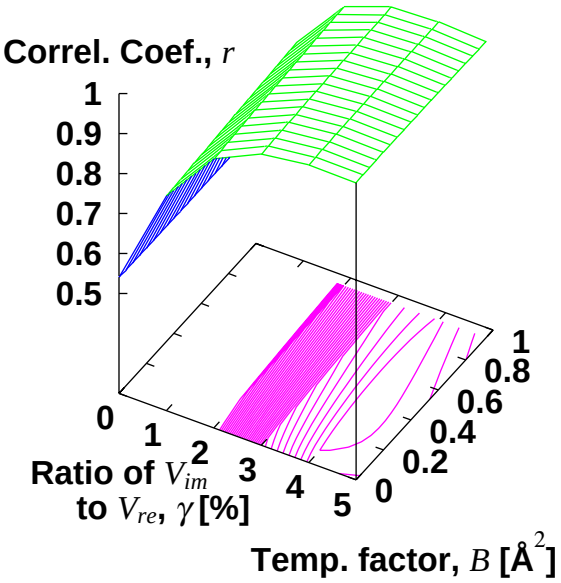
    Complex potential, V, is given by $V = V_{re} + iV_{im}$, where $V_{im} = \gamma V_{re}$



B = 0.45 Å^2

γ = 4 %

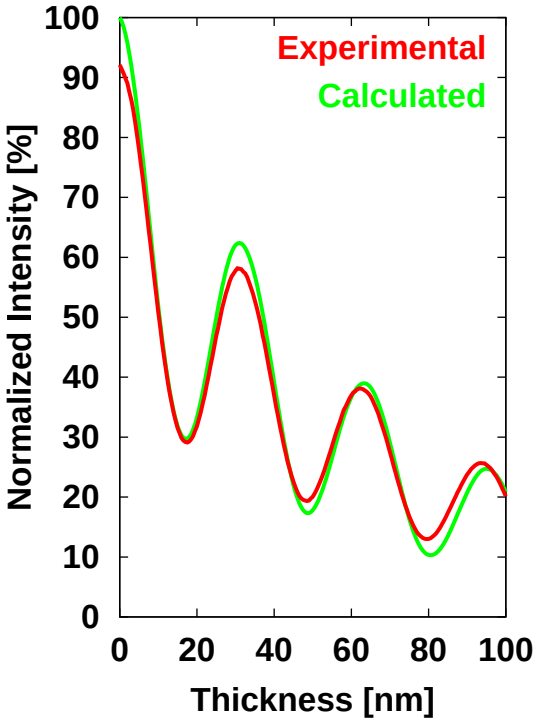
Fitting result for Si



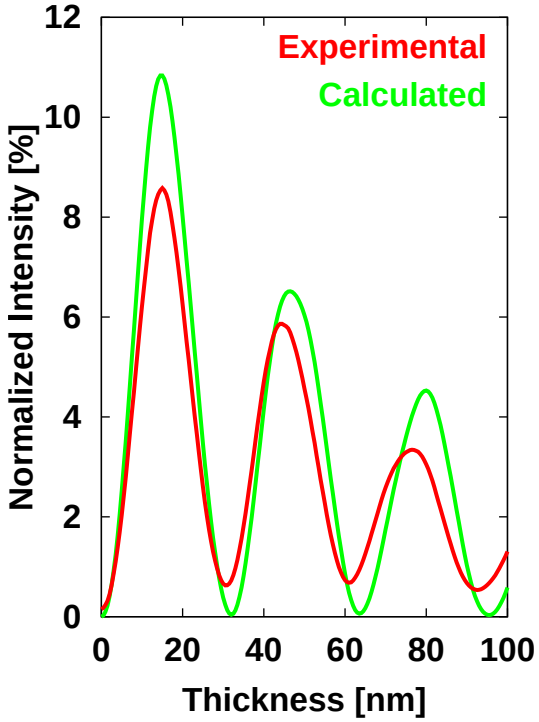
$B = 0.45$ Å^2

$\gamma = 4$ %

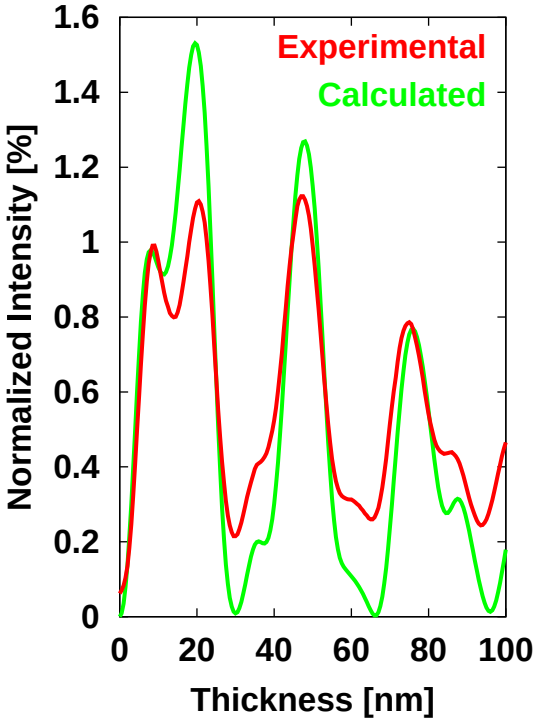
000 ($r = 0.998$)



022 ($r = 0.964$)

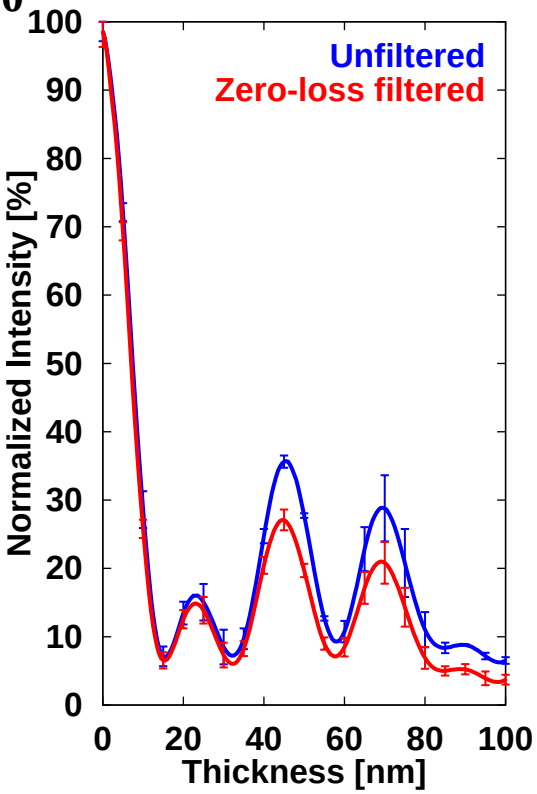


040 ($r = 0.958$)

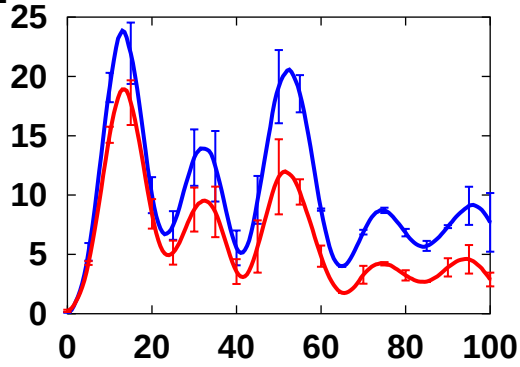


Intensity profiles of [1$\bar{1}$0] MgO

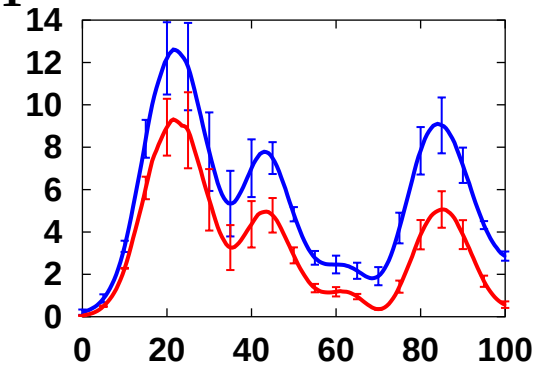
000



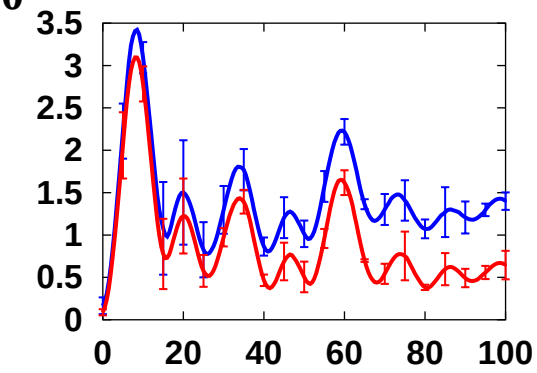
002



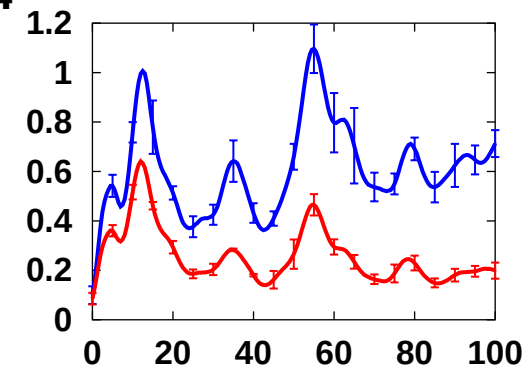
111



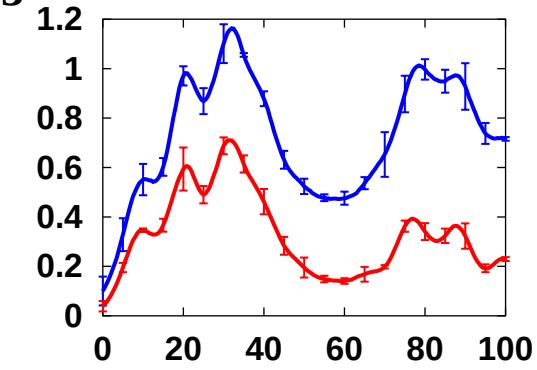
220



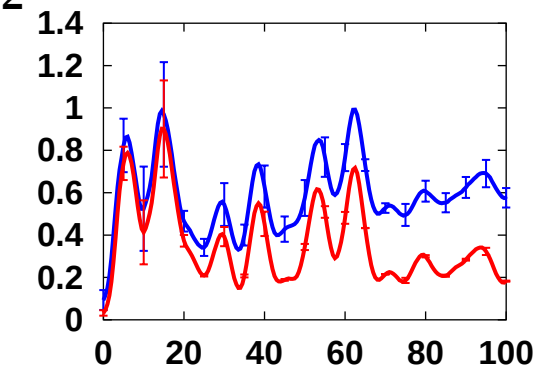
004



113



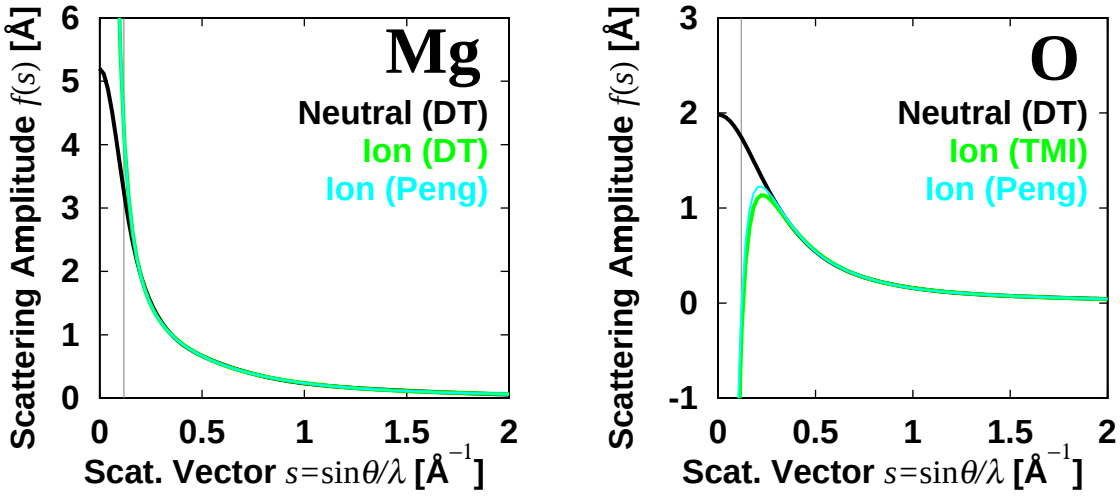
222



Fitting procedure for MgO

- **Scattering factors**

	Mg^{2+}	O^{2-}
Green	**DT**: Doyle and Turner, *Acta Cryst.* **A24** (1968) 390	**TMI**: Tanji, Masaoka and Ito, *J. Elec. Microsc.* **38** (1989) 409
Blue	**Peng**: Peng, *Acta Cryst.* **A54** (1998) 481	

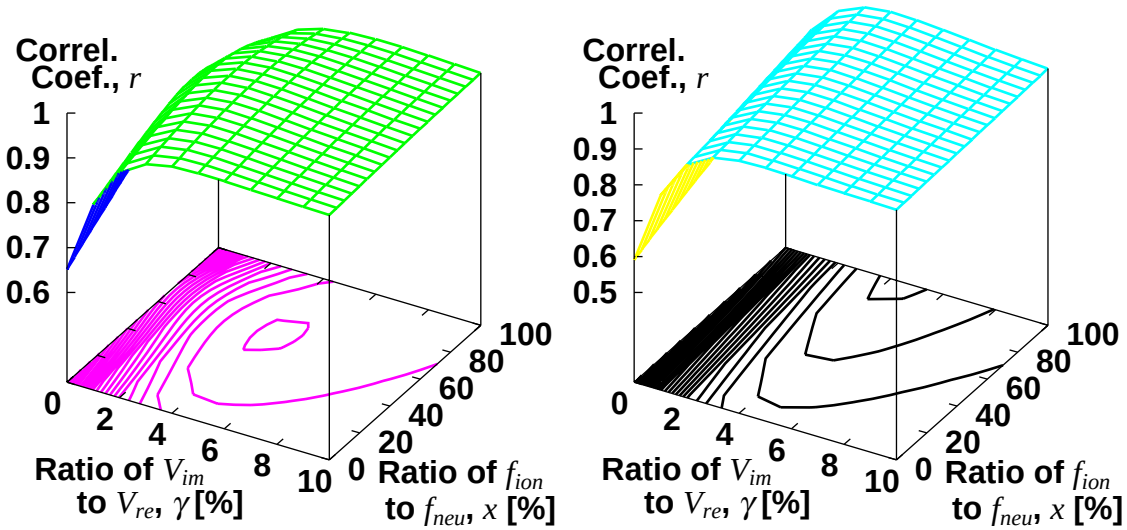


- **Temperature factors**

$B_{\mathrm{Mg}} = 0.305$ Å^2, $B_{\mathrm{O}} = 0.340$ Å^2 (Zuo, O'Keeffe, Rez and Spence, *Phys. Rev. Lett.* **78** (1997) 4777)

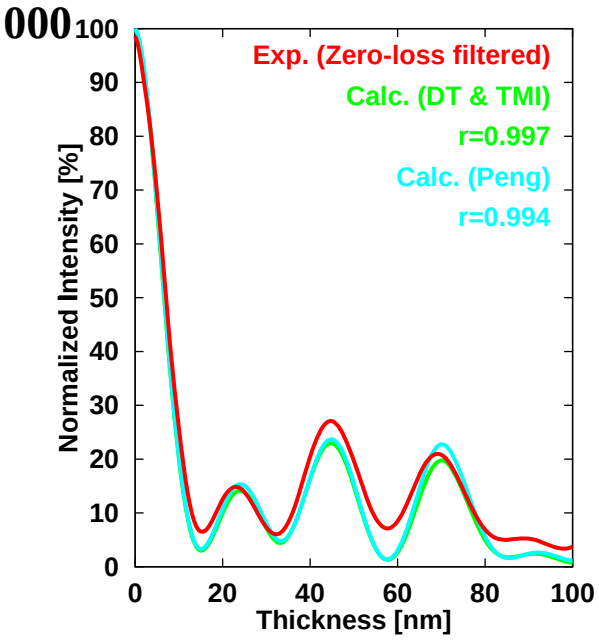
- **Fitting parameters**
  - γ: Absorption coefficient $(\gamma = 0, 1, \cdots, 10\ \%)$
  - x: Ionicity $(x = 0, 5, 10, \cdots, 100\ \%)$

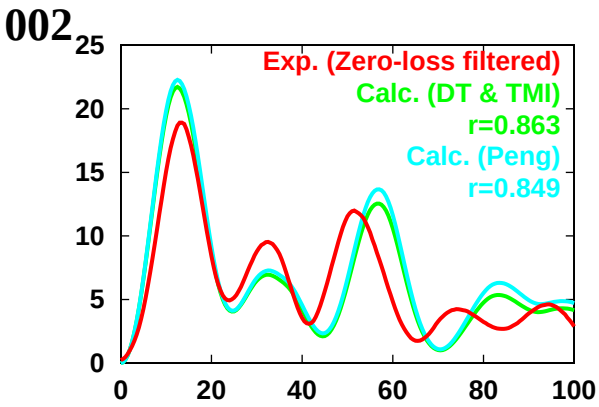
Scattering factor, f, is given by $f = x f_{ion} + (1-x) f_{neu}$

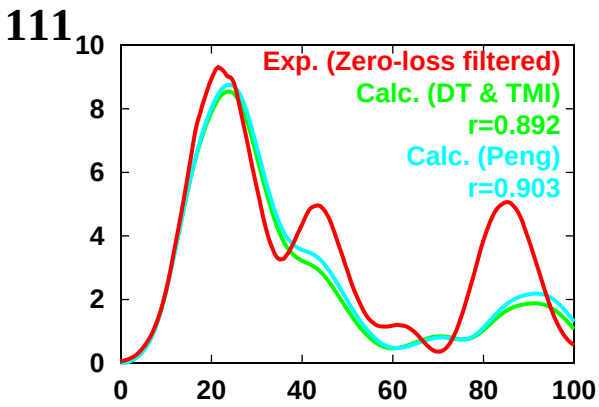


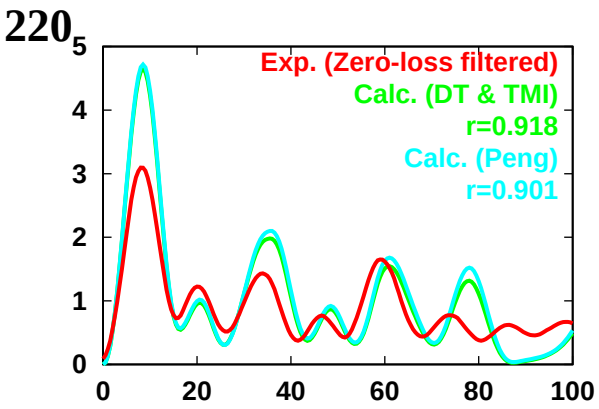
Fitting result for MgO

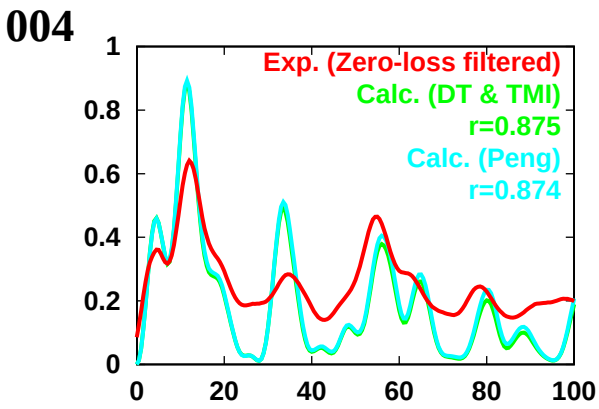
	f_{ion}	x	γ
Green	DT, TMI	65 %	4 %
Blue	Peng	100 %	4 %

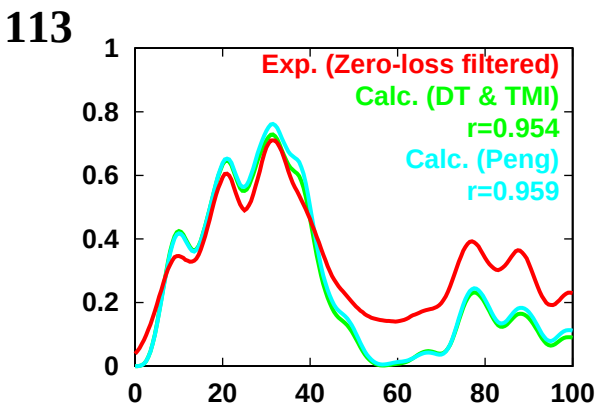


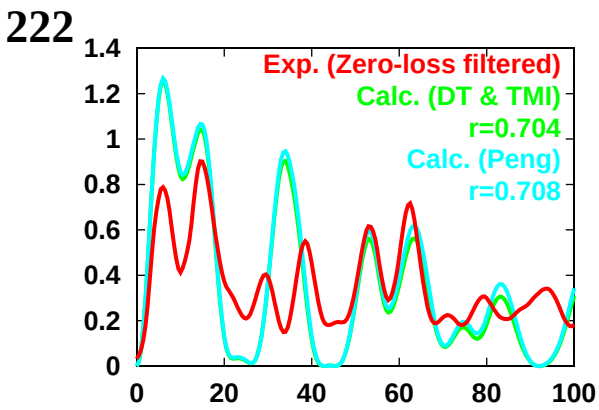












Summary

- **Intensity profiles obtained from zero-loss filtered and unfiltered equal thickness fringes are presented.**

  [100] Si: 000, 022, and 040
  [1$\bar{1}$0] MgO: 000, 111, 002, 220, 113, 222, and 004

- **Comparison between the experimental profiles and the calculated profiles was carried out.**

Si:

B	γ
0.45 Å^2	4 %

MgO:

f_{ion}	x	γ
DT, TMI	65 %	4 %
Peng	100 %	4 %

- The equal thickness fringe intensities can be obtained from

  K. Nishio, T. Isshiki and M. Shiojiri,
  J. Electron Microscopy **49** (2000) in print.

  or by making contact to

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