



Theoretical modeling of crystal properties

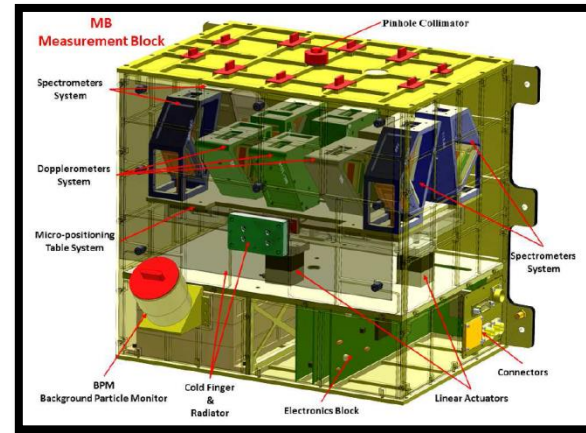
Żaneta Szaforz

1. Astronomical Institute, University of Wrocław; 2. Space Research Centre, PAS, Wrocław

Polish crystal spectrometers



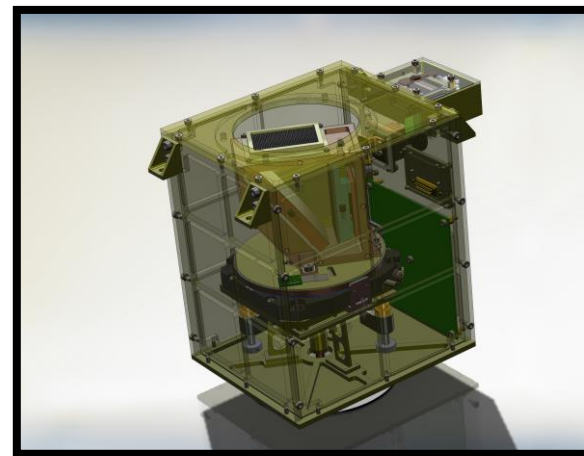
DIOPENESS



CHEMIX



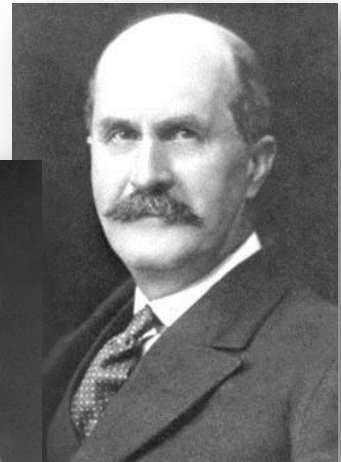
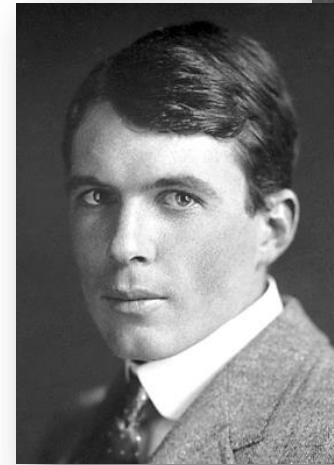
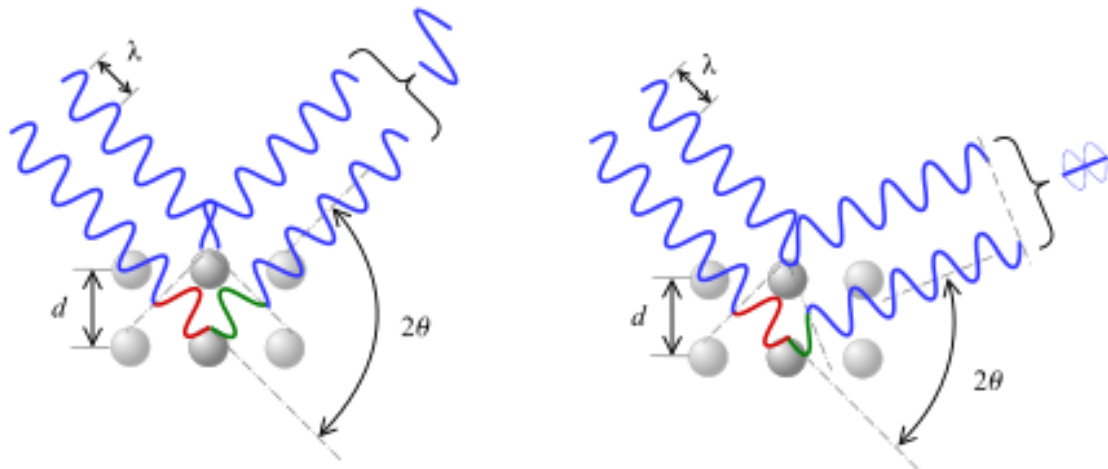
RESIK



SOLPEX

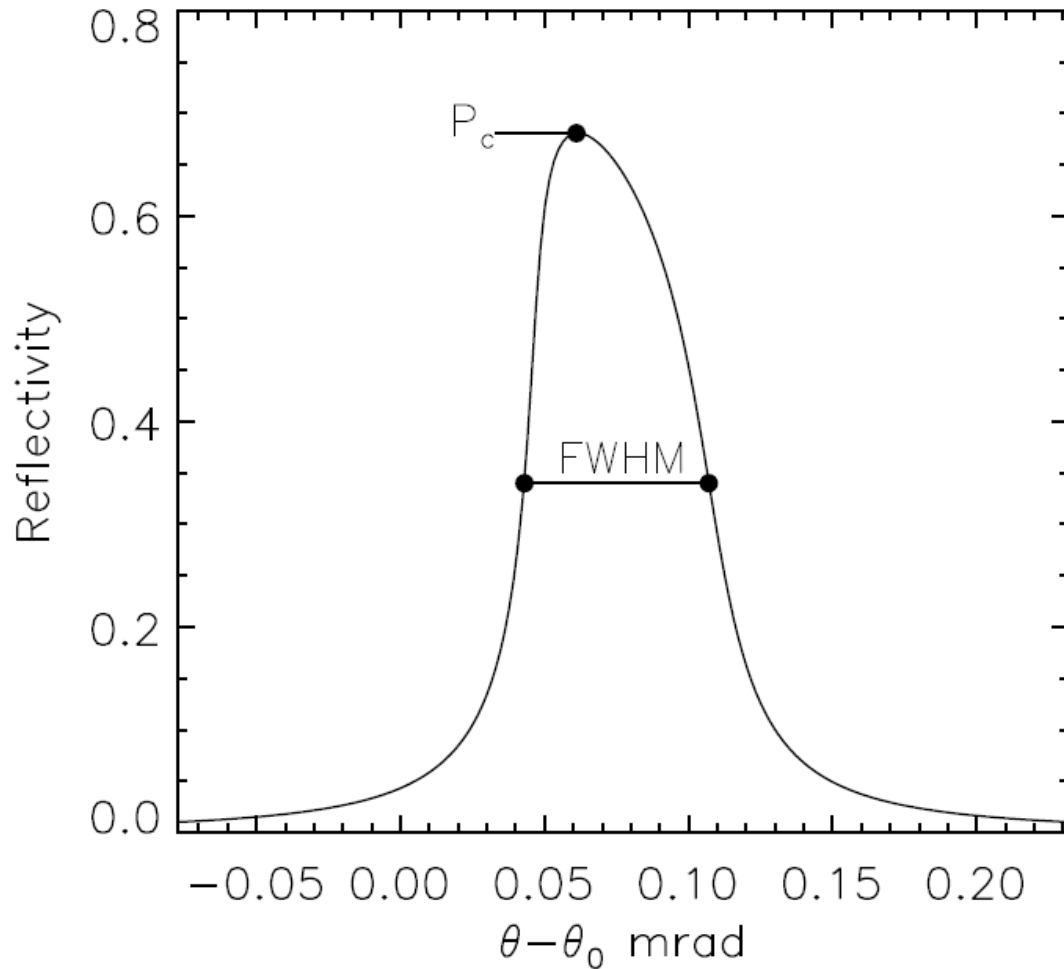
Bragg's law

$$2 d \sin \theta_B = n \lambda$$



Sir William Henry Bragg
Sir William Lawrence Bragg

Rocking curve



$$R = \frac{I_0}{I}$$

$$R_c(\theta) = \int R(\theta) d\theta$$

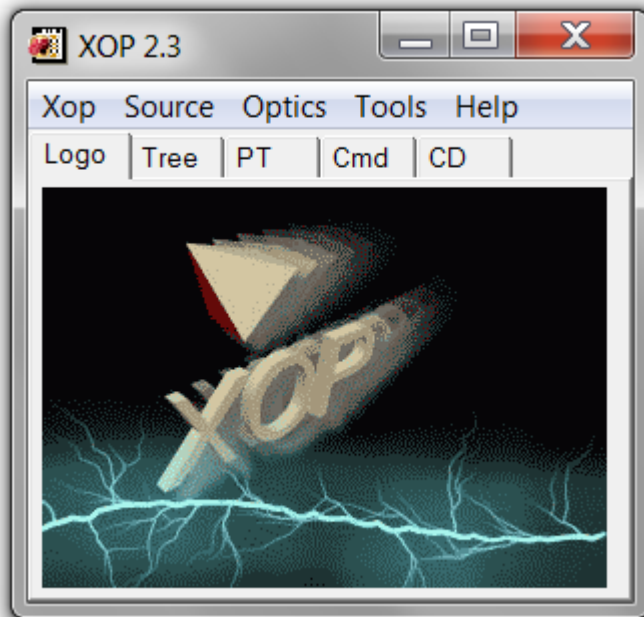
Dynamic Theory of Diffraction

- Dynamical diffraction theory for perfect crystal (Darwin, 1914; Ewald, 1917; von Lane, 1931; Zachariasen, 1967)
- Local application of the dynamical diffraction theory for perfect crystal to distorted crystals (Multilamellar method, Bonse, 1958; Authier, 1966)
- Geometrical optic (Penning-Polder theory, Penning & Polder, 1961a)
- Wave optic (Takagi-Taupin theory, Takagi, 1969; Taupin, 1964a)

Software

- REFLECT (Eteläniemi et al., 1989)
- REFLEX (Caciuffo et al., 1990)
- PEPO (Cchulze & Chapman, 1995)
- DIXI (Holzer et al., 1998)
- X-ray server/GID_SL (Stepanov, 2004)
- XOP: X-ray Oriented Programs (Sanchez del Rio & Dejus, 2011)

XOP (X-ray Oriented Programs)



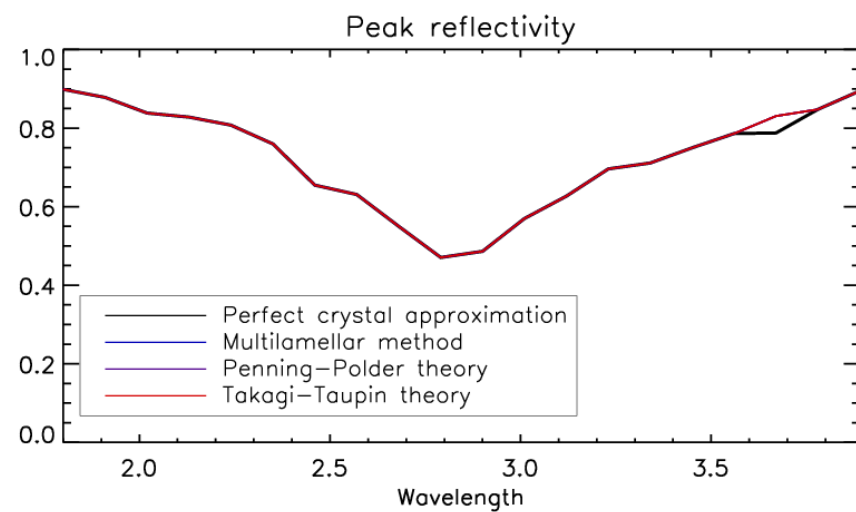
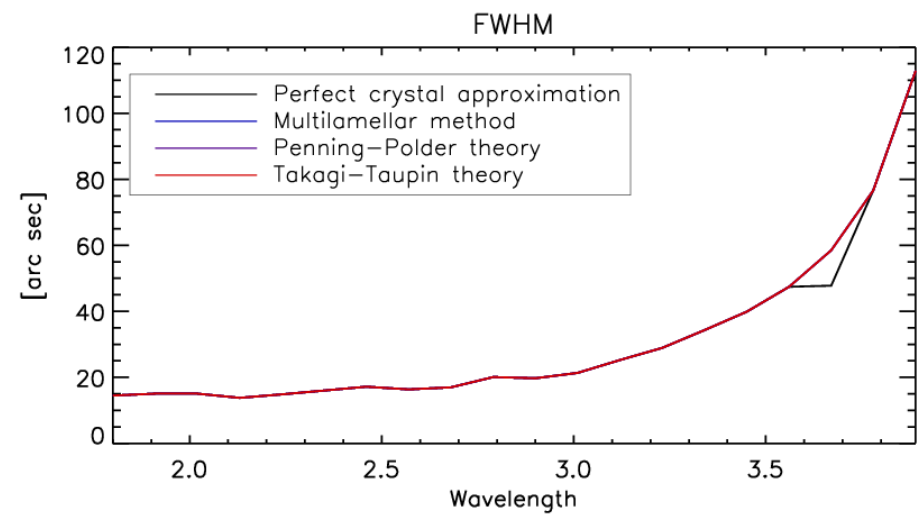
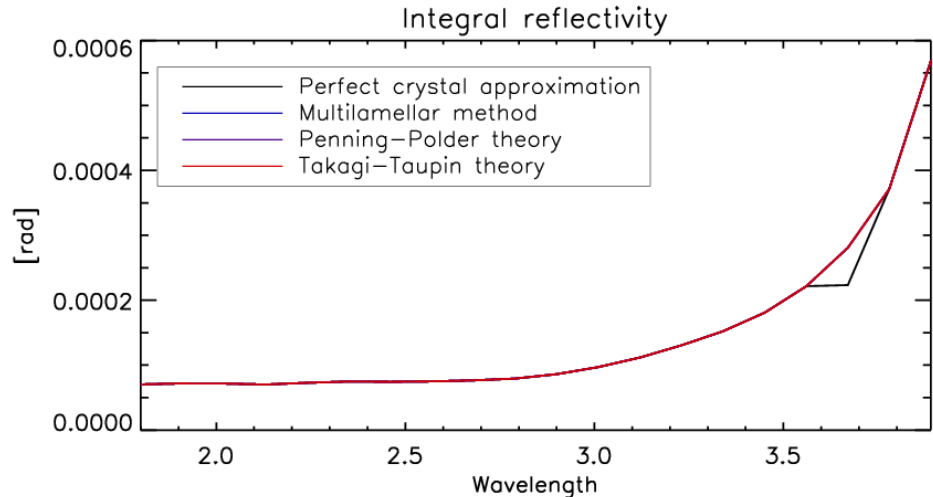
- XCRYSTAL
- XCRYSTAL_Bent

Accept Cancel Help

DABAX f0 file: f0_xop.dat	Crystal Model: Perfect crystal	Asymmetry angle [deg] (to surf.) 0.0000000
DABAX f1f2 file: f1f2_Windt.dat	Geometry: BRAGG: diffr beam	Crystal Thickness [cm]: 0.7000000
Crystal: Si	Scan: Th - Th Bragg	
h Miller index 1	Scan Units: micro rads	
k Miller index 1	Min Scan value: -100.00000	
l Miller index 1	Max Scan value: 100.00000	
	Scan Points: 200	
Temperature factor [see help]: 1.0	Fix value (E[eV] or Theta[deg]) 8000.0000	Use binary: Installed

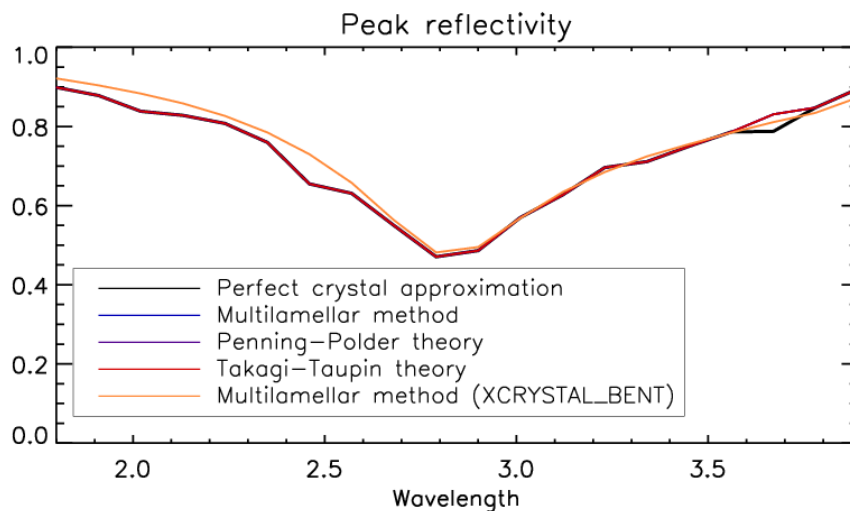
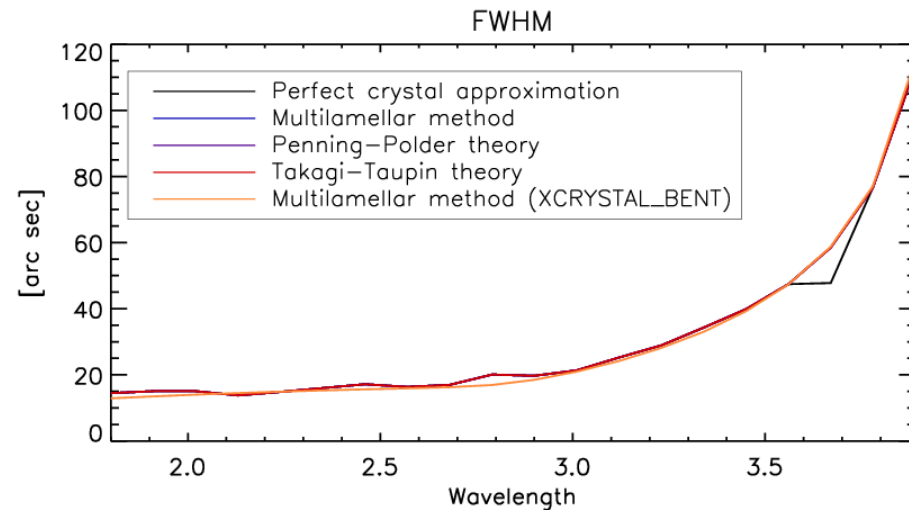
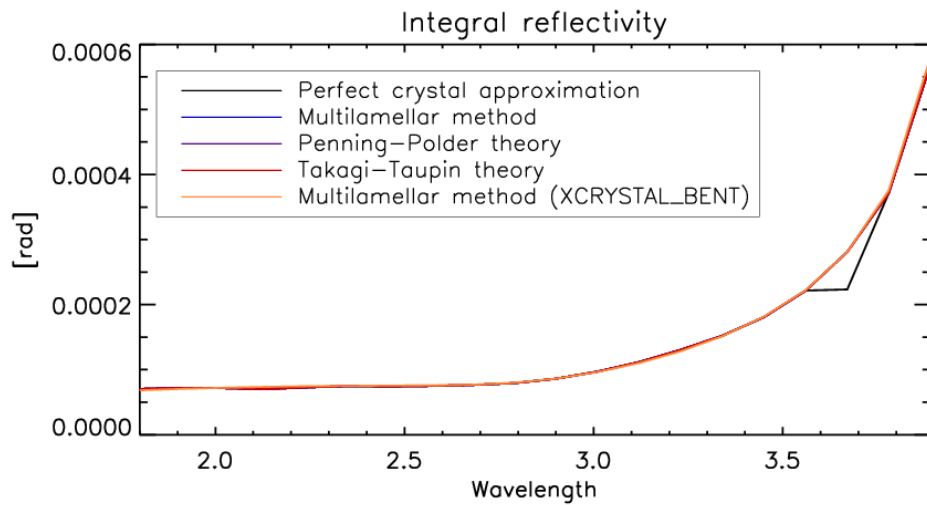
Crystal parameters- XOP/XCRYSTAL

Ge 220 crystal



Crystal parameters- XOP/XCRYSTAL_BENT

Ge 220 crystal



X-ray server/GID_SL

GID_SL on the Web

Dynamical x-ray diffraction from strained crystals, multilayers and superlattices at usual and grazing incidence angles

X-rays specified by: Wavelength (Å) Value=1.540562 Line=Cu-Kα1 Polarization=Sigma

Crystal: Germanium Auto DB for f',f'' Sigma=0. Å W0=1. Wh=1.

Bragg Reflection: 1 1 1 Substrate da/a=0.

Geometry specified by: angle of Bragg planes to surface ('+' for g0>gh) Value: 0. degr.

Scan: from -60. to +60. sec. Scan points: 401 Invert axis: Plot argument: scan angle

Approximations: alpha_max=1.E+8 *|xh|

watch progress (single click, please!)

Top layer profile (optional):

period=
t= sigma= da/a= code= x= code2= x2= code3= x3= code4= x0= xh= xhdf= w0= wh=
end period

(same "Submit" action as above; single click, please!)

Available codes:

[?] Crystals:


- ADP
- AlAs
- AlFe3
- AlN
- AlP
- alpha-Fe
- AlSb

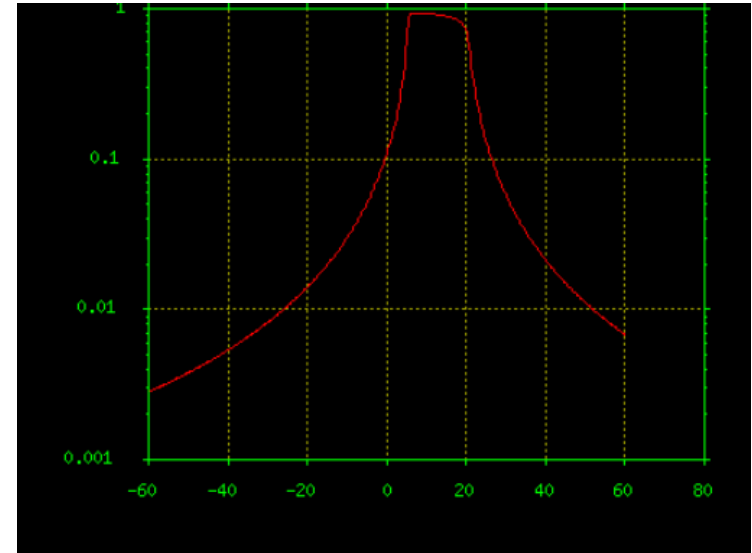
[?] Non-crystals:

- Al2O3
- B4C
- BeO
- BN
- C18H37Cl3
- Si

[?] Elements:


- Ac
- Ag
- Al
- Am
- Ar
- As
- At
- Au

 The profiles are restricted to 5000 layers after applying periods.
Do not use links or unusual words in surface layer profile!



Data plot

Download ZIPped results: [gd667714.zip](#)

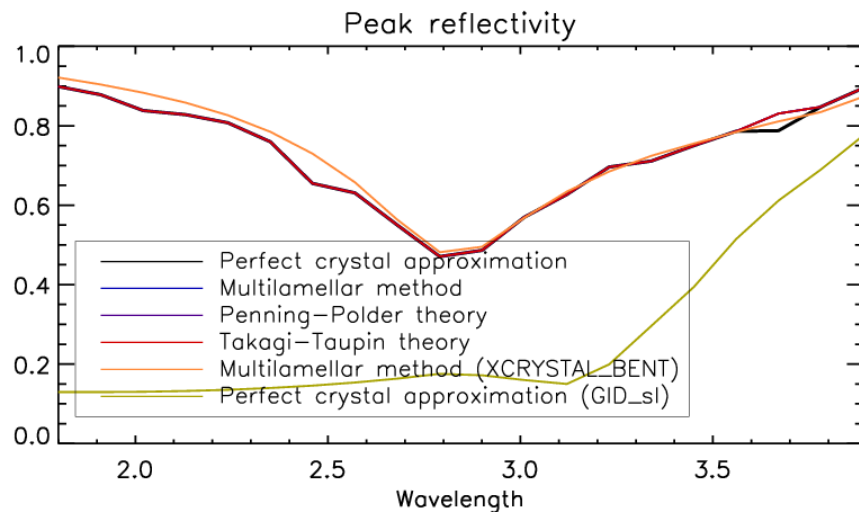
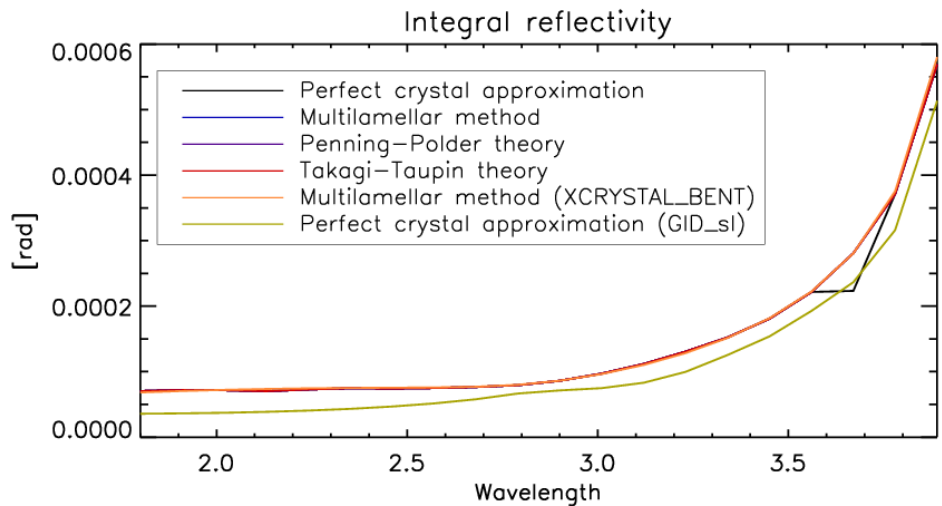
( Get a freeware UNZIP software for the most of platforms at [Info-Zip Web site](#))

Display inp file: [gd667714.inp](#)

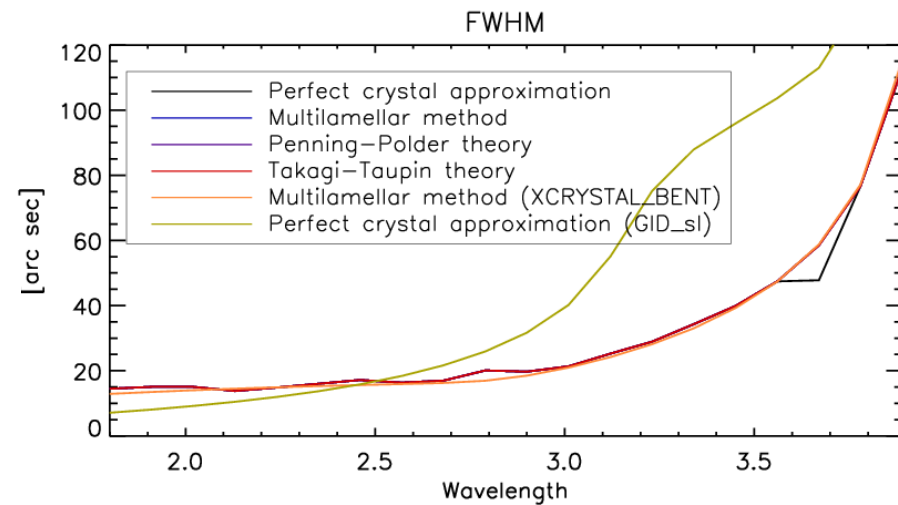
Display tbl file: [gd667714.tbl](#)

Display dat file: [gd667714.dat](#)

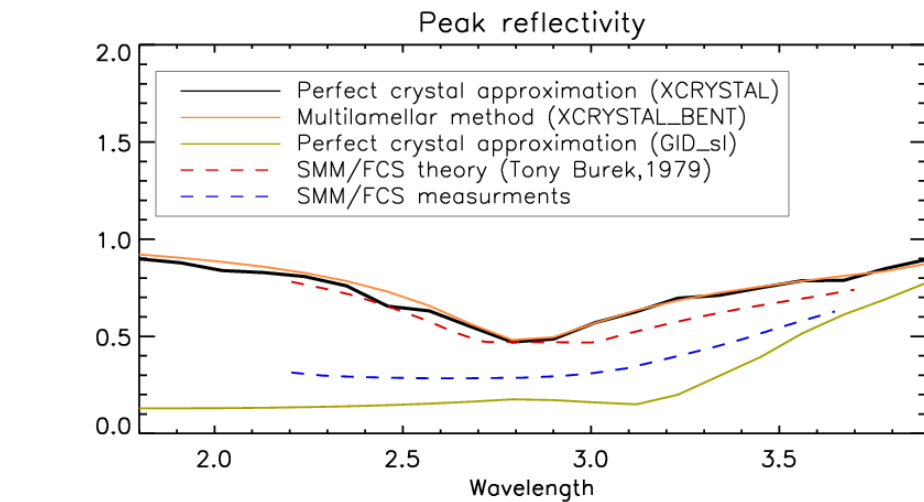
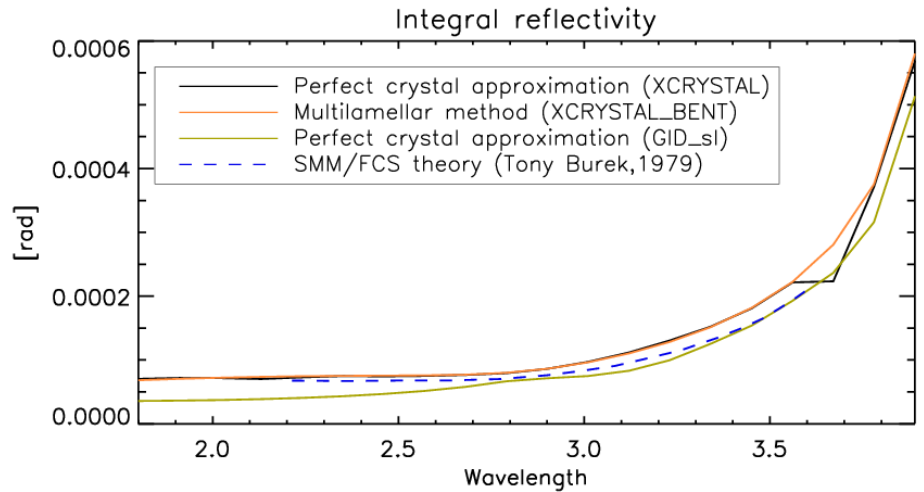
Crystal parameters- GID_SL



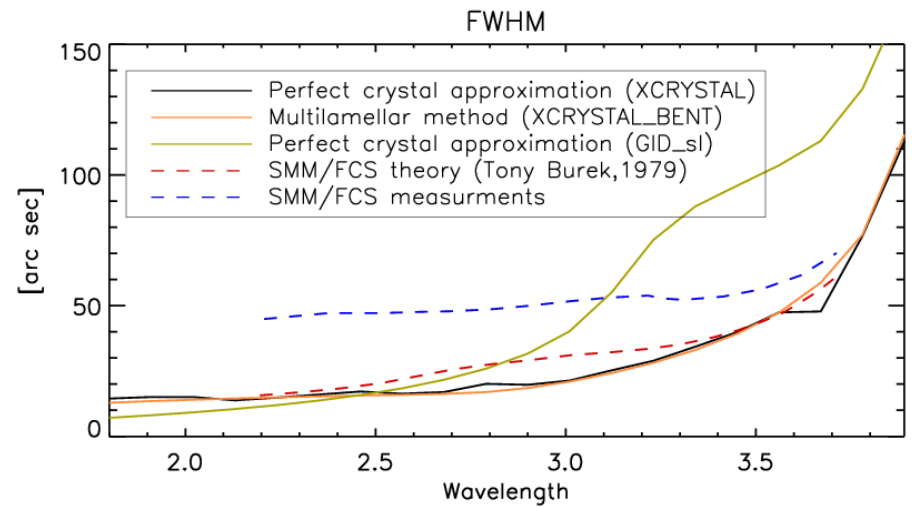
Ge 220 crystal



Theory vs measurements



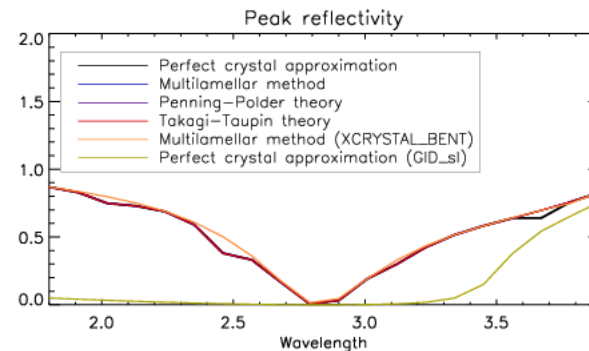
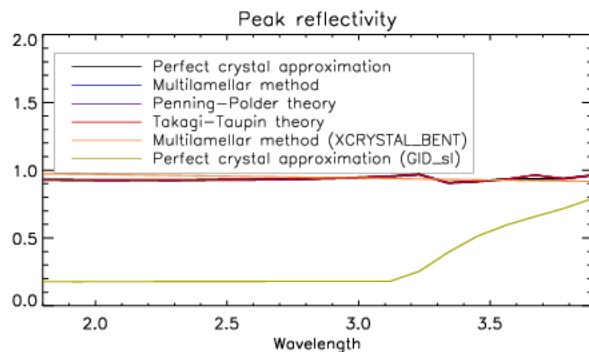
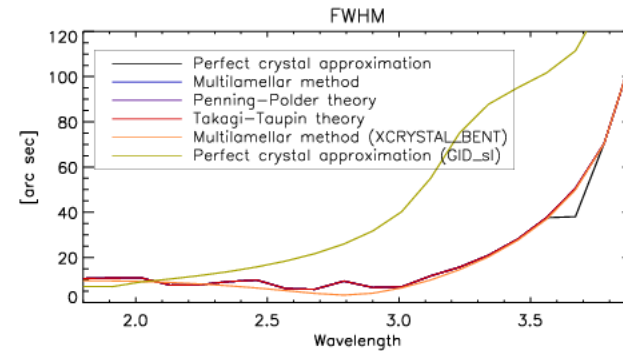
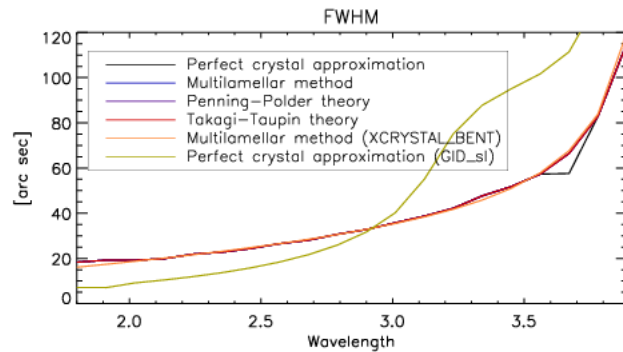
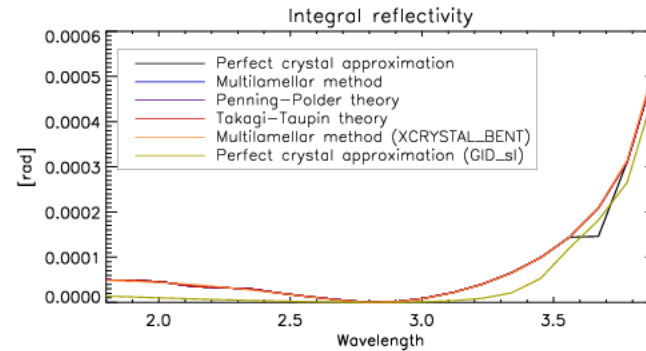
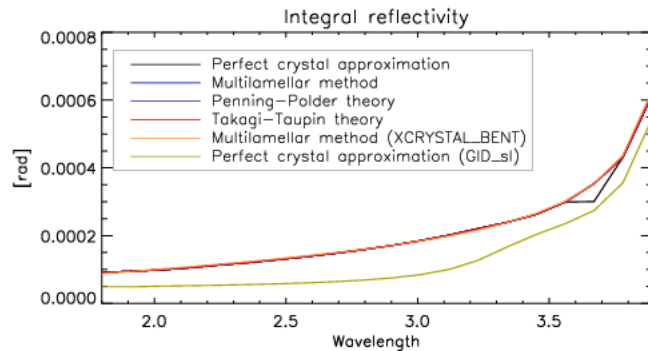
Ge 220 crystal



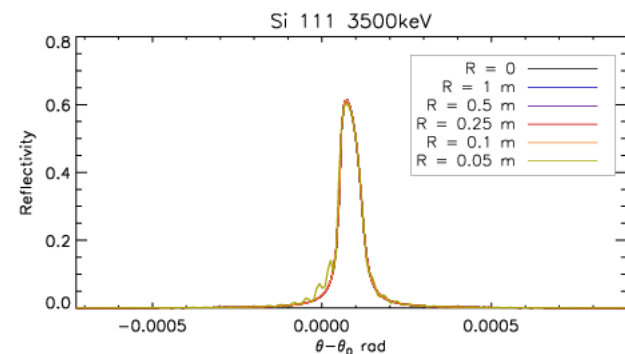
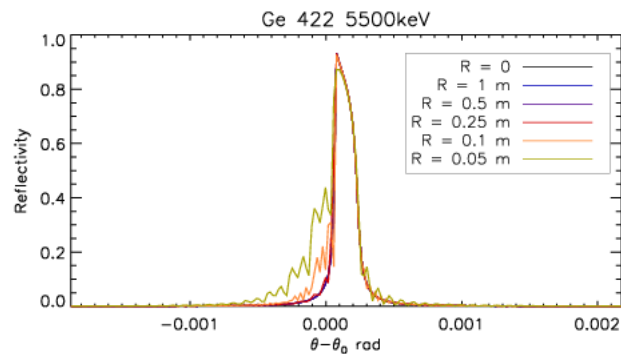
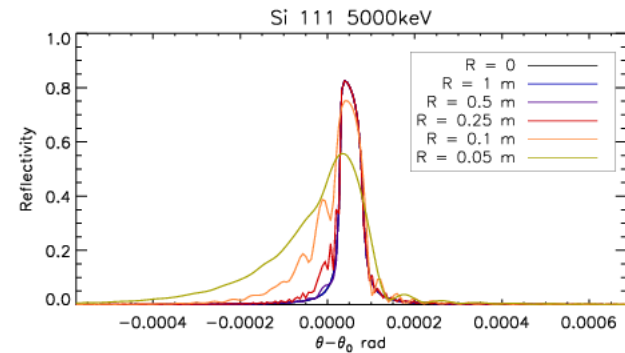
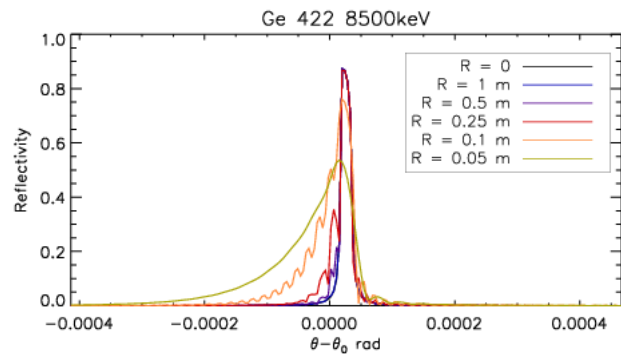
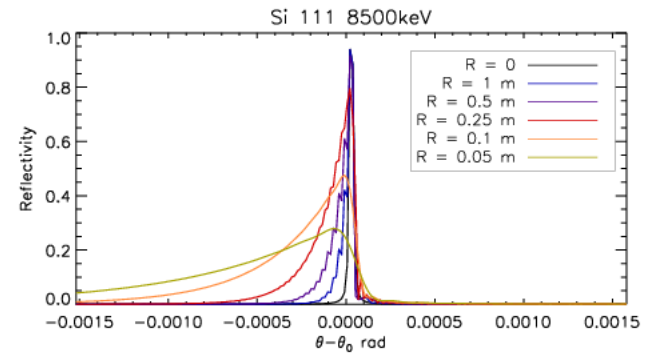
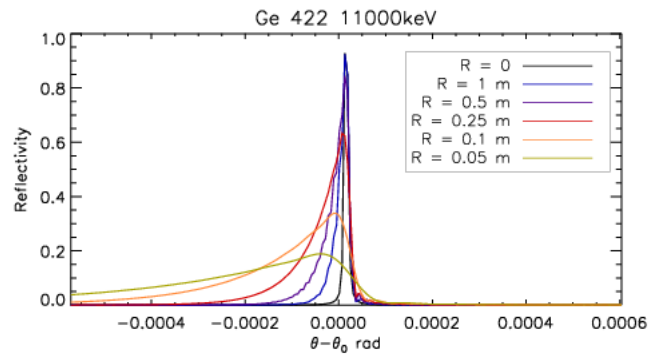
Polarization

S-polarized light

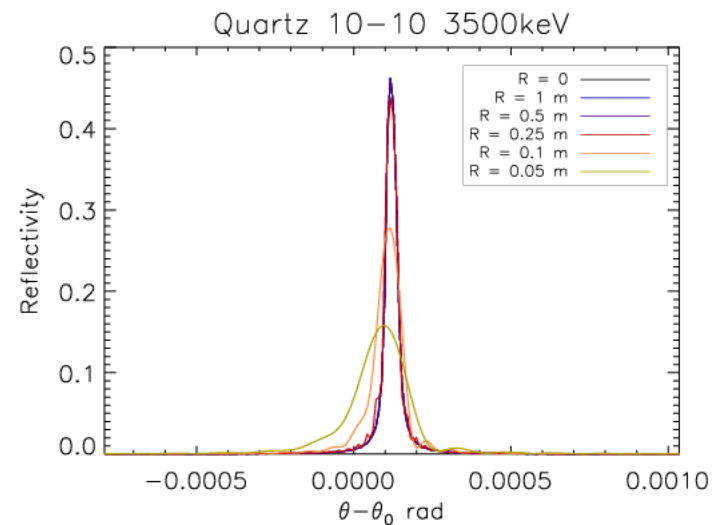
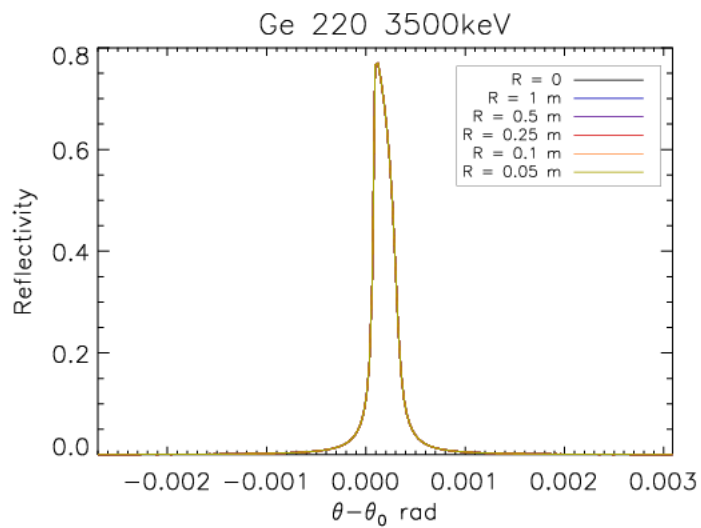
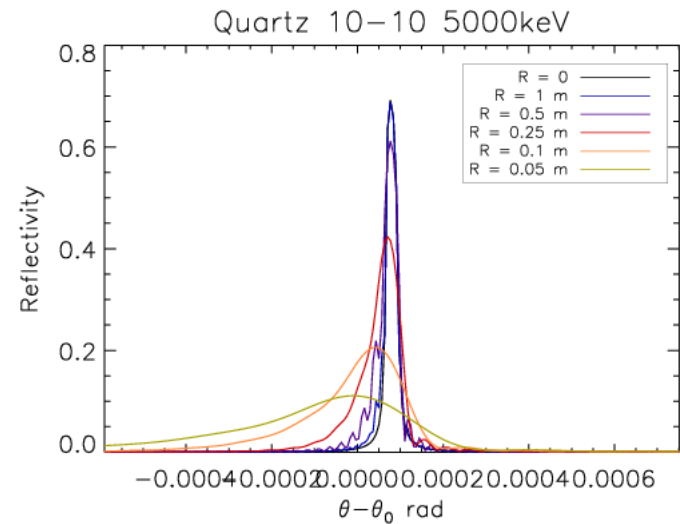
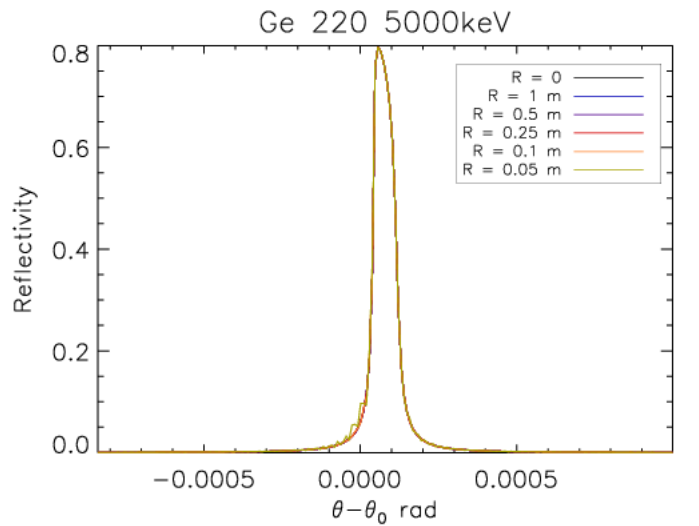
P-polarized light



Crystal bending



Crystal bending



A cluster of several translucent, faceted blue crystals or ice pieces is shown against a solid black background. The crystals have sharp, angular edges and are illuminated from the side, creating bright highlights and deep shadows that emphasize their three-dimensional structure. The overall appearance is that of a natural mineral specimen or a cluster of ice cubes.

Thank you for your attention