

Sergey Stepanov

X-Ray Server As A Resource For Studies Using Grazing Incidence X-Ray Techniques

What is X-ray Server?

X-ray Server is a public project that I launched in **1997** with the goals to provide scientific community with a wider access to personal research results, establish scientific collaborations, and refine X-ray scattering models and scientific software.

The Server provides Web-based access to a number of programs implementing author's models in the field of X-ray diffraction and scattering. Thus, the project is a combination of physics and programming with physics being a lead and software being a tool.

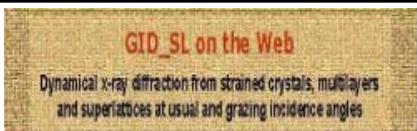
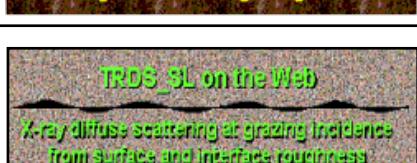
The software operates directly on the Server available for use without downloading. At present seven programs are accessible that have been used more than **120,000** times by more than **5,500** colleagues worldwide.

Currently at: <http://sergey.gmca.aps.anl.gov>

Formerly at: <http://sergey.bio.aps.anl.gov>

Software available through X-ray Server

This site has been online since 1997 and has served **122,102** x-ray jobs

 	<p>Xoh interpolates dielectric susceptibilities x_o and x_h for some crystals and other materials in wide range of x-ray wavelengths with the option to compare data from different databases.</p> <p>Xoh-search is a tool to search for Bragg planes under various conditions.</p>	58,245 jobs
 Dynamical x-ray diffraction from strained crystals, multilayers and superlattices at usual and grazing incidence angles	<p>GID SL on the Web calculates x-ray diffraction curves of strained crystals and multilayers for any Bragg-case diffraction with scans around arbitrary axis. It replaces Takagi-Taupin equations for extremely asymmetric and grazing incidence diffraction.</p>	31,534 jobs
 X-ray specular reflection from multilayers with rough interfaces at grazing incidence	<p>TER SL on the Web calculates x-ray specular reflection and standing waves from multilayers with interface roughness and transition layers. It uses a new recursive algorithm converging faster than the recursions by Parratt.</p>	12,438 jobs
 X-ray diffuse scattering at grazing incidence from surface and interface roughness	<p>TRDS SL on the Web calculates x-ray diffuse scattering from interface roughness. It implements several different models of roughness and can simulate effects of skew roughness transfer, dependence of interface-interface roughness correlations on lateral size of roughness and x-ray scattering from atomic steps.</p>	9,811 jobs
 X-ray resonant specular reflection from magnetic multilayers	<p>MAG SL on the Web calculates x-ray resonant specular reflection from magnetic multilayers with interface roughness and transition layers. It can also supply wavefields for calculations of diffuse scattering from magnetic roughness.</p>	8,749 jobs
 X-ray multiple Bragg/Laue diffraction	<p>BRL on the Web applies a novel algorithm to calculate multiple Bragg diffraction of x-rays including the cases of x-ray waves grazing along the crystal surface and Bragg angles at 90 degr.</p>	1,325 jobs

Based on ~17 research papers

X0h calculates material susceptibilities χ_0 and χ_h for x-ray wavelength range by interpolating data tabulated in the International Tables for X-ray Crystallography and several other tables.

The highlight of **X0h** is the way it interpolates the dispersion corrections df' and df'' [1]. The dispersion corrections are calculated with the formulae given by Don Cromer [Acta Crystallogr. vol.18 (1965) p.17-23]:

$$df' = \sum_{k=1}^{N_s} g_k P(X_k, N_k)$$

$$df'' = 0.5\pi \sum_{k=1}^{N_s} g_k (N_k - 1) / X_k^{N_k - 1}$$

First, **X0h** applies the above equations to known tabulated dispersion corrections and evaluates oscillator strengths g_k . Then, it uses calculated g_k to find the dispersion corrections of interest.

Once the χ_0 and χ_h are found, **X0h** can fulfill a lot of useful service tasks like evaluating the HWFM of Bragg peaks, searching for Bragg reflections that satisfy certain conditions, and etc.

Originally developed for the studies of parametric X-ray radiation by relativistic electrons, now **X0h** is primarily used for synchrotron radiation and automatically called by all other server programs.

[1] O.M.Lugovskaya & S.A.Stepanov, (1991) Sov. Phys. Crystallogr. **36**, 478-471.

X-rays:

- Wavelength (Å):
- Energy (keV):
- Characteristic line: Cu-Kα1

Target:

- Crystal: Silicon
- Other material:
- Chemical formula: and density (g/cm³):

Reflection:

Miller indices:

Database Options for dispersion corrections df1 , df2:

- Use XOh data (5-25 keV or 0.5-2.5 Å) -- recommended for Bragg diffraction.
- Use Henke data (0.01-30 keV or 0.4-1200 Å) -- recommended for soft x-rays.
- Use Brennan-Cowan data (0.03-700 keV or 0.02-400 Å)
- Compare results for all of the above sources.

Background algorithm

GID_si (Grazing Incidence Diffraction from Superlattices) was originally developed for GID (Fig.1a) from multilayers, but then extended to arbitrary Bragg case including coplanar (Fig.1b) and non coplanar asymmetric diffraction (Fig.1c).

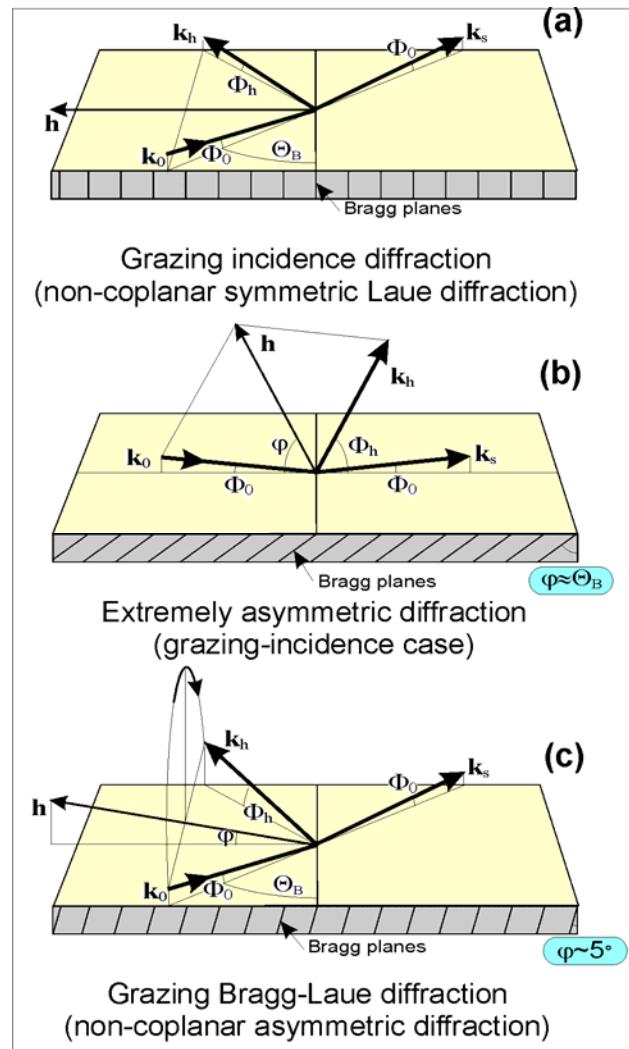
The program can calculate Bragg diffraction from imperfect crystals with given profiles of normal lattice strains $da(z)/a$, dielectric susceptibilities $\chi_0(z)$, $\chi_h(z)$, and interface roughness height $\sigma(z)$.

The advantage of **GID_si** over most of other Bragg diffraction simulation software is that it takes into account specular reflection and refraction of X-rays at crystal surface and interfaces in multilayers.

Replaces Takagi-Taupin equations for Grazing Incidence Diffraction!

S.A.Stepanov, E.A.Kondrashkina, R.Koehler, D.V.Novikov,
G.Materlik, and S.M.Durbin,

Phys. Rev. B, v.57, No 8, p. 4829-4841, (1998).



GID_SL on the Web

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

Web input form

X-rays: Wavelength(A) / Energy(keV) = 1.540562 Line= Cu-Ka1 Polarization= Sigma

Crystal: GaAs X0h data (0.5-2.5A) Sigma=0. A W0=1. Wh=1.

Bragg Reflection: [4] [0] [0] Substrate da/a=0.

Geometry specified by: [5]. Surface orientation & condition of symmetric Bragg case

-- Geometry parameter ([1,7]=incidence angle, [2,8]=exit angle, [6]=Bragg planes angle, [9]=g0/gh): [] []

-- Surface plane ([1-5]): [1] [0] [0] Miscut direction: [0] [1] [1] Miscut angle: [0.] degr.

Scan axis: [k0 x h] Indices, if other scan axis: [] [] [] Invert scan axis

Scan limits: from [-2000.] to [+2000.] sec. Scan points= 401 Plot argument= incidence angle

watch progress (single click, please!)

Top layer profile (optional):

```
period=
t= sigma= da/a= code= x= code2= x2= code3= x3= code4= x0= xb= xhdf= w0= wh=
end period
period=20
t=100 code=GaAs sigma=2
t=70 code=AlAs sigma=2 da/a=a
end period
```

Available codes:

[?] Crystals:

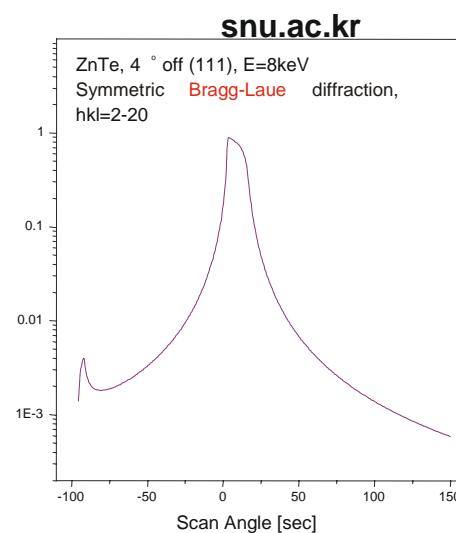
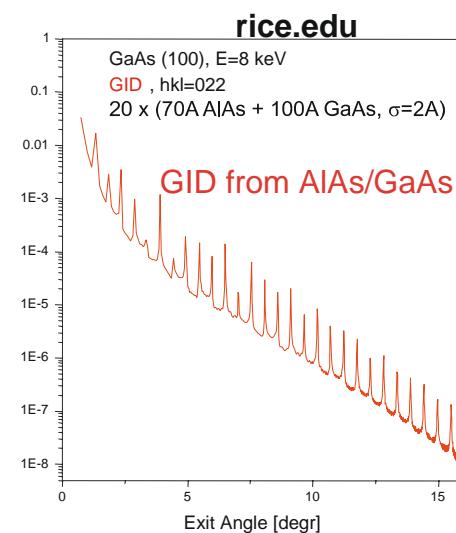
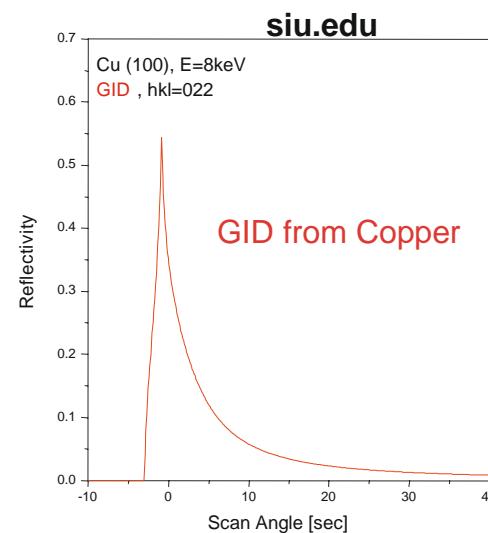
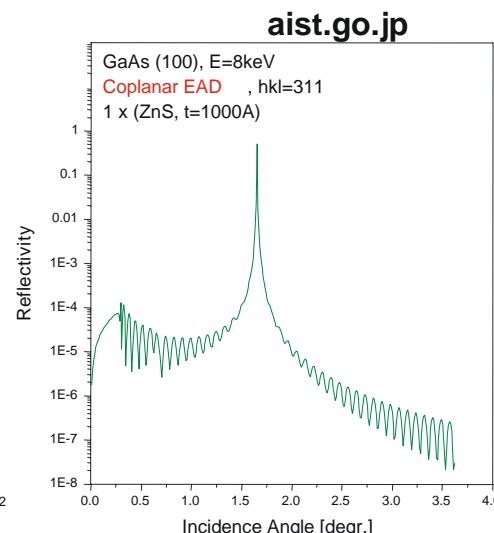
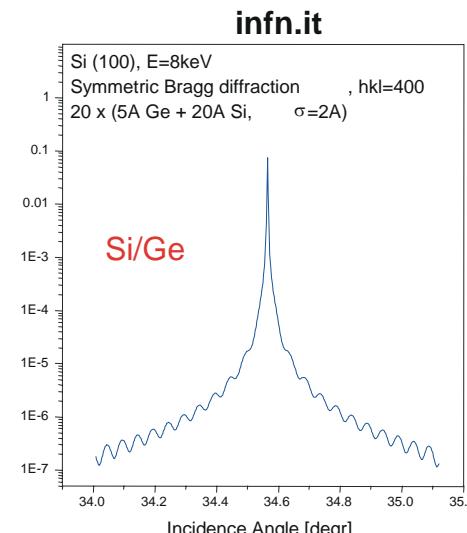
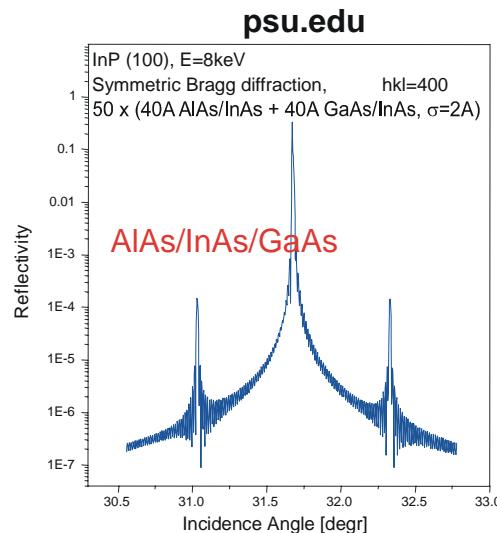
AlAs
AlP
AlSb
AlYO3
BaTiO3
Beril
Beryllium

[?] Non-crystals:

Al2O3
B4C
BeO
BN
Cr2O3
CsI
Fluorite

[?] Elements:

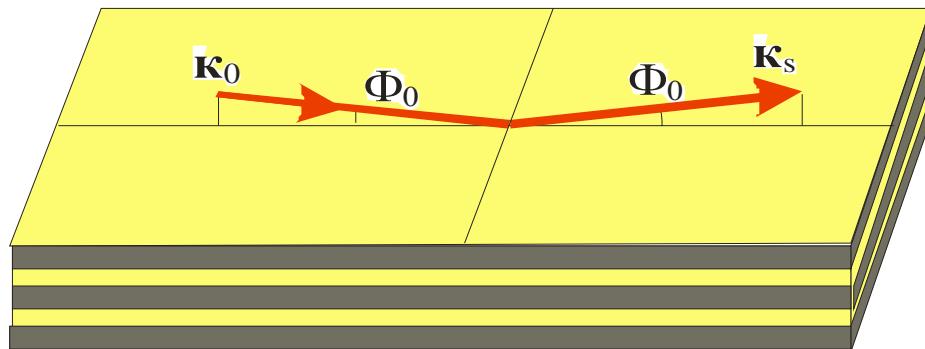
Example web results



Background model

TER_sl (Total External Reflection) software simulates X-ray specular reflection from multilayers with the account for interface roughness or transition layers using the same recursion algorithm as in **GID_sl**.

The advantage of **TER_sl** over the well know **Parratt** recursive technique is a faster convergence of recursions because **TER_sl** expresses the reflection from a stack of N layers through the reflectivity of (N-1) layers, while the Parratt technique expresses the reflectivity of N-th layer via that of the underlying (N-1)-th layer.



By-product of **GID_sl**:
same recursion algorithm !

S.A.Stepanov, E.A.Kondrashkina, R.Koehler, D.V.Novikov, G.Materlik, and S.M.Durbin,
Phys. Rev. B, v.57, No 8, p. 4829-4841, (1998).



Web form

X-rays: Wavelength(A) / Energy(keV) = 1.540562 Line=Cu-Ka1 ? Polarization=Sigma

Substrate: Database code: GaAs ? X0h data (5-25keV; 0.5-2.5A)
 Chemical formula: _____ rho= _____ g/cm³
 Susceptibility x0 = (_____) / format: x0=(Re(x0), Im(x0)); note: x0=2*delta /
x0 correction: w0 = 1. / this is used as: x0 = w0 * x0 /
Roughness: sigma = 4. Angstrom OR Transition layer tr = 0. Angstrom

Incidence angle limits: from 0. to 3. degr. Scan points=601

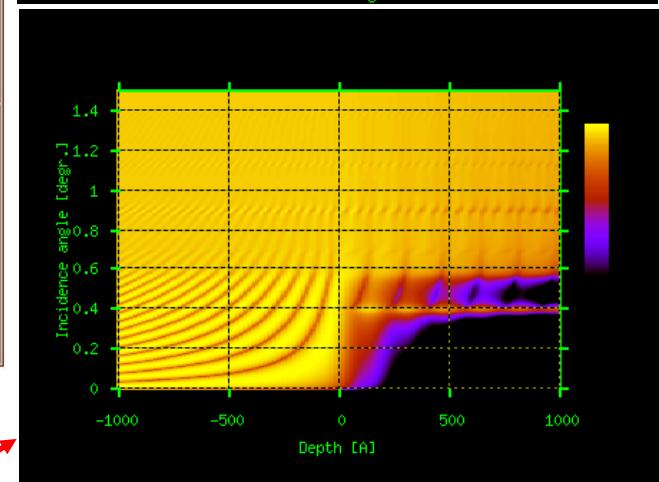
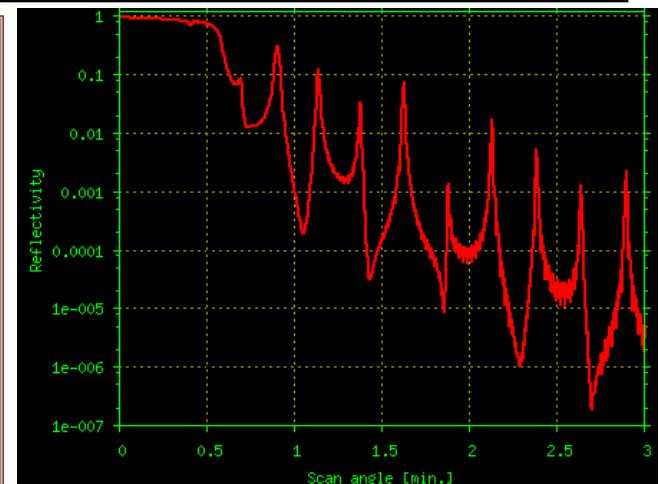
Standing waves: Reference interface = 0 (0=surface)
Start offset = 0. Angstrom
End offset = 1000. Angstrom
Number of offsets = 101 (max = 401)

watch progress Submit Query (single click, please!)

Top layer profile (optional):
t=20 w0=0.5 sigma=5 lsurface oxide, organic contamination or dust
period=20
t=100 code=GaAs sigma=4
t=70 code=AlAs sigma=4
end period

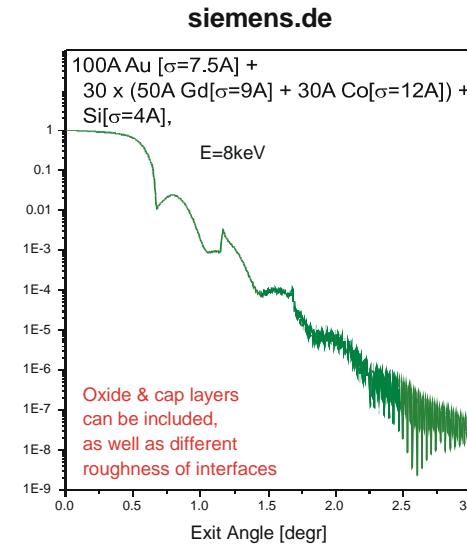
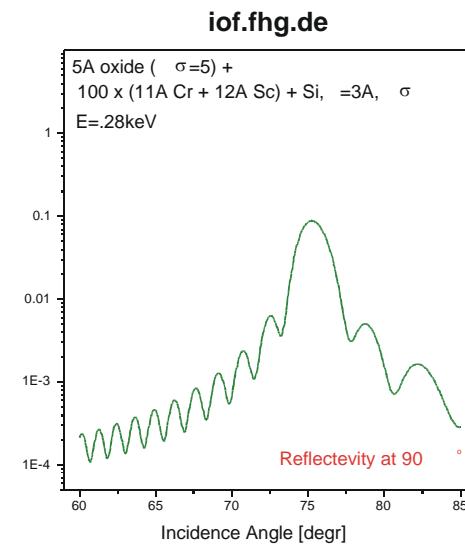
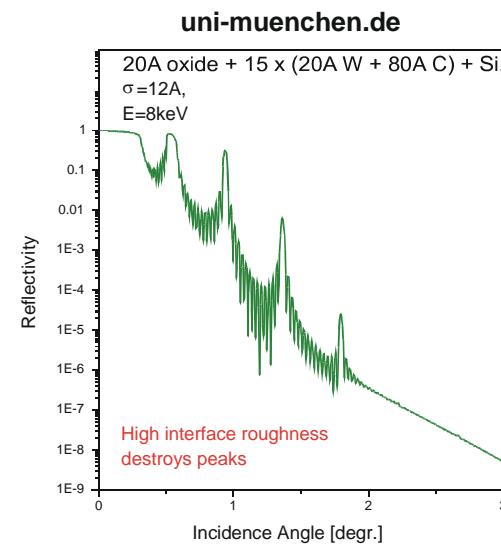
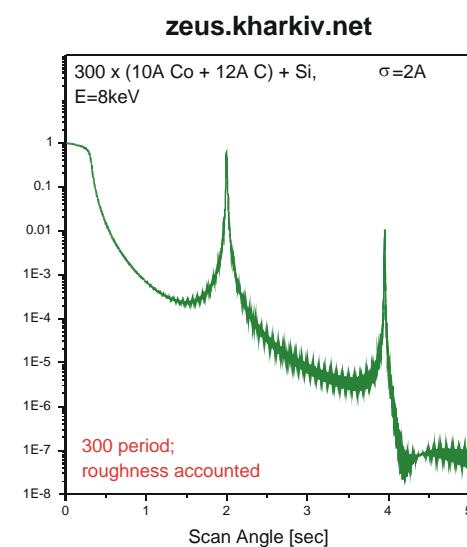
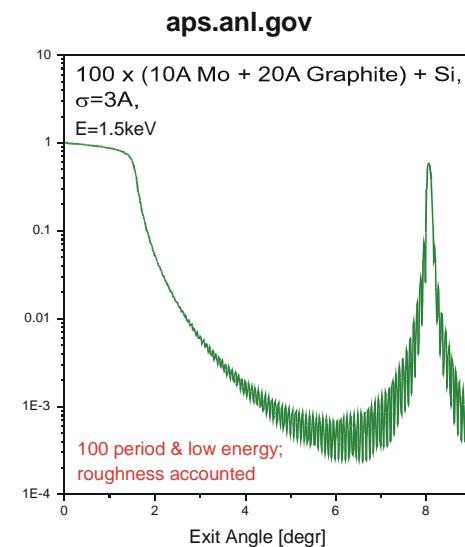
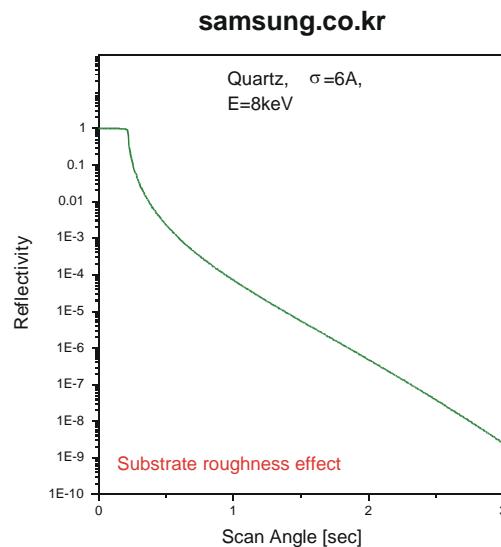
Submit Query (same "Submit" action as above; single click, please!)

Available codes:
(use Copy/Paste)
Ac
Ag
Al
Al2O3
AlAs
AlFe3
AIN
AlP



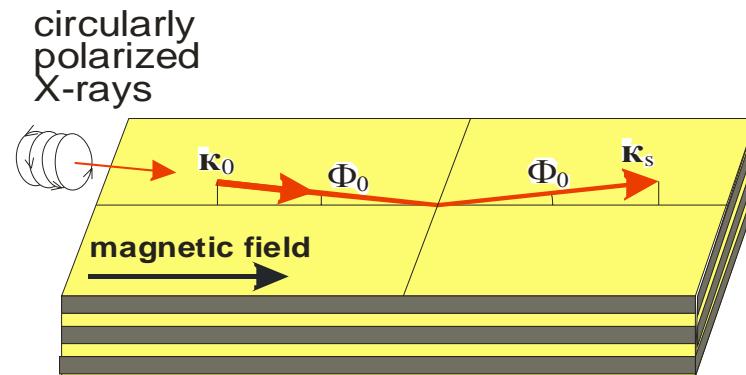
Recently added wavefields calculations for applications like fluorescence yield analysis, X-ray standing waves method, GISAXS, and etc.

Example web results



Background algorithm

The **MAG_sl** program solves the problem of resonant X-ray reflectivity from magnetic multilayers. The major application of X-ray resonant magnetic scattering is to probe thin magnetic films and magnetic multilayers. This is a hot topic related to studying magnetic heads for computer hard drives. However, since in this case the media susceptibility is a tensor, the conventional Parratt technique for calculating X-ray specular reflection is not applicable. The problem is solved in **MAG_sl** applying a recursive algorithm for (2x2) scattering matrices similar to that of **GID_sl**.



S.Stepanov and S.Sinha, Phys. Rev. B, **61** (2000) 15302-15311.

D.R.Lee, S.K.Sinha, D.Haskel, Y.Chi, J.C.Lang, S.A.Stepanov, and G.Srajer, Phys. Rev. B, **68** (2003) 224409-224427.

MAG_SL on the Web

X-ray resonant specular reflection
from magnetic multilayers

Web form

X-rays: Wavelength(A) / Energy(keV) = 7.243 Line=

Polarization: 4. Circular - 0.

Substrate: Database code: Silicon X0h data (5-25keV; 0.5-2.5A)
 Chemical formula: rho= g/cm³
 Susceptibility x0 = () / format: x0=(Re(x0), Im(x0)); note: x0=2*delta /
x0 correction: w0 = / this is used as: x0 = w0 * x0 /
Roughness: sigma = Angstrom OR Transition layer tr = Angstrom
Magnetic atoms share(0..1) / density(1/cm³) =
Magnetic orientation X = Y = Z =
Magnetic amplitudes F10 = , F11 = , F1T = ,

Scan (incidence angle or qz): from to degr.

Magnetic model: generic (may have numeric problems for hard x-rays) / hard x-rays (E>6keV)

watch progress (single click, please!)

Top layer profile (optional):

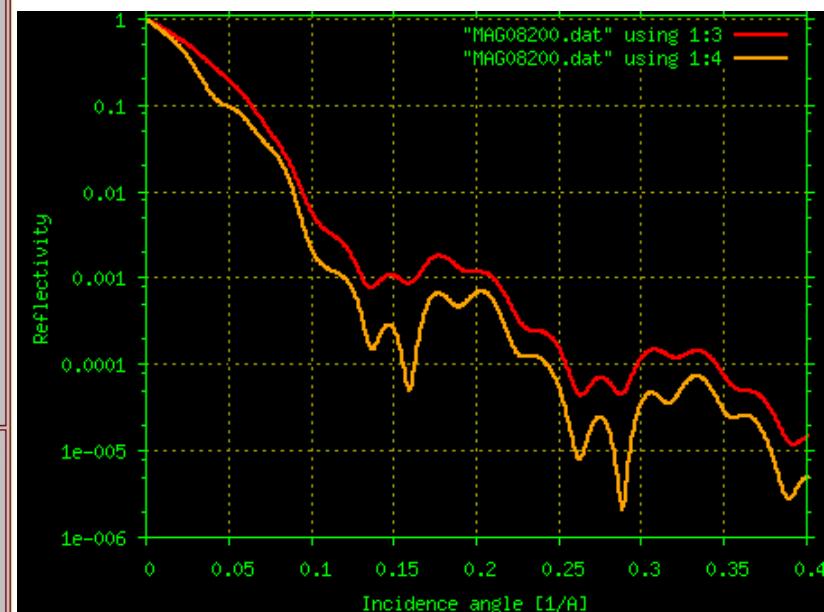
```
period=
t= sigma= tr= code= rho= x= code2= x2= code3= x3= code4= x0= w0=
mshare= mdensity= mvector= F10= F11= F1T=
end period
period=15
code=Gd t=50 F11=(-0.22,9.35) F1T=(0.37,9.65) mshare=1 mvector=(1 0 0)
code=Fe t=35
end period
```

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

Available codes: (use Copy/Paste)

- Ac
- Ag
- A1
- Al2O3
- AlAs
- AlP
- AlSb
- AlYO3
- Am
- Ar
- As
- At
- Au
- B
- B4C

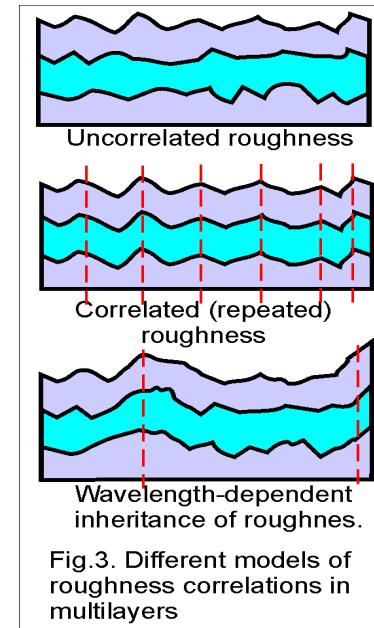
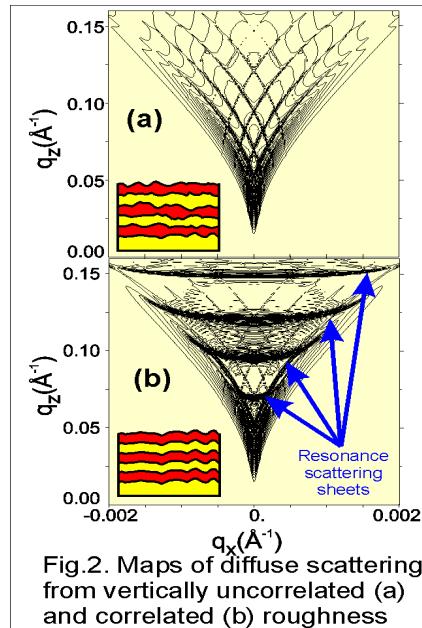
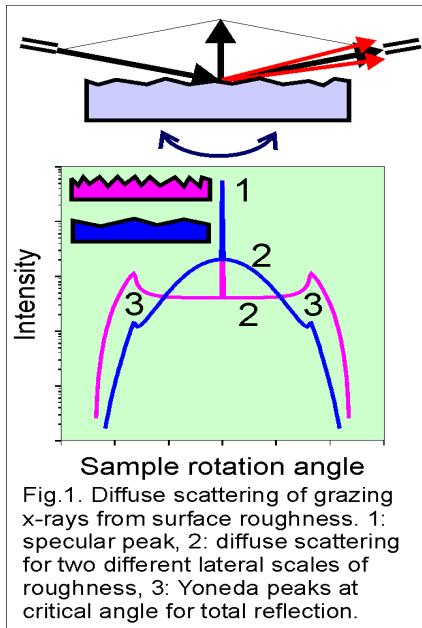
[More details](#)



MAG_sl example: difference between reflectivity of circular-plus and circular-minus polarized X-rays at E=849eV from 47Å capped Ni film.

Background algorithm - I

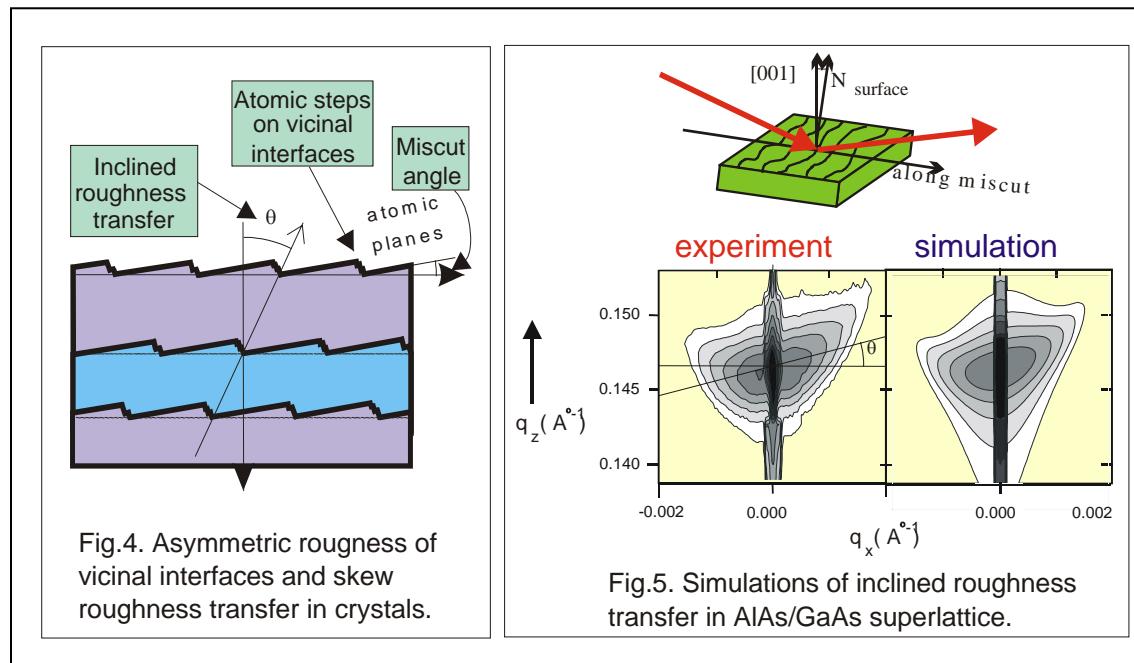
TRDS_SI (Total Reflection Diffuse Scattering from Superlattices) was developed for the simulations of X-ray diffuse scattering from interface roughness in multilayers (Fig.1). This program implement a number of different models for interface roughness and for correlations between roughness at different interfaces in multilayers (Fig.2). Notable is the implementation of the model allowing to study wavelength-dependent inheritance of roughness in layer-by-layer grown multilayers (Fig.3).



V.M.Kaganer, S.A.Stepanov & R.Koehler, (1995) Phys. Rev. B **52**, 16369-16372.

Background algorithm - II

Other notable models implemented in **TRDS_sl** are the X-ray scattering from atomic steps on vicinal interfaces and the scattering due to inclined roughness transfer in crystalline multilayers (Fig.4). Both of those effects provide asymmetry of x-ray diffuse scattering (Fig.5), but each of different kind.



E.A.Kondrashkina, S.A.Stepanov, R.Opitz, M.Schmidbauer, R.Koehler, R.Hey,
M.Wassermeier, and D.V.Novikov,
Phys. Rev. B, v.56, No 16, p. 10469-10482, (1997).



Web form

X-rays: Wavelength(Å) / Energy(keV) = 1.540562 Line= Cu-Kα1 ? Polarization= Sigma

Substrate: Database code: GaAs ? XRD data (5-25keV; 0.5-2.5Å)
 Chemical formula: rho= g/cm³
 Susceptibility x0 = () / format: x0=(Re(x0), Im(x0)); note: x0=2*delta /
x0 correction: w0 = 1. / this is used as: x0 = w0 * x0 /
Roughness: sigma = 3. Angstrom / this is rms roughness height /

Type of scan: Q-scans at fixed 2Q Units for Q,2Q: degr. Units for qx,qz: 1/Å
Scan limits: from 0. to 2. points=201
Offset limits: from 2. to 2. points=1
Compute at specular rod: scattering reflection

Accelerators: Use K instead of exp(K)-1 Use semi-Born approximation

Roughness: lateral correlation length= 1000. Å vertical correlation length= Å jaggedness= 1.
angle of skew transfer= 0. degr.

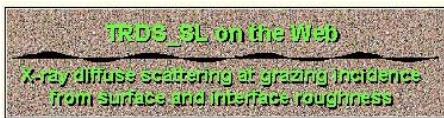
Models:	<input checked="" type="radio"/> Uncorrelated roughness
	<input checked="" type="radio"/> Completely correlated roughness
	<input type="radio"/> Ming's model
	<input type="radio"/> Lagally's model lateral size of vertically correlated roughness= Å
	<input type="radio"/> Holy's model
	<input type="radio"/> Spiller's model (*very slow!*)
Data for all Pukite's models:	miscut angle= degr. <input type="checkbox"/> Add affine roughness
	<input type="radio"/> Classic Pukite's model
	<input type="radio"/> Smoothed Pukite's model effective rms height of steps= Å
	<input type="radio"/> Pershan's model terraces size spread= Å

watch progress Submit Query (single click, please!)

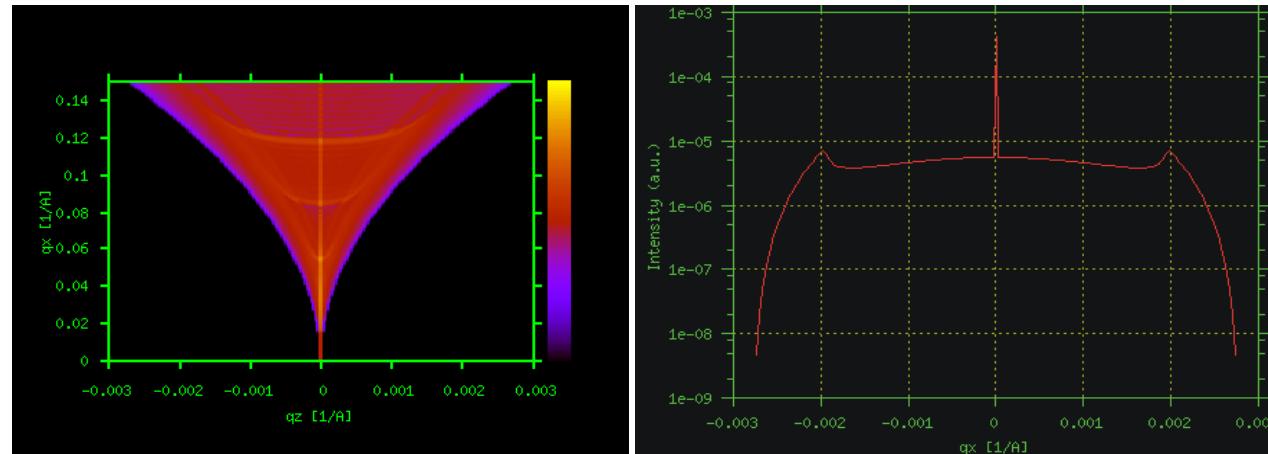
Top layer profile (optional):
period=
t= sigma= tr= code= rho= x= code2= x2= code3= x3= code4= x0= w0=
end period

Available codes:
(use Copy/Paste)

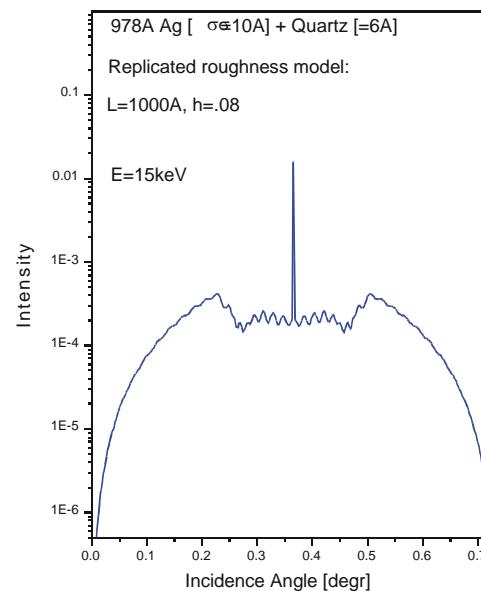
Ac
Ag
Al
Al2O3
...



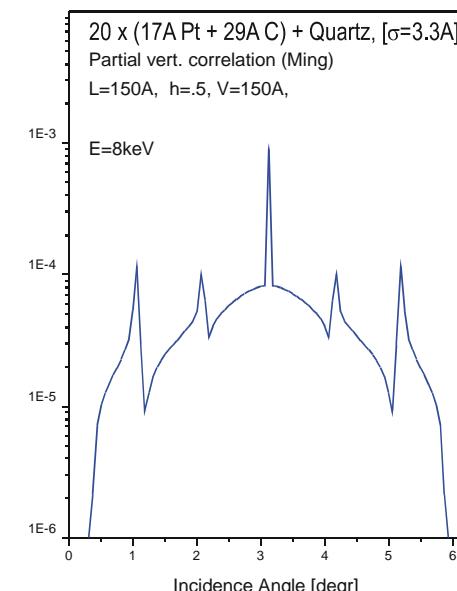
Example web results



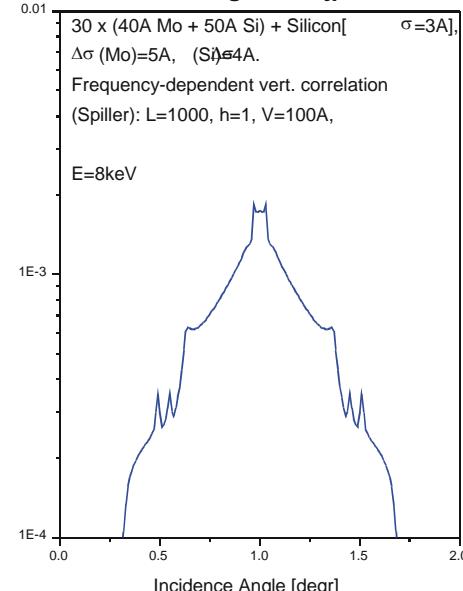
uni-duesseldorf.de



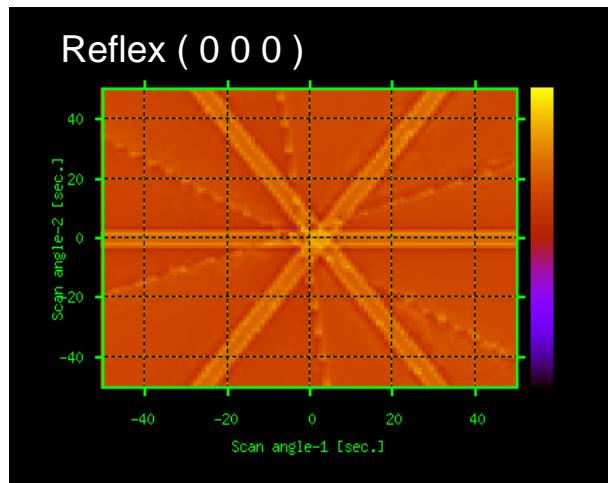
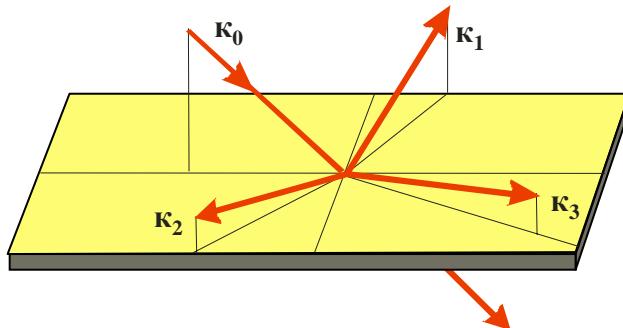
iisc.ernet.in



rigaku.co.jp



Background algorithm



Kossel lines in case of
multiple Bragg diffraction

BRL (Bragg/Laue) calculates multiple Bragg diffraction patterns with the algorithm based on the extended dynamical diffraction theory.

Typically the calculations of multiple Bragg diffraction are reduced to the eigenvalue problem for a **$2N \times 2N$** scattering matrix. However, when the diffraction geometry involves grazing X-ray waves, the calculations are reduced to the eigenvalue problem for **$4N \times 4N$** scattering matrix [Colella, Acta Cryst. **A30** (1974) 413].

BRL implements an algorithm where the calculations are reduced to a *generalized* eigenvalue problem for **$2(N+N_s) \times 2(N+N_s)$** scattering matrix where N_s is the number of grazing waves. Thus, if there are no grazing waves, the matrix size is $2N \times 2N$ and if all of the waves are grazing it becomes $4N \times 4N$. In some cases the calculations are reduced dramatically.

S.Stepanov and A.Ulyanenkov, Acta Cryst. **A50** (1994) 579-585.

BRL on the Web

X-ray multiple Bragg/Laue diffraction

Web form

Target:

Crystal: Silicon

Surface: Base plane:

1	1	1
---	---	---

Miscut direction:

1	-1	0
---	----	---

Miscut angle: 0.

Reflections:

Reflex-1:

1	1	1
---	---	---

Reflex-2:

2	2	0
---	---	---

Index search range: 5

Min. Intensity filter:
 $(|xh/x_0|*100\% > \dots)$

X-rays:

Wavelength (Å):

Energy (keV):

Characteristic line: Cu-K α 1

Fixed by coplanar case

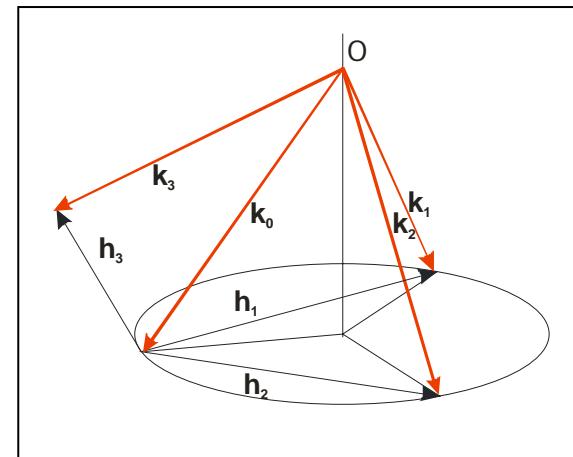
Fixed by Reflex-3:

Database Options for dispersion corrections df1, df2:

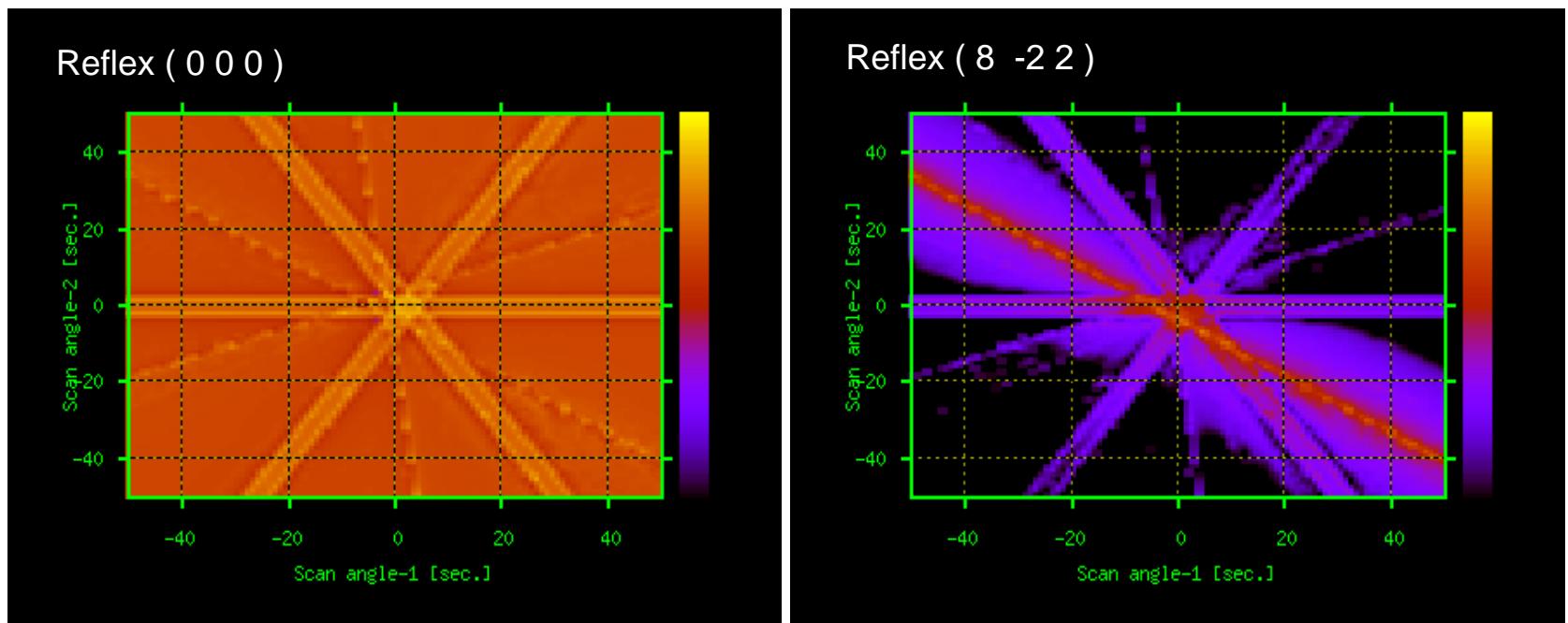
- Use X0h data (5-25 keV or 0.5-2.5 Å) -- *recommended*
- Use Henke data (0.01-30 keV or 0.4-1200 Å)
- Use Brennan-Cowan data (0.03-700 keV or 0.02-400 Å)

This is a Step-1 input form where one defines diffraction geometry. It calls an auxiliary program that looks for multiple diffraction combinations and generates Step-2 form.

At Step-2 user can enter scan parameters and include additional reflections if they were found and then call **BRL** to perform the multiple diffraction calculations.

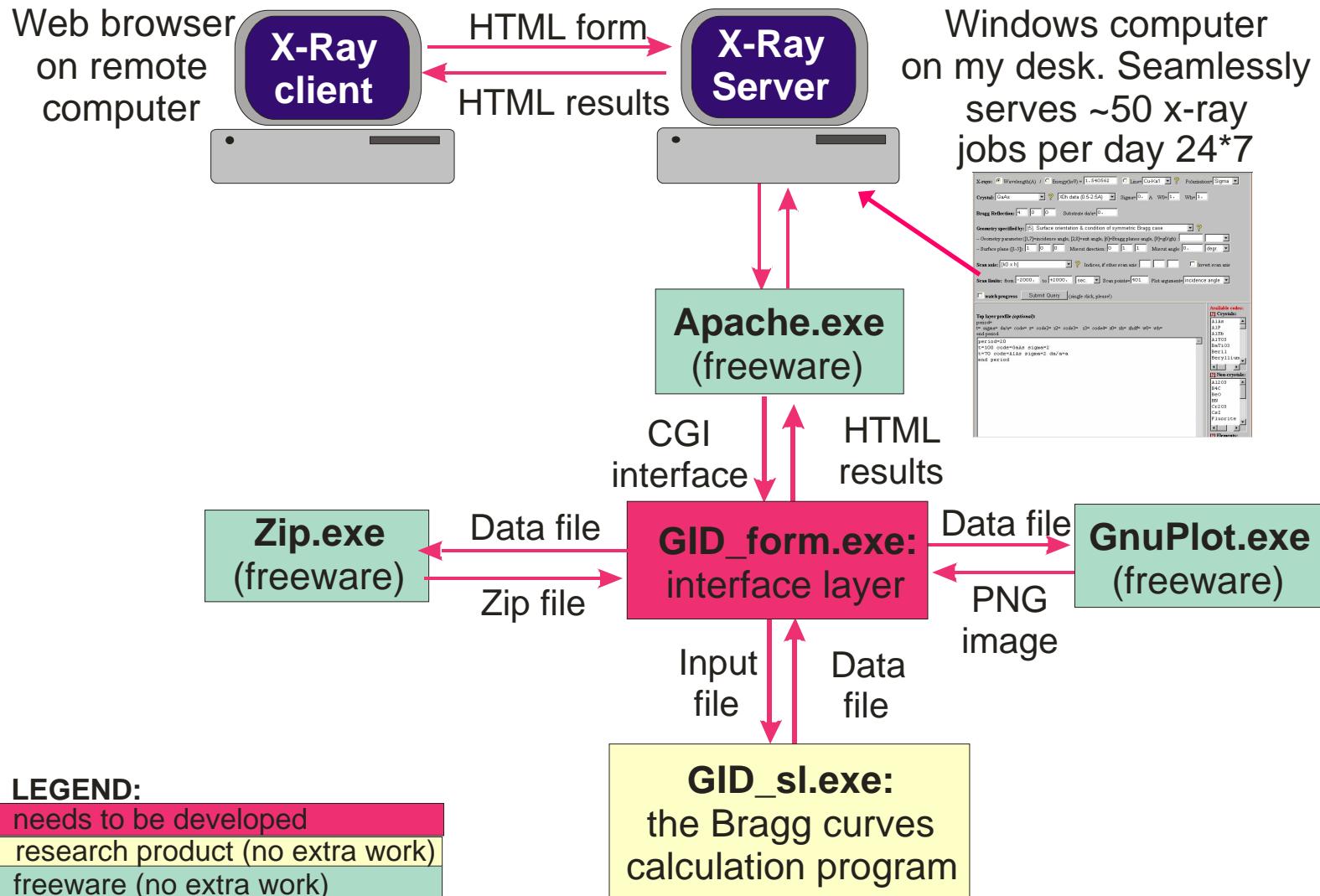


monash.edu.au

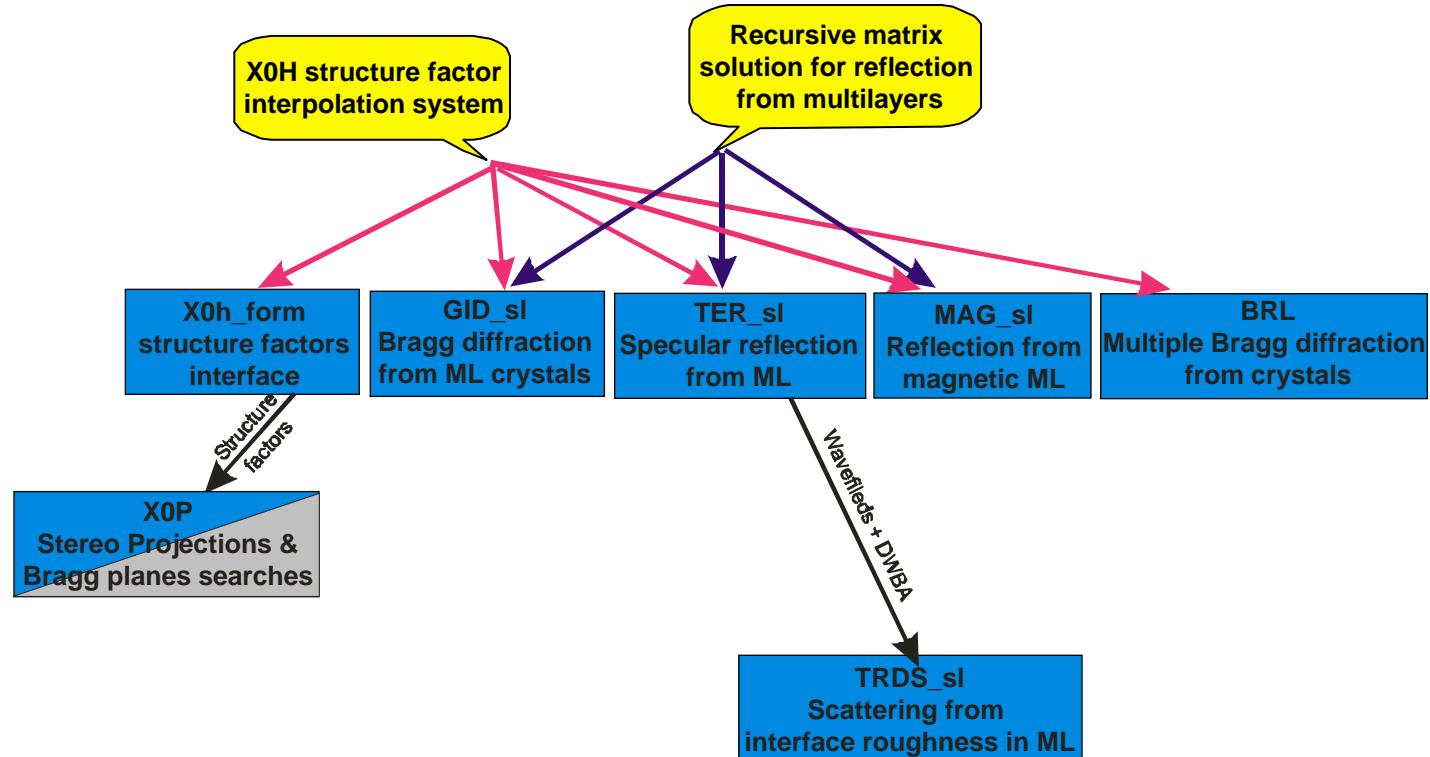


Some maps produced by 10-wave case calculations
(Silicon, $\lambda = 0.6968004107\text{\AA}$)

How it works: is it much effort to make software WWW-accessible?

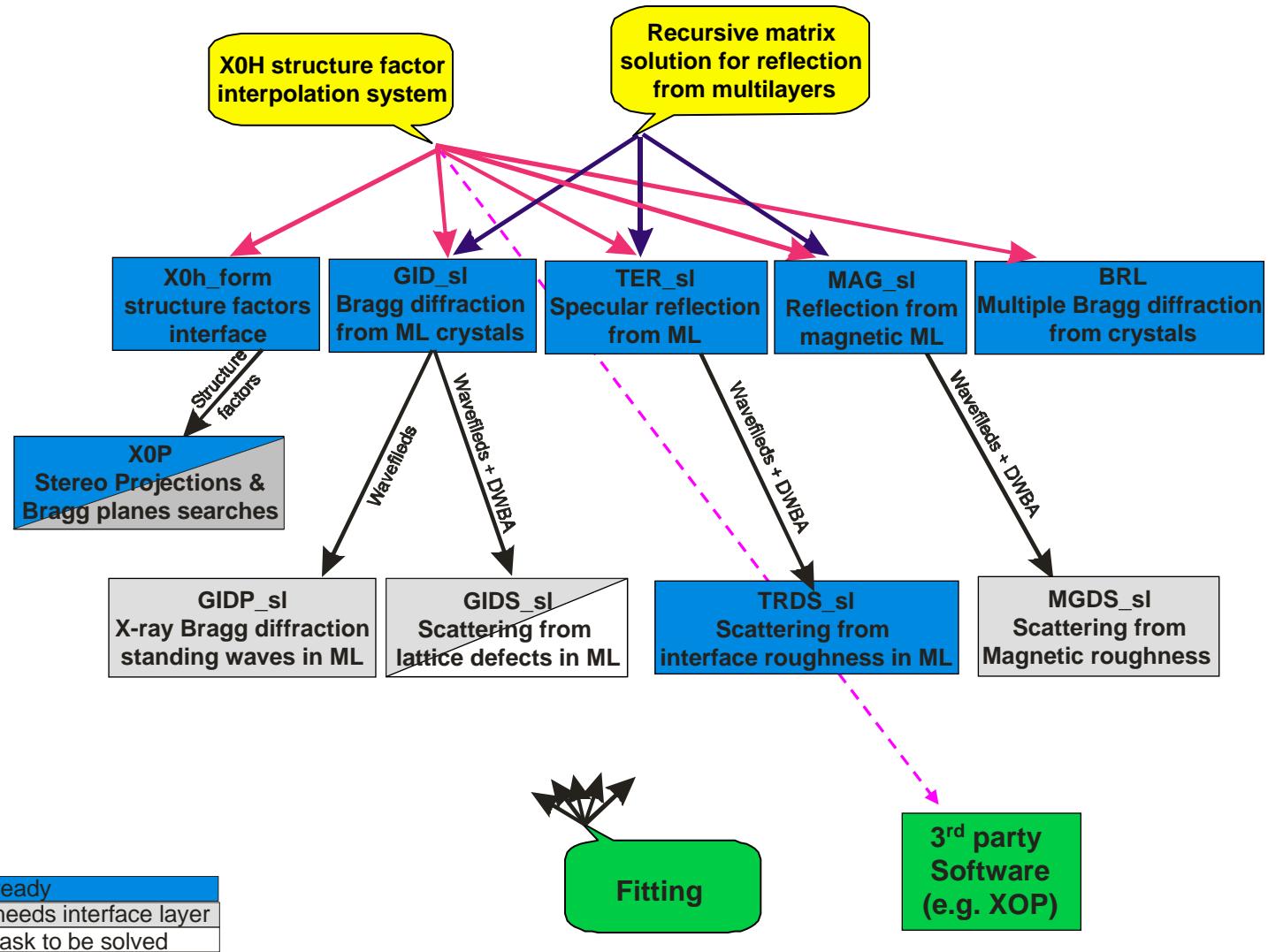


Server development: present structure



ready
needs interface layer
task to be solved

Server development: future plans



Server development: fitting vs. automation – I

The screenshot shows a software interface for X-ray diffraction analysis. At the top, there are several input fields: 'X-rays' (radio buttons for Wavelength(A) or Energy(keV), set to 1.540562), 'Line' (Cu-K α 1), 'Polarization' (Mixed), 'Crystal' (SiC-4H), 'Sigma' (0. A), 'W0' (1.), 'Wh' (1.), 'Bragg Reflection' (0, 0, 12), 'Substrate da/a' (0), 'Geometry specified by' (angle of Bragg planes to surface), 'Value' (0. degr.), 'Scan' (from -14000 to +4000 sec., 401 points), 'Invert axis' (unchecked), 'Plot argument' (incidence angle), and 'Approximations' (alpha_max = 1.E+8 * |xh|). Below these are buttons for 'watch progress' and 'Submit Query' (with a note: '(single click, please!)'). A large text area displays a 'Top layer profile (optional)' with 72 lines of parameter assignments, such as t=800 da/a = 0.00048 wh= 0.971610767. To the right, there are three scrollable lists under the heading 'Available codes': 'Crystals' (AlAs, AlFe3, AlN, AlP, alpha-Fe, AlSb, AlYO3), 'Non-crystals' (Al2O3, B4C, BeO, BN, Cr2O3, CsI, Fluorite), and 'Elements' (Ac, Ag, Al, Am, Ar, As, At, Au).

Providing fitting for general case is non-practical:

Too many parameters!

The form at the left is a typical material science application submitted from univ-poitiers.fr. The profile contains 72 lines, i.e. more than 200 parameters.

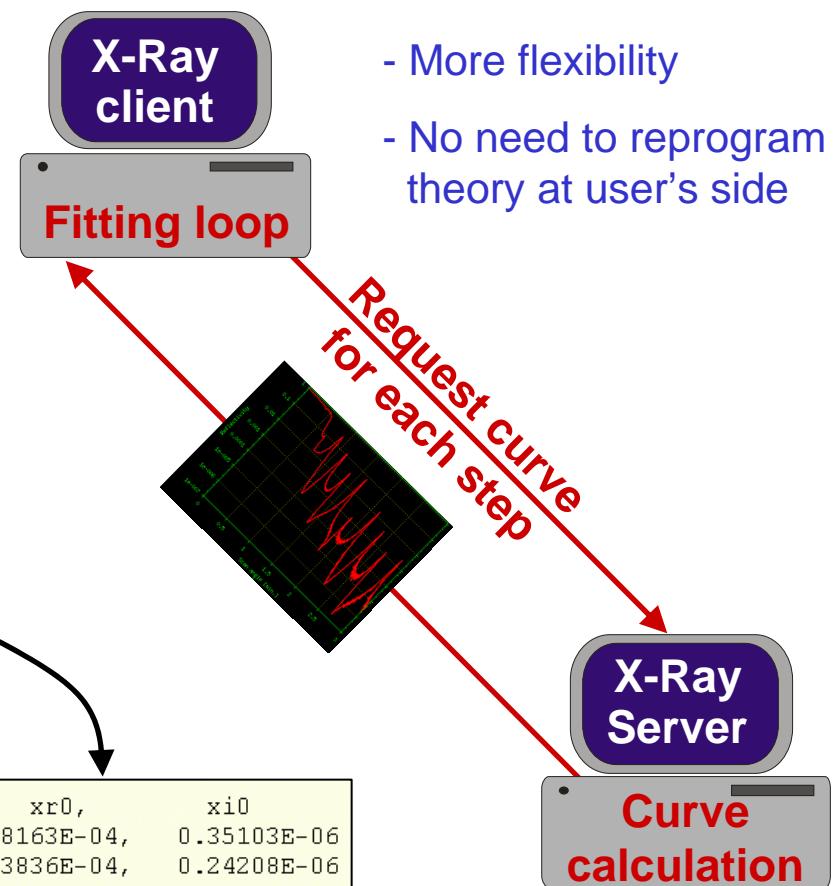
Server development: fitting vs. automation – II

```
#!/usr/bin/perl -W
use LWP::Simple;      # World-Wide Web library for Perl (libwww-perl)
my $file = "example.dat";
my ($E1,$E2) = (10,12); # start and end energy
my $n = 3;              # number of pts (please stay within a few dozen!)
my $dE = ($E2-$E1)/($n-1);
my $url = "http://sergey.gmca.aps.anl.gov/cgi/X0h_form.exe";
my $xway = 2;           # 1 - wavelength, 2 - energy, 3 - line type
my $wave = 0;            # works with xway=2 or xway=3
my $line = '';           # works with xway=3 only
my $coway = 0;           # 0=crystal, 1=other material, 2=chemicalformula
my $code = 'Germanium'; # works with coway=0 only
my $amor = '';           # works with coway=1 only
my $chem = '';           # works with coway=2 only
my $rho = '';             # works with coway=2 only
my ($i1,$i2,$i3) = (0, 0, 0); #Miller indices
my $df1df2 = 0;          # DB Option for dispersion corrections:
my $modeout = 1;          # 0 - html out, 1 - quasy-text out with keywords
my $detail = 0;            # 0 - don't print coords, 1 = print coords
open (DAT,>"$file") || die "Can't open ${file}\n";
print DAT "#Energy,          xr0,          xi0\n";
for (my $i=0; $i<$n; $i++) {                      # Energy loop
    $wave = $E1 + $dE * $i;
    my $addr = "$url?xway=$xway&wave=$wave&line=$line&coway=$coway" .
               "&code=$code&amor=$amor&chem=$chem&rho=$rho" .
               "&i1=$i1&i2=$i2&i3=$i3&df1df2=$df1df2" .
               "&modeout=$modeout&detail=$detail";
    my $buffer = get($addr);                         #Request X0h data from WWW
    my @content = split /\n/, $buffer;                # split page into lines
    my $ncon = $#content + 1;                        # number of lines on page
    print DAT "  $wave,";                            # loop over page lines
    for (my $j=0; $j<$ncon; $j++) {
        my $x = $content[$j]; chop $x;                 #strip LF/CR
        if ( $x =~ m/xr0=/ ) { $x =~ s/^.*xr0=/g; print DAT "  $x,"; }
        if ( $x =~ m/xi0=/ ) { $x =~ s/^.*xi0=/g; print DAT "  $x\n"; }
    }
}
```

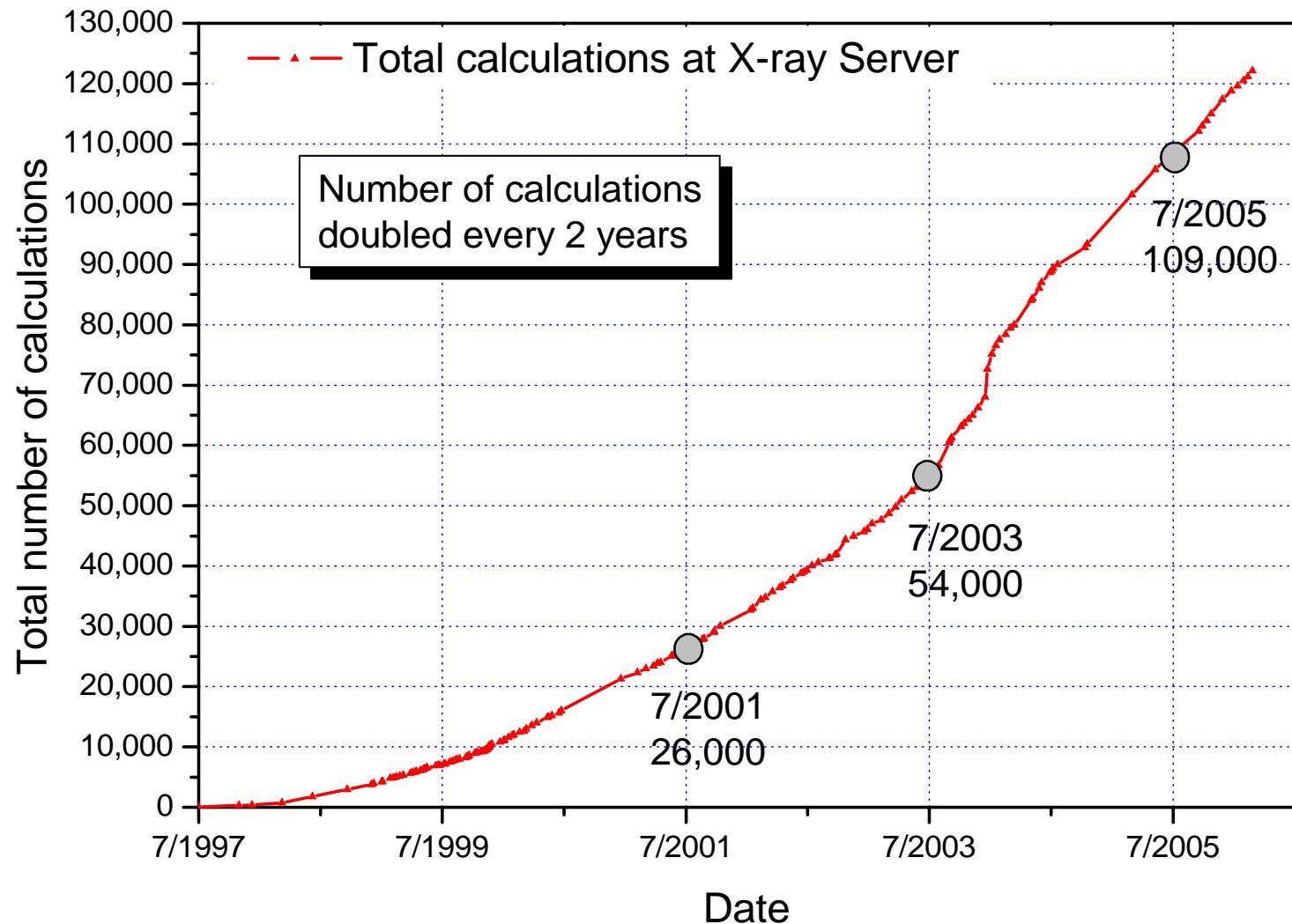
Example script provided on the server to request & save χ_{0r} and χ_{0h} as a function of X-ray energy

#Energy	xr0	xi0
10,	-0.18163E-04,	0.35103E-06
11,	-0.13836E-04,	0.24208E-06
12,	-0.12809E-04,	0.14516E-05

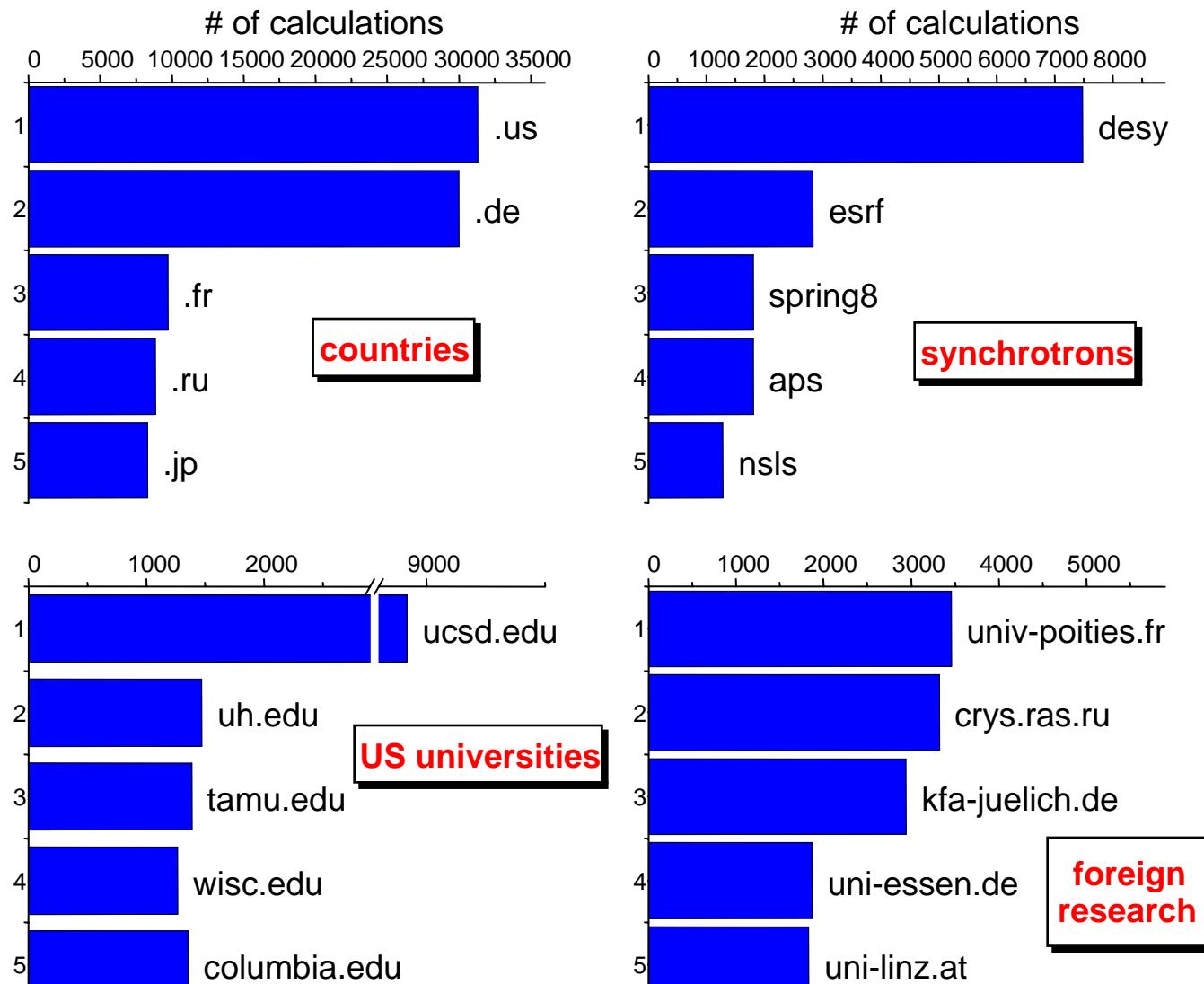
Perhaps a more productive idea than online fitting is to provide tools to grab data by a fitting procedure running at a remote computer:



Some X-ray Server statistics



Some X-ray Server statistics (continued)



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Acknowledgements

Co-authors of algorithm presented through the X-ray Server:

S.Durbin, T.Jach, B.Jenichen, V.Kaganer, R.Koehler, E.Kondrashkina, O.Lugovslaya, G.Materlik, D.Novikov, U.Pietsch, S.Sinha, A.Souvorov, A.Ulyanenkov.

X-ray Server users contributed by their feedback:

B.Barnes, A.Van der Lee, G.Bertschinger, D.Black, C.Blome, W.Cai, G.Ceriola, K. Chandrasekaran, H.Chapman, Y.Danon, A.Declemy, C.Dufour, R.Forrest, M.Dias Franco, M.Grundmann, E.Gullikson, L.Hudson, E.Ikonen, C.-C.Kao, J.Langer, B.Lings, J.Santiso, R. Medicherla, A. Fontcuberta-i-Morral, P.Muduli, P.Nilsson, C.Noyan, R.Osgood, F. Pfeiffer, E.Roa, X.Huang, D. Satapathy, D. Schroff, M. Servidori, X.Su, S.Warren, M.Weimer, M.Zhong, and many others!

X-ray Server hosts:

Management of BIO and GM/CA Collaborative Access Teams at the Advanced Photon Source for hosting X-ray Server on their computers. The GM/CA and BIO CATs are the research centers sponsored by the National Institutes of Health.