NOBUGS'2006

Transformation of X-ray Server into WWW-based library with simple API

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What is X-ray Server (http://x-server.gmca.aps.anl.gov)?

X-ray Server is a public project launched in **1997** with the goals to explore using WWW for providing scientific community with a wider access to personal research results, establishing scientific collaborations, and refining X-ray scattering models and scientific software.

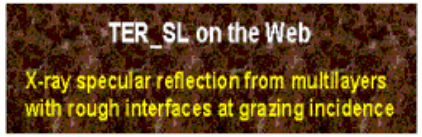
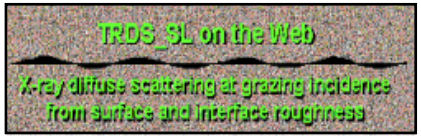
The Server delivers Web interface to a number of programs implementing author's models in the field of X-ray diffraction and scattering, i.e. the software operates directly on the Server available for use without downloading. At present 7 programs have been made operational; they will be briefly described on the next slides.

After 10 years of development and experience the Server has become one of the most reputable Web resources in the X-ray field. The server programs have been used more than **135,000** times by more that **5,500** colleagues worldwide with the base of ~**1,500** regular users who performed 10 or more calculations. About **55%** of the usages are the simulations of X-ray curves and the rest are the X-ray structure factors requests and related services for planning X-ray experiments.

This wide usage suggested to extend access beyond web browser sessions and to convert the server into a kind of web-accessible X-ray library.

Software available through X-ray Server

This site has been online since 1997 and has served **135, 644** x-ray jobs

	X0h interpolates dielectric susceptibilities x_0 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. ***X0h-search*** is a tool to search for Bragg planes under various conditions.	**63,821 jobs**
	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.	**36,390 jobs**
	***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.	**13,749 jobs**
	***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.	**10,882 jobs**
	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.	**8,795 jobs**
	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.	**2,007 jobs**

Based on ~17 research papers

Interpolation of X-ray structure factors

X-rays:

- Wavelength (A):
- Energy (keV):
- Characteristic line: Cu-Ka1 ?

Target:

- Crystal: Silicon ?
- Other material: ?
- Chemical formula: and density (g/cm^3):

Reflection:

Miller indices: 1 1 1

Database Options for dispersion corrections df1 , df2:

- Use X0h data (5-25 keV or 0.5-2.5 A) -- recommended for Bragg diffraction.
- Use Henke data (0.01-30 keV or 0.4-1200 A) -- recommended for soft x-rays.
- Use Brennan-Cowan data (0.03-700 keV or 0.02-400 A)
- Compare results for all of the above sources.

Get X0h! Reset

Structure :	Silicon
Symmetry :	Cubic
Density (gm/cm^3) :	2.3293
Unit cell constants (A) :	5.4309 , 5.4309 , 5.4309
Unit cell angles (degr.) :	90.000 , 90.000 , 90.000
Poisson Ratio :	0.2800
Composition: Element -- N_sites (Sites occupation)	Si -- 8 (1.000)
X-ray line :	Cu-Ka1
Wavelength (A) :	1.54056
Energy (keV) :	8.04778
Closest absorption edge (keV) :	1.84 (for element **Si**)
Database for df_1, df_2 :	*** X0h (International Tables), 5-25 keV ***
x_{r0} , x_{i0} ($n = 1 + x_{r0}/2 + i*x_{i0}/2$) :	-0.15127E-04 , 0.34955E-06
delta , *eta* ($n = 1$ - *delta* - i*eta) :	0.75634E-05 , -0.17477E-06
? Absorption factor (1/cm) and length (um) :	142.56 , 70.144
? Extinction length at TER (A) :	63.033
? Critical angle for TER (degr., mrad) :	0.22287 , 3.8898 GET THE CURVE !
Reflection :	(1 1 1)
Bragg angle (degr.) :	14.221
Interplanar spacing (A) :	3.1355
sin(QB) , cos(QB) :	0.24566 , 0.96936
tan(QB) , cotan(QB) :	0.25343 , 3.9459
sin(2*QB) , cos(2*QB) :	0.47627 , 0.87930
Polarization :	***Sigma***
$\lvert x_{rh}\rvert$, $\lvert x_{ih}\rvert$:	0.79801E-05 , 0.24314E-06
Phase difference (x_{rh} - x_{ih}) :	1.0000 * pi
Relative intensity (x_h / x_0) :	52.765 %
? Symmetric Laue-case extinction length (um) :	18.705
? Symmetric Bragg-case extinction length (um) :	1.5089
? ..... Double-crystal curve FWHM (arcsec., urad) :	9.7797 , 47.413
? ..... Darwin curve FWHM (arcsec., urad) :	6.9153 , 33.526 GET THE CURVE !
Polarization :	***Pi***
$\lvert x_{rh}\rvert$, $\lvert x_{ih}\rvert$:	0.70169E-05 , 0.21274E-06
Phase difference (x_{rh} - x_{ih}) :	1.0000 * pi
Relative intensity (x_h / x_0) :	46.396 %
? Symmetric Laue-case extinction length (um) :	21.273
? Symmetric Bragg-case extinction length (um) :	1.7160
? ..... Double-crystal curve FWHM (arcsec., urad) :	8.5992 , 41.690
? ..... Darwin curve FWHM (arcsec., urad) :	6.0806 , 29.479 GET THE CURVE !

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

Tool for searching Bragg reflections

X-rays:

- Wavelength (A):
- Energy (keV):
- Characteristic line: Cu-Ka1

Crystal:

Select code: Silicon

Bragg planes range:

From: 1 0 0 To: 1 1 1

Bragg angle range:

From: 0. To: 30.

Intensity control:

Minimum |xh/x0| (%): 0.

Database option for dispersion corrections df1, df2:

- Use X0h data (5-25 keV or 0.5-2.5 A) -- recommended for Bragg diffraction.
- Use Henke data (0.01-30 keV or 0.4-1200 A) -- recommended for soft x-rays.
- Use Brennan-Cowan data (0.03-700 keV or 0.02-400 A)

Find only those Bragg planes which make certain angles to the surface:

Surface plane indices: 1 0 0

- Planes make angles from Theta1 to Theta2
- Planes make angles from Theta1 to (Bragg_Angle - Theta2)
- Planes make angles from (Bragg_Angle - Theta1) to (Bragg_Angle - Theta2)

Theta1: 0. Theta2: 180.

Find Planes! Reset

SEARCH CONDITIONS :

Crystal:	Silicon
Symmetry group:	Cubic
Density (gm/cm^3) :	2.3293
Unit cell constants (A) :	5.4309 , 5.4309 , 5.4309
Unit cell angles (degr.) :	90.000 , 90.000 , 90.000
X-ray wavelength (Angstrom) :	1.540562
X-ray energy (keV) :	8.047777
X-ray characteristic line :	Cu-Ka1
Bragg planes range :	(1 0 0) -- (1 1 1)
Bragg angles range :	0.0000 -- 30.0000
Minimum intensity (xh/x0) :	0.0000%
Surface :	(1 0 0)
Planes angles to surface :	From Theta1 to Theta2
Theta1, Theta2 :	0.0000 -- 180.0000

SEARCH RESULTS :

Planes found: 4. Planes being displayed: 4

hkl	Angle to surface	Bragg angle
(1 0 0)	0.0000	8.1540
(1 0 1)	45.0000	11.5711
(1 1 0)	45.0000	11.5711
(1 1 1)	54.7356	14.2211

GID_SL on the Web

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

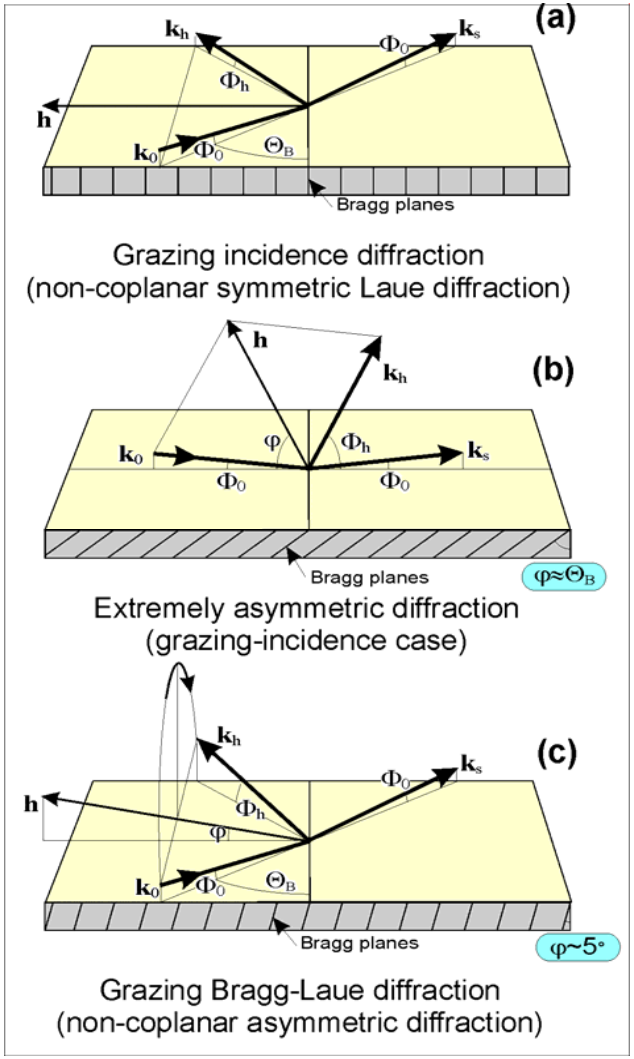
Bragg diffraction simulation program – 1

GID_sl (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 $\sigma(z)$.

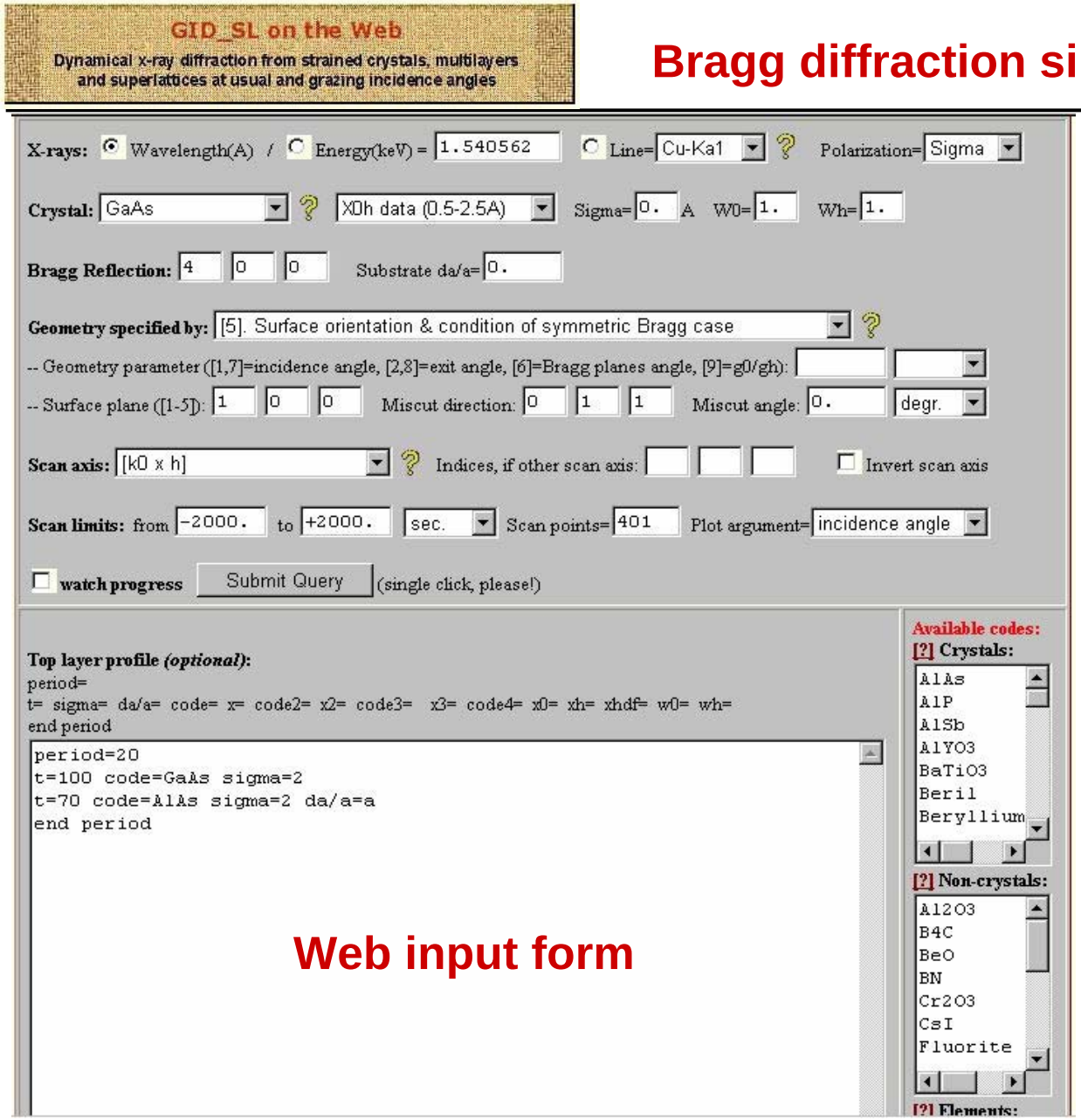
The advantage of ***GID_sl*** over most of other Bragg diffraction simulation software is that it takes into account specular reflection and refraction of X-rays at crystal surface and interfaces in multilayers.

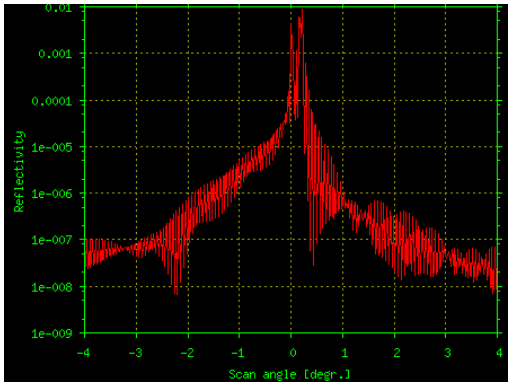
Replaces Takagi-Taupin equations for Grazing Incidence Diffraction!

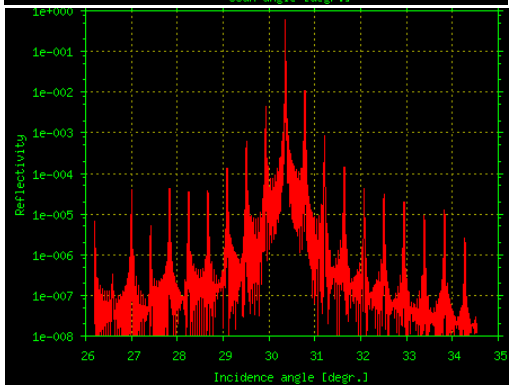


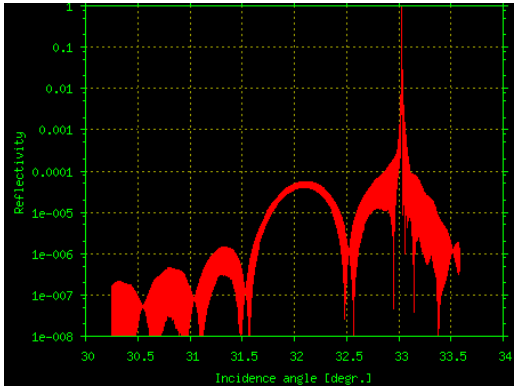
S.Stepanov, E.Kondrashkina, R.Koehler, D.Novikov, G.Materlik, and S.Durbin, PRB, **57**, (1998) 4829-4841.

Bragg diffraction simulation program - 2









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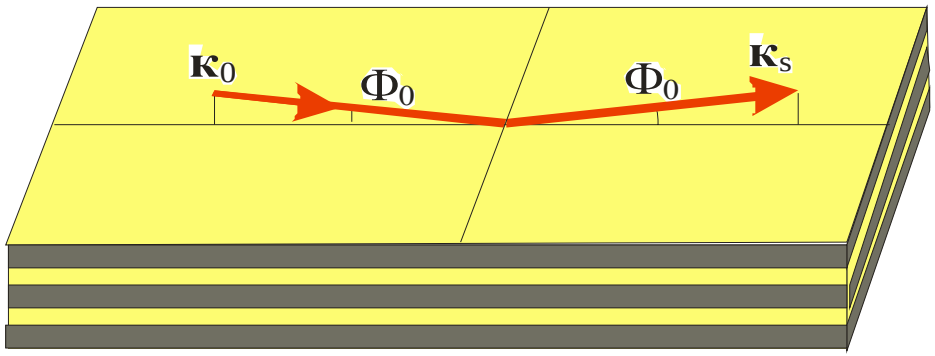
TER_SL on the Web

X-ray specular reflection from multilayers with rough interfaces at grazing incidence

Specular reflectivity simulation program - 1

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***.

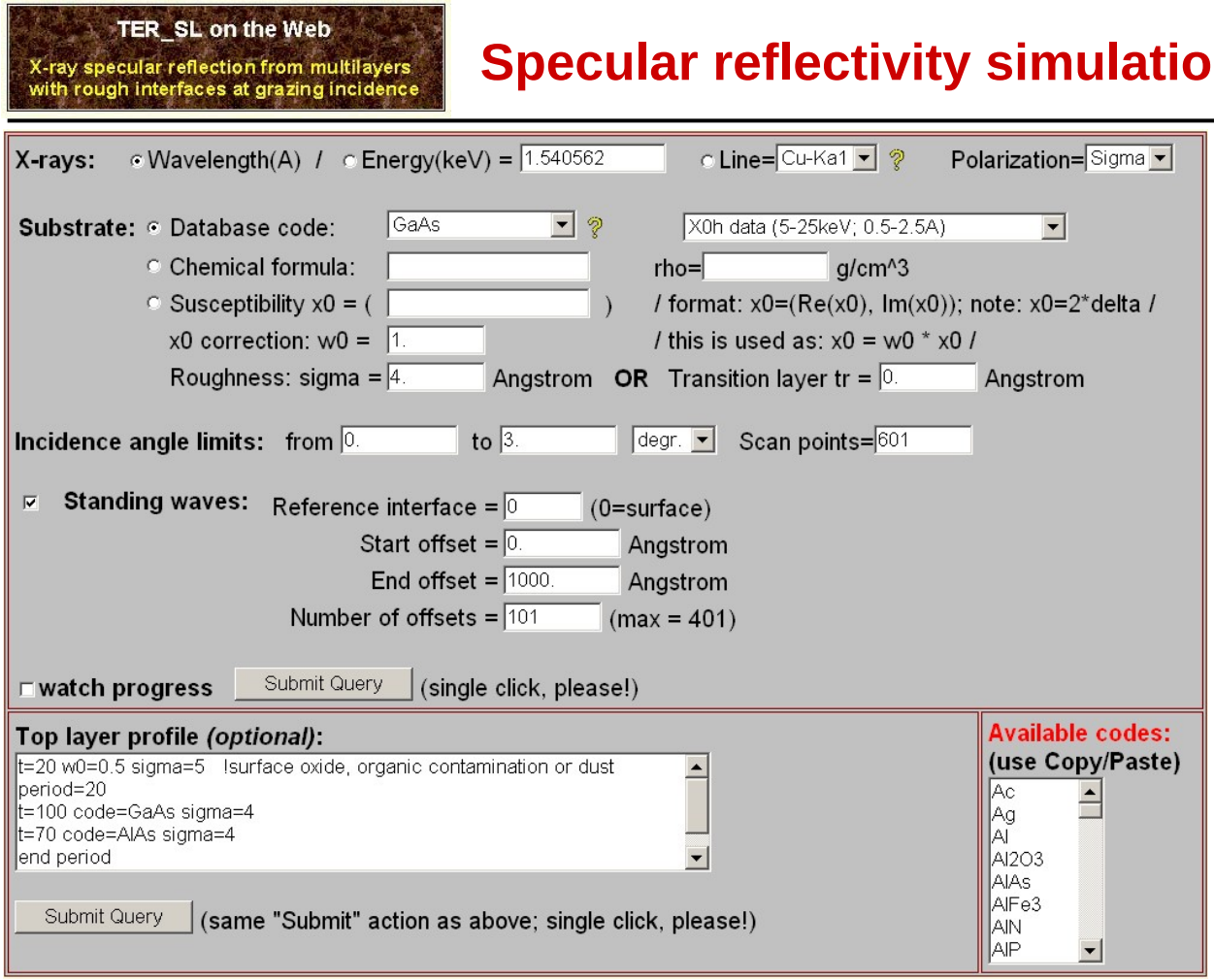
The advantage of ***TER_sl*** over the well know Parratt recursive technique is a faster convergence of recursions because ***TER_sl*** expresses the reflection from a stack of N layers through the reflectivity of (N-1) layers, while the Parratt technique expresses the reflectivity of N-th layer via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

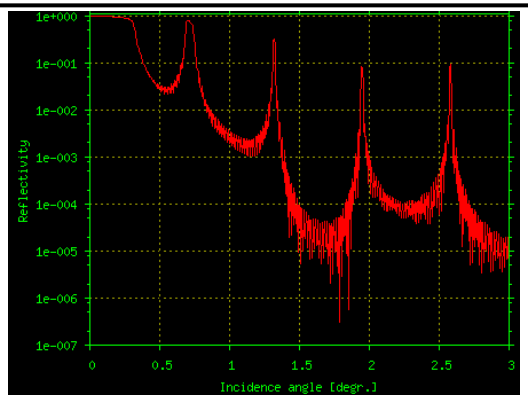


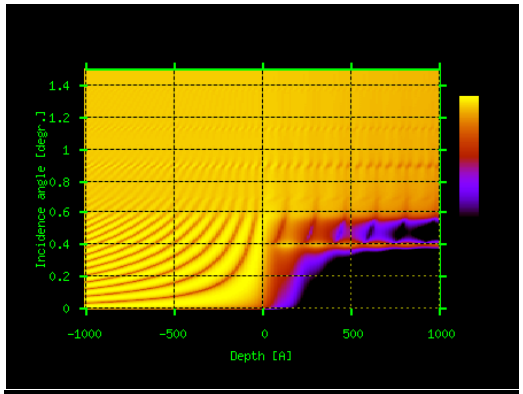
By-product of ***GID_sl:***
same recursion algorithm !

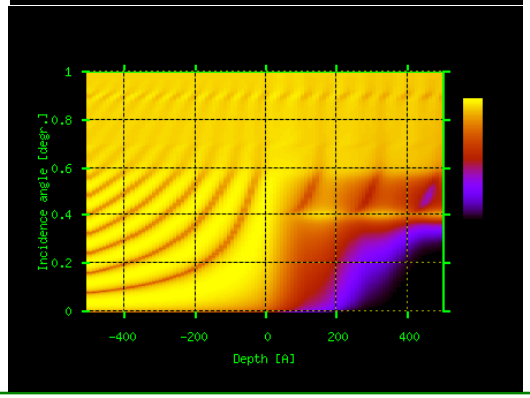
S.Stepanov, E.Kondrashkina, R.Koehler, D.Novikov, G.Materlik, and S.Durbin, PRB, **57**, (1998) 4829-4841.

Specular reflectivity simulation program - 2







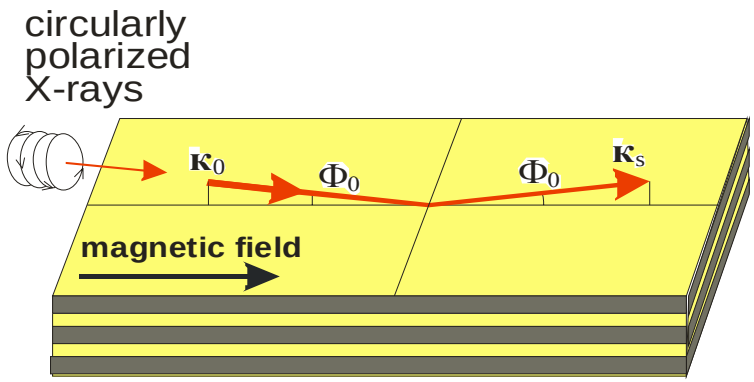


Recently added wavefields calculations for applications like fluorescence yield analysis, X-ray standing waves method, GISAXS, and etc.

MAG_SL on the Web
X-ray resonant specular reflection from magnetic multilayers

Resonance magnetic reflectivity program - 1

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. Since the resonant 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, PRB, **61** (2000) 15302-15311.

D.R.Lee, S.K.Sinha, D.Haskel, Y.Choi, J.C.Lang, S.Stepanov, and G.Srajer, PRB, **68** (2003) 224409-224427.

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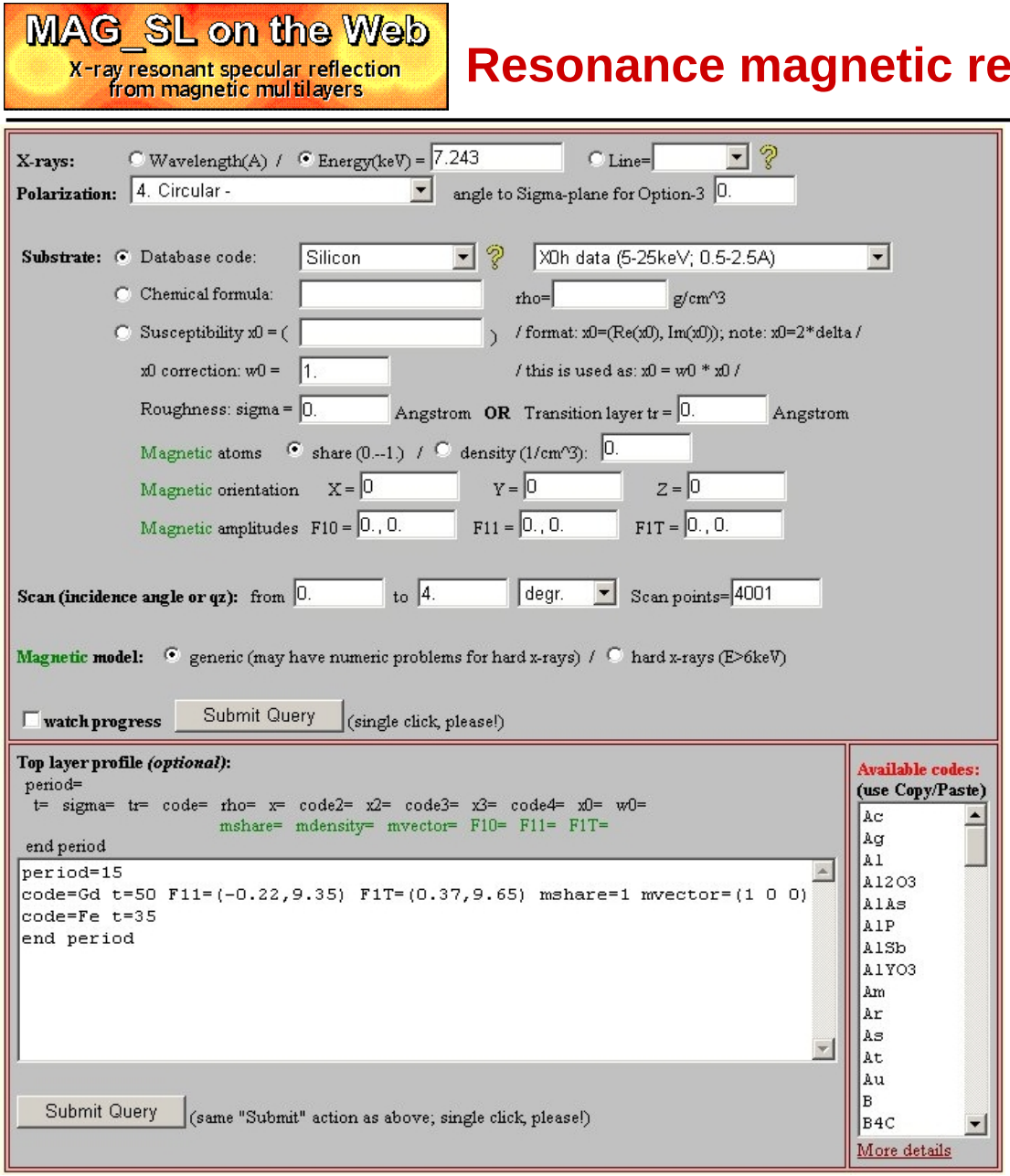
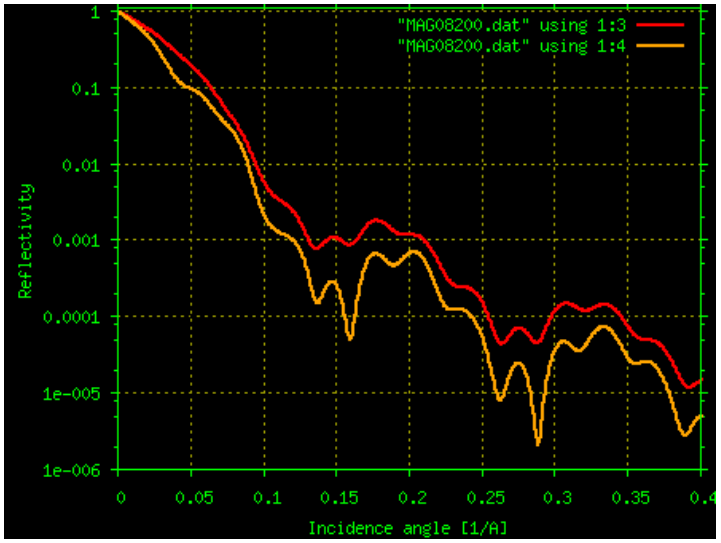
Resonance magnetic reflectivity program - 2





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

TRDS_SL on the Web
X-ray diffuse scattering at grazing incidence from surface and interface roughness

Grazing incidence diffuse scattering program - 1

The ***TRDS_sl*** program calculates GISAX from interface roughness in multilayers with 10 models of roughness formation and propagation. These include wavelength-dependent inheritance of roughness in multilayers, scattering from atomic steps on vicinal interfaces and scattering due to inclined roughness transfer in crystalline multilayers.

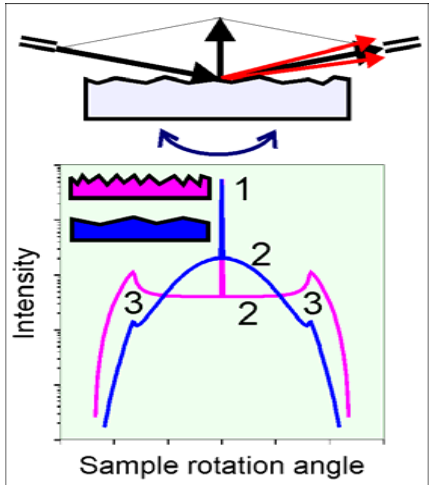


Fig.1. Diffuse scattering of grazing x-rays from surface roughness. 1: specular peak, 2: diffuse scattering for two different lateral scales of roughness, 3: Yoneda peaks at critical angle for total reflection.

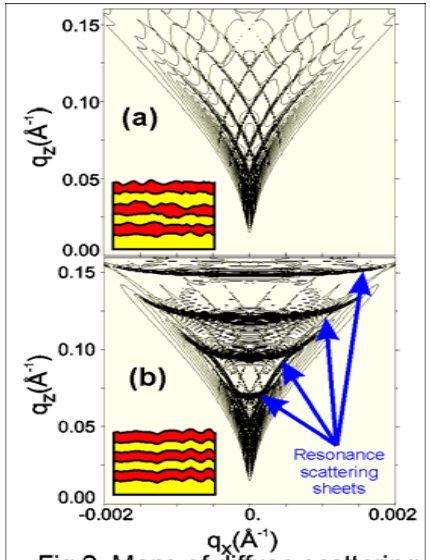


Fig.2. Maps of diffuse scattering from vertically uncorrelated (a) and correlated (b) roughness

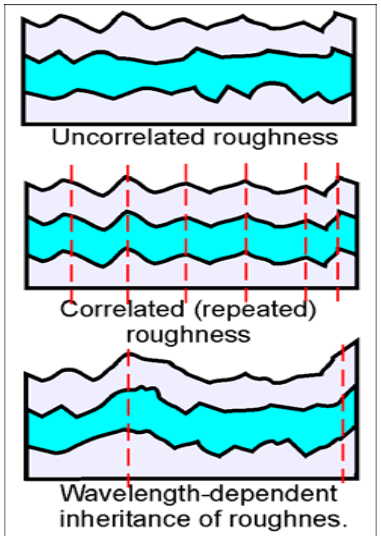


Fig.3. Different models of roughness correlations in multilayers

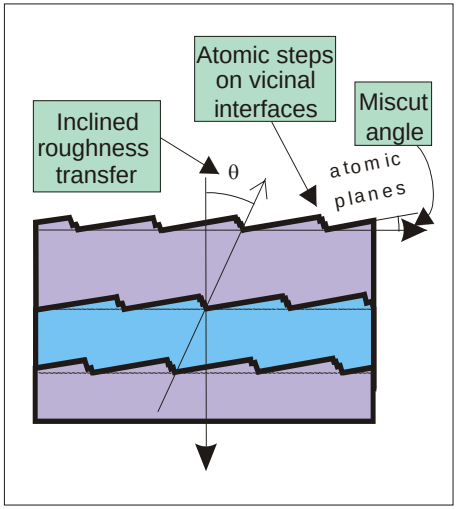
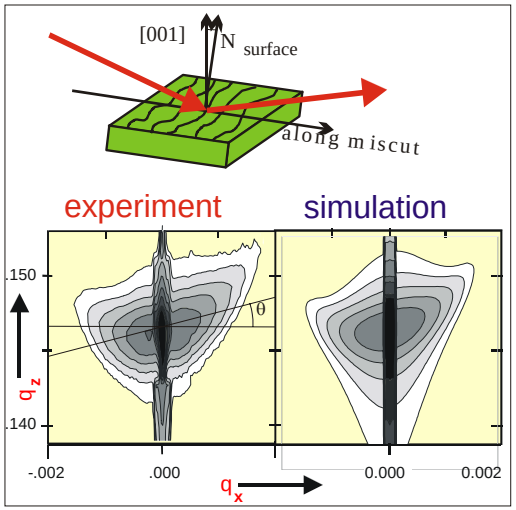


Fig.4. Asymmetric rougness of vicinal interfaces and skew roughness transfer in crystals

Fig.5. Simulations of GISAX due to inclined roughness transfer in 20 x (AlAs/GaAs)



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

E.A.Kondrashkina, S.A.Stepanov, *et al*, PRB **56** (1997) 10469-10482.

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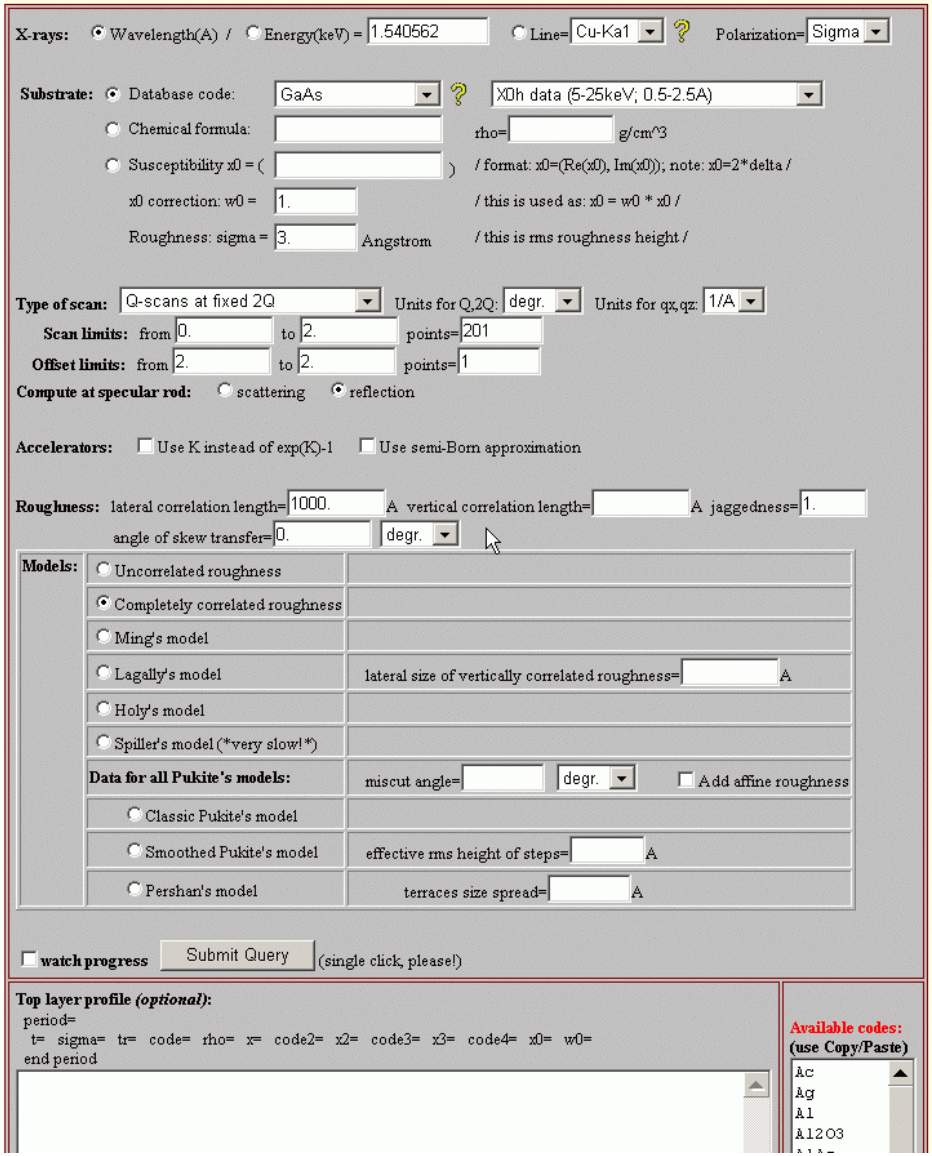
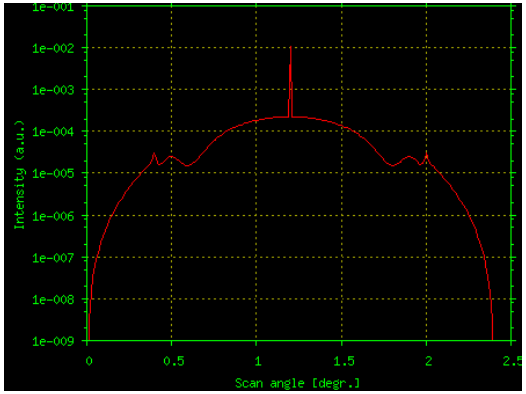
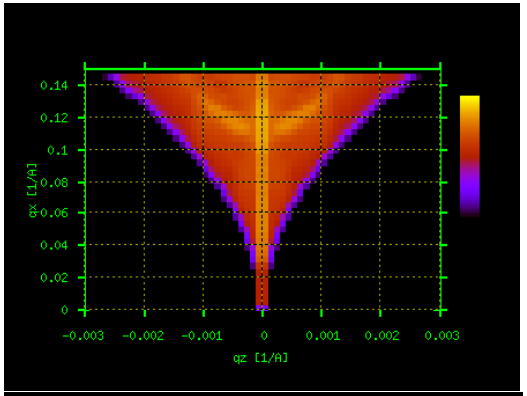
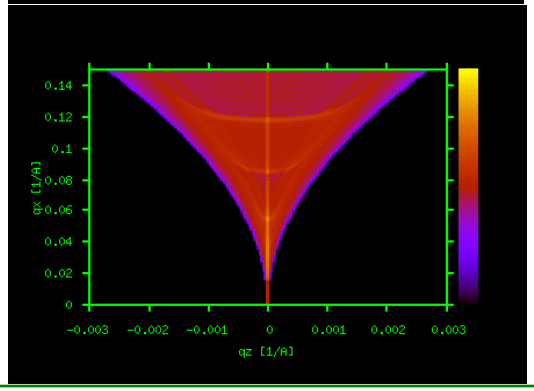
Grazing incidence diffuse scattering program - 2









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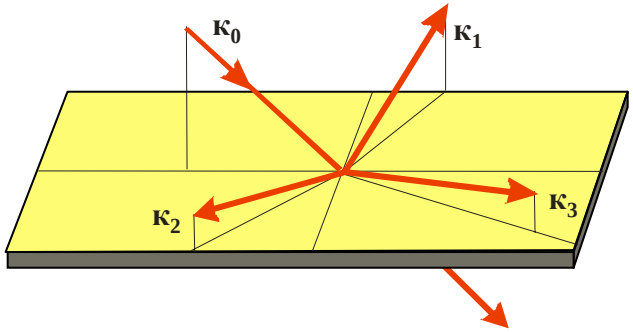
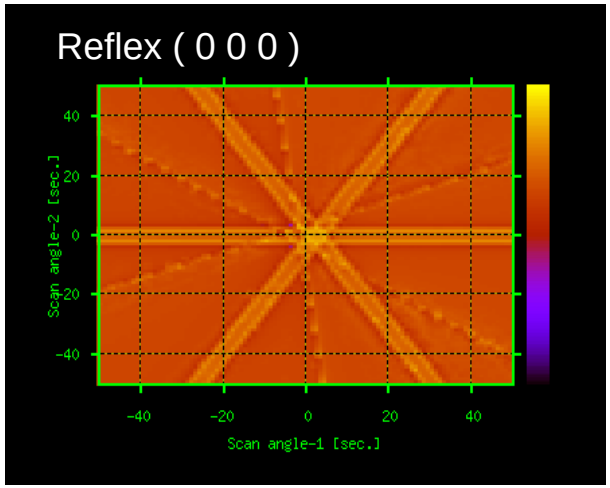
BRL on the Web
X-ray multiple Bragg/Laue diffraction

Multiple Bragg diffractrion program - 1





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*2N** scattering matrix. However, when the diffraction geometry involves grazing X-ray waves, the calculations are reduced to the eigenvalue problem for **4N*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+Ns)*2(N+Ns)** scattering matrix where Ns is the number of grazing waves. Thus, if there are no grazing waves, the matrix size is 2N*2N and if all of the waves are grazing it becomes 4N*4N. In some cases the calculations are reduced dramatically.

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

BRL on the Web
X-ray multiple Bragg/Laue diffraction

Multiple Bragg diffractrion program - 2

Target:

Crystal: Silicon ?

Surface: Base plane: 1 1 1

Miscut direction: 1 -1 0

Miscut angle: 0. degr.

Reflections:

Reflex-1: 1 1 1

Reflex-2: 2 2 0

Index search range: 5

Min. Intensity filter: 0.1
(|xh/x0|*100% > ...)

X-rays:

- ○ **Wavelength (A):**
- ○ **Energy (keV):**
- ◉ **Characteristic line:** Cu-Ka1 ?
- ○ **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 A) -- *recommended***
- ○ **Use Henke data (0.01-30 keV or 0.4-1200 A)**
- ○ **Use Brennan-Cowan data (0.03-700 keV or 0.02-400 A)**

Submit Reset

Step-1

Crystal: Silicon Symmetry: Cubic X0h data: Automatic DB choice

Surface: base plane=(1 1 1) miscut direction=(1 -1 0) miscut angle=0. degr.

Thickness (microns): 100.

X-rays: wavelength= 2.6344 A energy= 4.7063 keV line=*none*

X-ray polarization: [1] Mixed (unpolarized) Angle to pi0 for mode [2]: 0.

Scan limits (Theta1): from -50. to 50. points = 101

Scan limits (Theta2): from 0. to 0. points = 1

Scan axes: [1] Theta2 along sigma0 **Scan angle units:** sec.

Specified reflections:

Reflex1 = (1 1 1) QB = 24.840 degr. |xh/x0| = 52.895% |alpha/x0| = 0.105E-10

Reflex2 = (2 2 0) QB = 43.314 degr. |xh/x0| = 60.859% |alpha/x0| = 0.210E-10

Reflex3 = (3 1 1) QB = 53.552 degr. |xh/x0| = 39.863% |alpha/x0| = 0.700E-11

Additional reflections search results (you can select up to 8 planes if available):

Searching from (-5 -5 -5) to (5 5 5) Intensity filter |xh/x0| > 0.100%

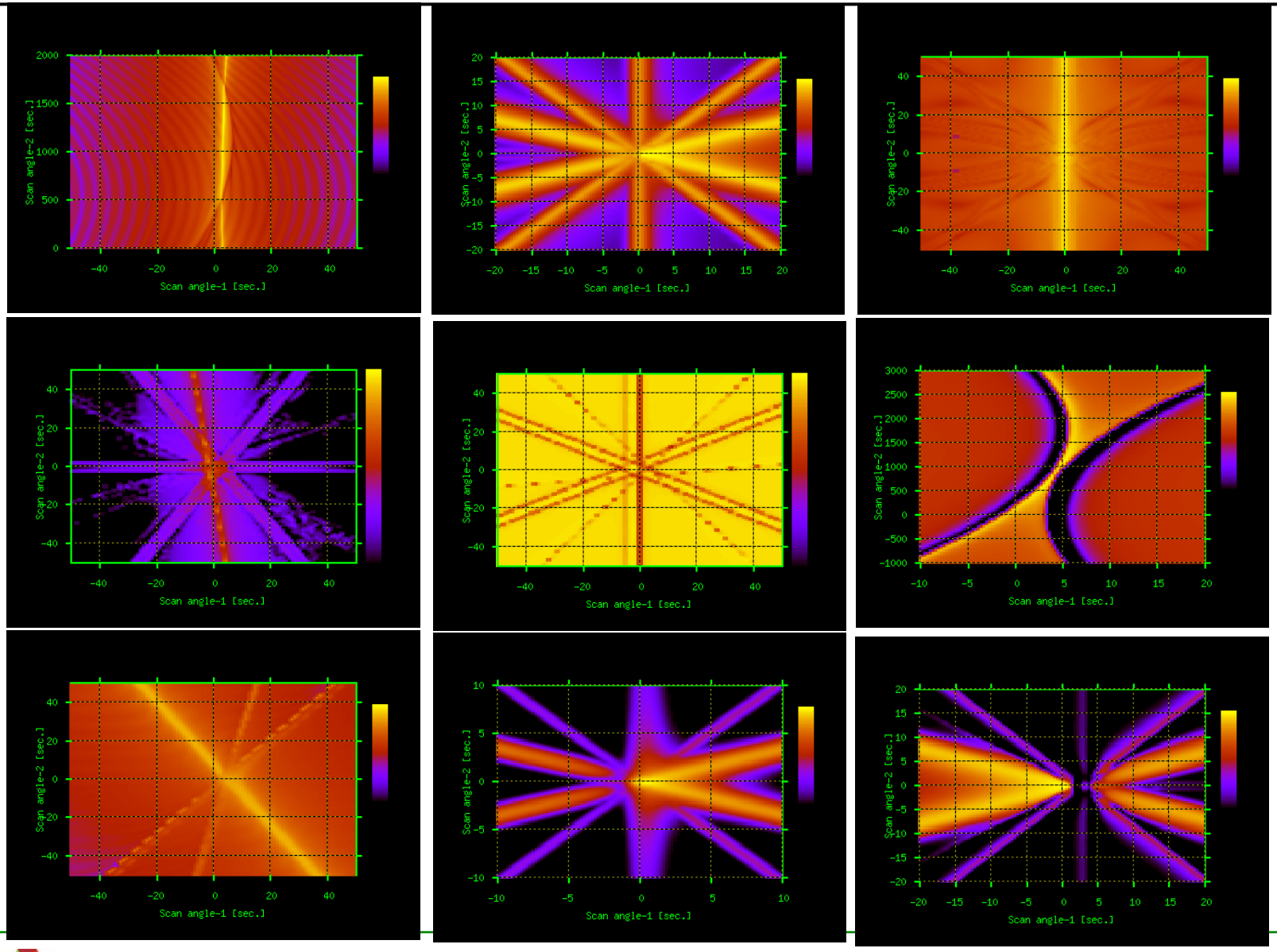
- ☐ **Reflex4** = (1 -1 1) QB = 24.840 degr. |xh/x0| = 52.895% |alpha/x0| = 0.105E-10
- ☐ **Reflex5** = (2 -2 0) QB = 43.314 degr. |xh/x0| = 60.859% |alpha/x0| = 0.210E-10
- ☐ **Reflex6** = (3 -1 1) QB = 53.552 degr. |xh/x0| = 39.863% |alpha/x0| = 0.350E-10
- ☐ **Reflex7** = (4 0 0) QB = 75.964 degr. |xh/x0| = 50.816% |alpha/x0| = 0.280E-10

Submit Reset

Step-2

BRL on the Web
X-ray multiple Bragg/Laue diffraction

Multiple Bragg diffractrion program - 3



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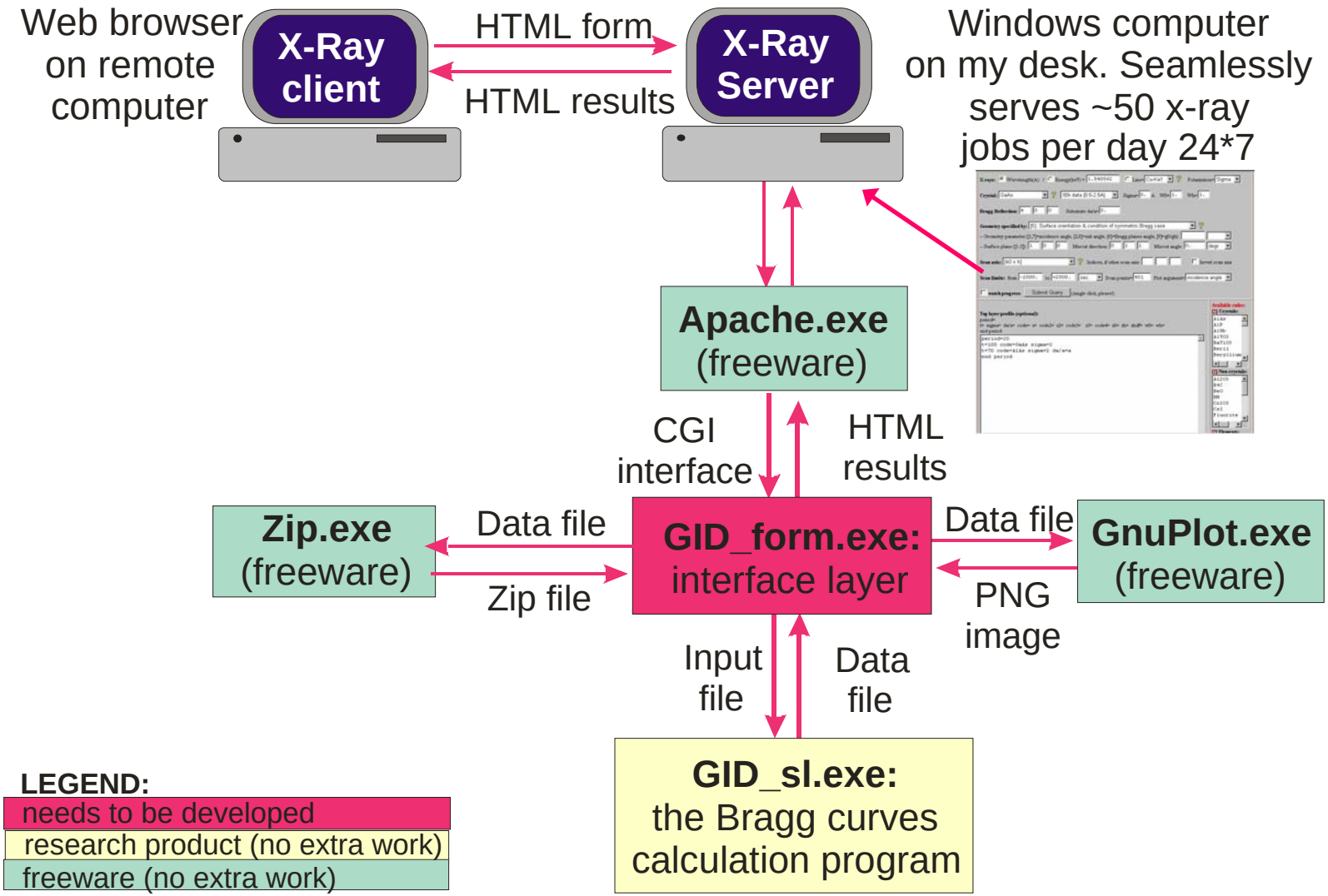
How it works: what is the effort to make software WWW-accessible?

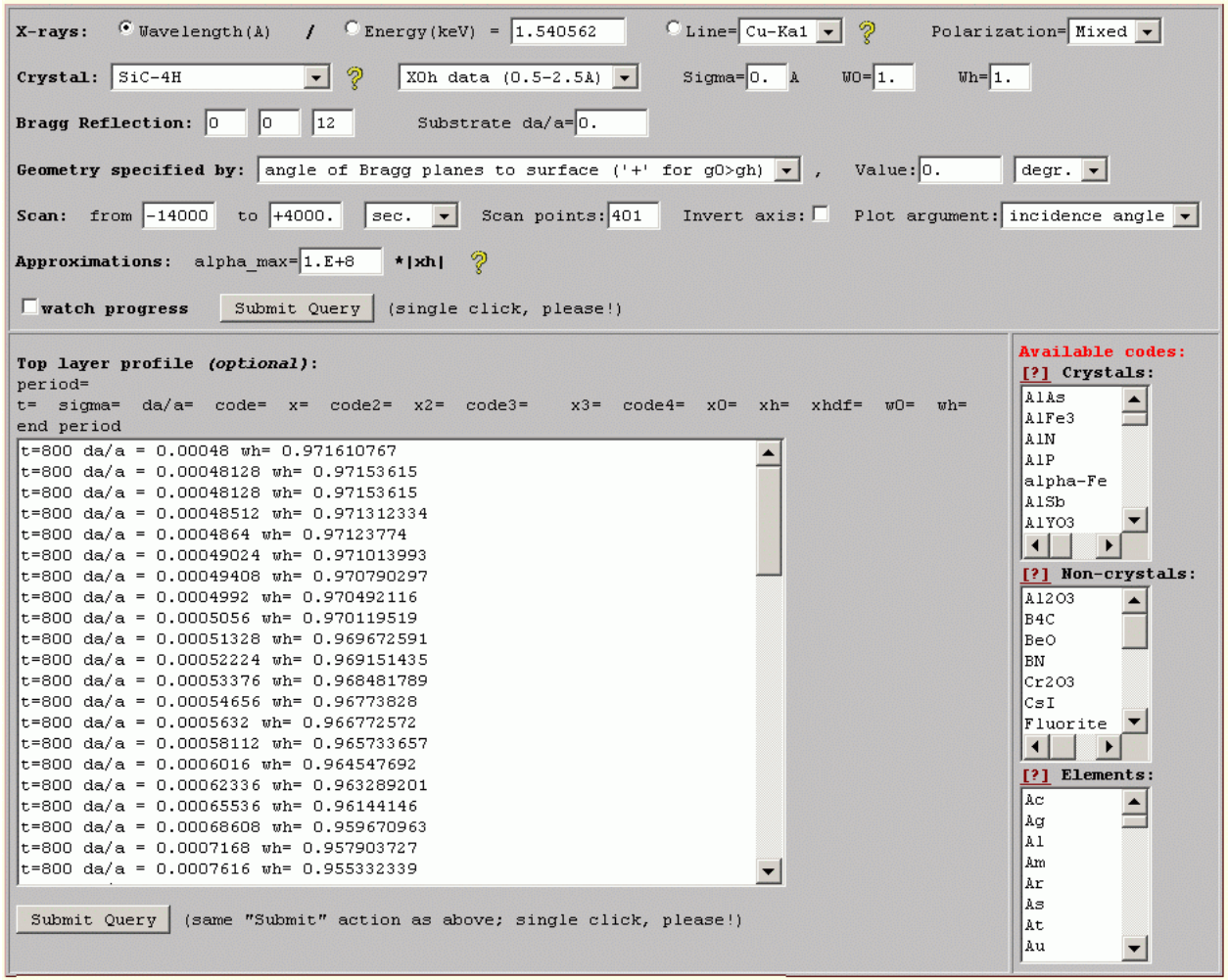


Most frequent Server development requests from users

With a big diversity of models presented through the Server and big variety of calculations one can do, there are two most frequent requests coming from the community:

- **Provide automation**
- **Provide fitting**

Server development: fitting *vs.* automation – I



Providing fitting for general case is non-practical:

Too many parameters!

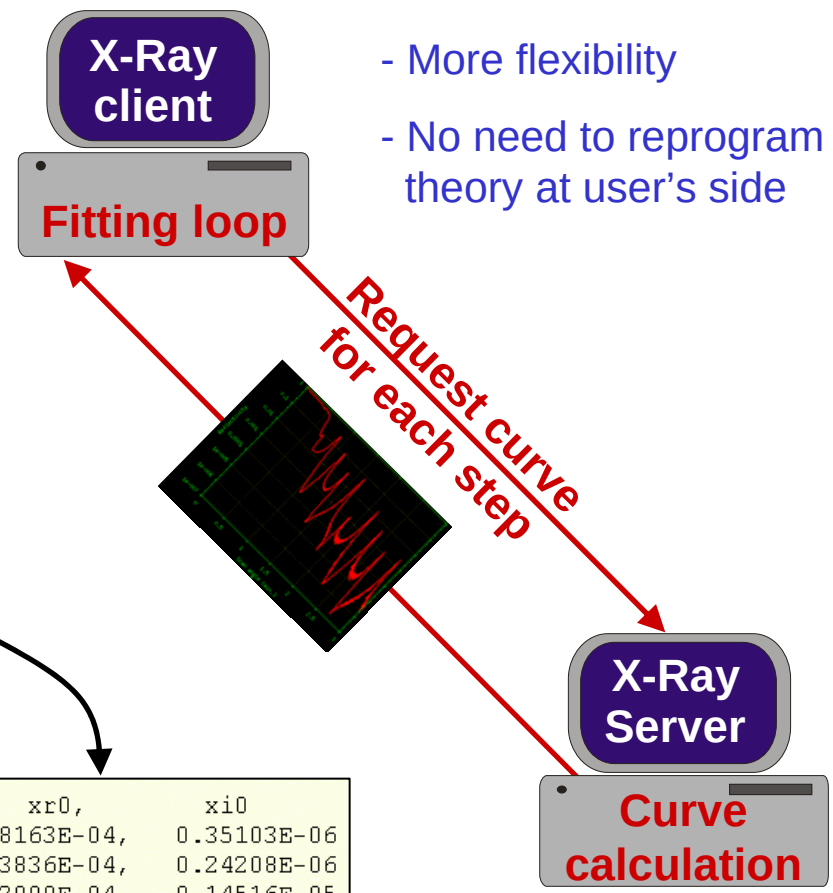
The form at the left is a typical material science application submitted from univ-poitiers.fr. The profile contains 72 lines, i.e. more than 200 parameters.

Also, account for the geometry or resolution of experiment would make the programs case-specific vs gerenal.

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},";
    for (my $j=0; $j<$ncon; $j++) {               # loop over page lines
      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";}
    }
  }
```

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



- More flexibility
- No need to reprogram theory at user's side

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
```

Server Templates

getX0h.pl	Script interfacing ***X0h***	(equivalent to *X0h* form)
getGID.pl	Script interfacing ***GID_sl***	(equivalent to *GID_sl* form)
getTER.pl	Script interfacing ***TER_sl***	(equivalent to *TER_sl* form)
getTER_sw.pl	A script interfacing ***TER_sl*** and additionally requesting standing waves	(equivalent to *TER_sl* form)

The scripts can be called from user's software written in any language using the **system** function. If one needs to vary a parameter, it can be passed to the script as a command line argument.

Basically, these scripts present a practical example of a CGI client program accessing the server programs. They are simple, but they **should be simple** to become useful since they address a wide auditory of physicists presumably unfamiliar or poorly familiar with the CGI.

Inspecting the Server logs has shown that the community perceived the idea very well: there have been many cases of using the template scripts since they were introduced in July'07. Moreover, only a month after posting the templates, a group at HASYLAB used this idea to develop their own Igor Pro macros for accessing the wavefields provided by ***TER_sl***.

Conclusions

We have presented a simple solution how to extend the accessibility of scientific software working through the WWW. A set of documented CGI wrappers available for download allows to educate users and let them embed the server programs into their own software as a remote library or implement remote fitting.

This experience shows that the remote interface should be as simple as possible because the only way to make it generic and flexible (i.e. of wide interest) is when scientists can link it directly to their own software without long learning or help from professional software guru.

The next steps in the X-ray Server development will head towards adding more remote access templates and providing intermediate data from server programs, for example the X-ray wavefields inside the samples in addition to the X-ray scattering curves.

This experience may be helpful for newly emerging scientific software projects like DANSE or Digital Lab.