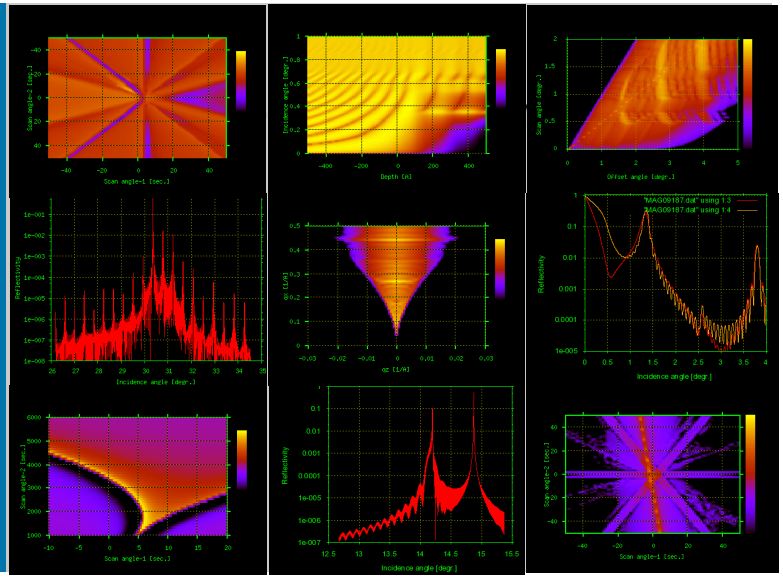
X-RAY SERVER: DYNAMICAL DIFFRACTION ON THE WEB. SCOPE, HISTORY, CAPABILITIES, AND PLANS



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Advanced Photon Source,
Lemont, IL, USA

October 2016, SOS Workshop, Trieste, Italy

What is X-ray Server?

X-Ray Server (x-server.gmca.aps.anl.gov) is a WWW-based computational server for modeling of X-ray diffraction, reflection and scattering. All software operates directly on the server and can be accessed remotely either from web browsers or from user software so that the server can be deployed as a software library or data fitting engine.

Goals:

- explore simplest ways to share scientific software with community using WWW.
- avoid porting software to multiple platforms and maintaining multiple versions.
- be able to collect feedback from users, correct errors and prevent misuse of programs beyond the limits of X-ray scattering models they implement.

Technology:

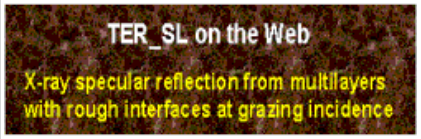
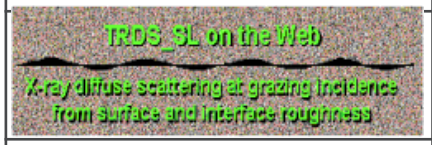
- http interface (CGI wrappers) to *unchanged* scientific software

History:

- online since 1997; free and no registration,
- served more than 2 million jobs,
- about 5000 IPs used it 10 or more times

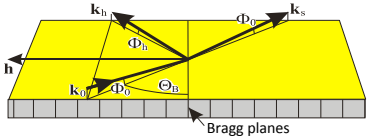
Software available through X-ray Server

http://x-server.gmca.aps.anl.gov (online since 1997)

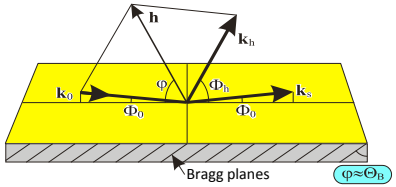
	***X0h*** interpolates dielectric susceptibilities for crystals and other materials in wide range of X-ray energies with the option to compare data from different DBs. ***X0h+*** provides search for Bragg planes in crystals under various conditions (Bragg angle, strong reflections…).	**1,262,567**
	***GID_sl*** models X-ray diffraction curves from perfect and strained crystals, as well as multilayers for any Bragg-case diffraction with scans around arbitrary axes.	**724,776**
	***TER_sl*** calculates X-ray specular reflection and respective X-ray standing waves from multilayers with interface roughness.	**150,728**
	***BRL*** models multiple Bragg diffraction of X-rays by perfect crystals including the cases of X-rays grazing along the surface and Bragg angles close to 90°.	**52,007**
	***TRDS_sl*** calculates X-ray diffuse scattering for several models of interface roughness in multilayers.	**22,012**
	***MAG_sl*** calculates X-ray resonant specular reflection from magnetic multilayers with interface roughness and transition layers.	**19,032**

Based on 17 research papers; as of 2016/08/31 served 2,231,122 jobs.

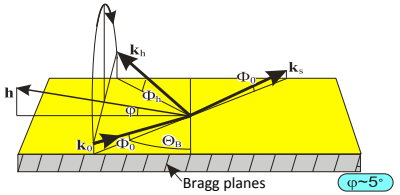
X-Server scope: GID_sl (diffraction)



Grazing incidence diffraction



Extremely asymmetric diffraction



Any non-coplanar diffraction

- Calculates Bragg diffraction from 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 profiles are specified layer-by-layer, which allows for flexibility
- Takes into account specular reflection and refraction of X-rays at crystal surface and interfaces in multilayers
- Works for any Bragg-case geometry and scans around any axis
- **Applications**: X-ray optics (monochromators) and semiconductor material science; examples:
  Stepanov, *et.al.* PRB **57**, 4829 (1998);
  Stepanov & Forrest, J.Appl.Cryst. **41**, 958 (2008);
  Stoupin *et.al.* PRB 86, 054301 (2012)
- **Limitations**: No Laue cases, no bent crystals, no lateral strains, no instrumental convolutions

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

Crystal: GaAs XOh 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 Submit Query (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

```
period=20
t=100 code=GaAs sigma=2
t=70 code=AlAs sigma=2 da/a=a
end period
```

Available codes:

[?] Crystals:

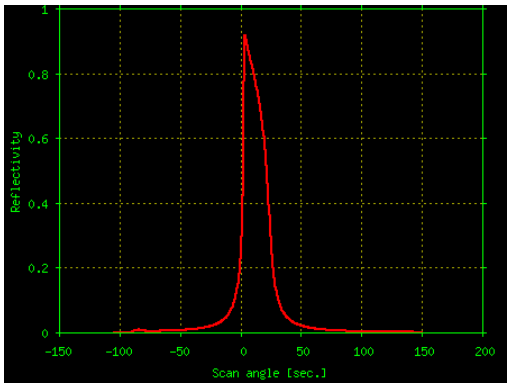
AlAs
AlP
AlSb
AlYO3
BaTiO3
Beril
Beryllium

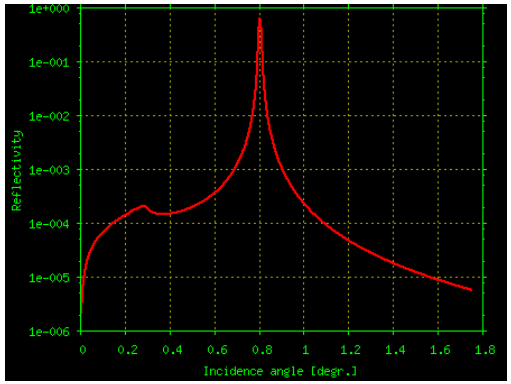
[?] Non-crystals:

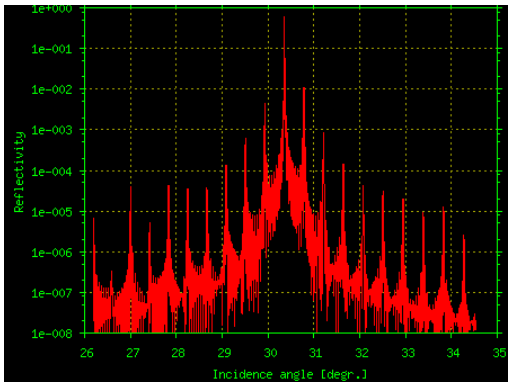
Al2O3
B4C
BeO
BN
Cr2O3
CsI
Fluorite

[?] Elements:

Web input form







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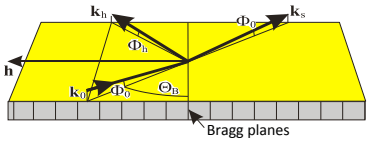
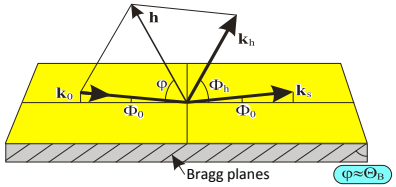
X-Server scope: TER_sl (specular reflection)

GID_SL on the Web

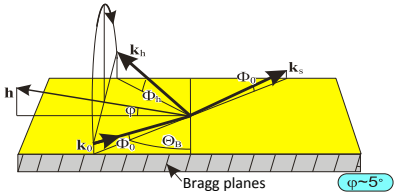
Dynamical x-ray diffraction from strained crystals, multilayers and superlattices at usual and grazing incidence angles



Grazing incidence diffraction



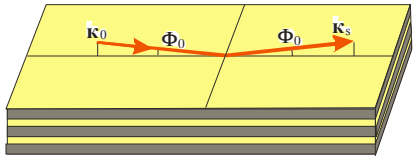
Extremely asymmetric diffraction



Any non-coplanar diffraction

TER_SL on the Web

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



- Calculates X-ray specular reflection from plain mirrors and multilayers with given profiles of electronic density (dielectric susceptibility) $\chi_0(z)$ and interface roughness height $\sigma(z)$ or transition layers.
- Converges faster than the Parratt recursive technique
- Also optionally calculates X-ray standing waves in multilayers
- **Applications**: X-ray optics (mirrors and multilayer mirrors and monochromators) and semiconductor material science
- **Limitations**: no curved mirrors, no instrumental convolutions

X-Server scope: TER_sl

TER_SL on the Web

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

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/cm^3

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!)

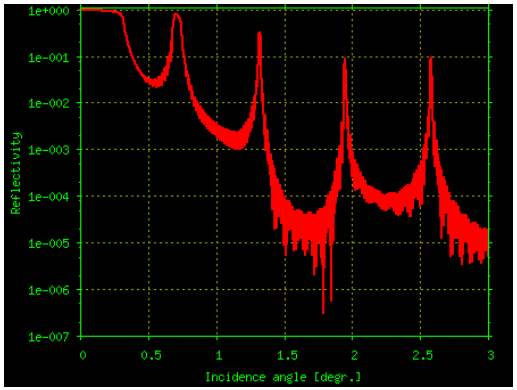
Top layer profile *(optional)*:

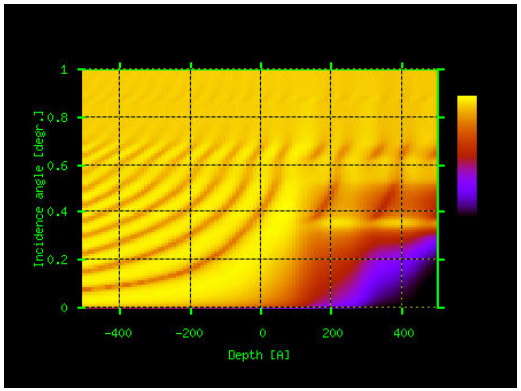
```
t=20 w0=0.5 sigma=5   !surface oxide, organic contamination or dust
period=20
t=100 code=GaAs sigma=4
t=70 code=AlAs sigma=4
end period
```

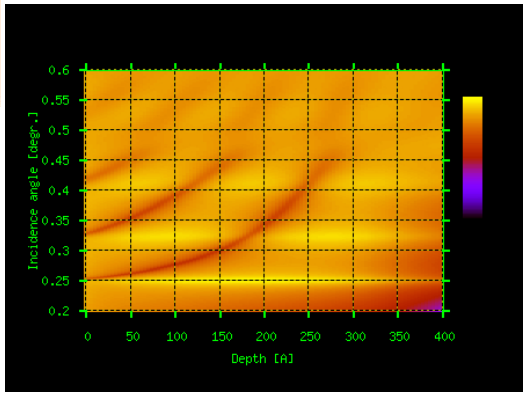
Submit Query (same "Submit" action as above; single click, please!)

Available codes:
(use Copy/Paste)

Ac
Ag
Al
Al2O3
AlAs
AlFe3
AlN
AlP







Web input form

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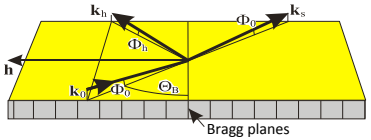
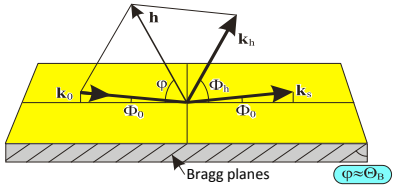
X-Server scope: BRL (multiple diffraction)

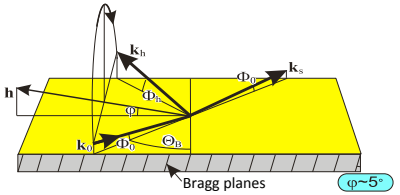
GID_SL on the Web
Dynamical x-ray diffraction from strained crystals, multilayers and superlattices at usual and grazing incidence angles



Grazing incidence diffraction

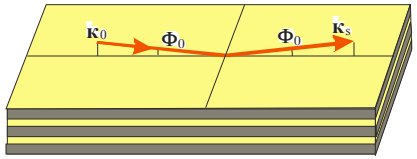


Extremely asymmetric diffraction

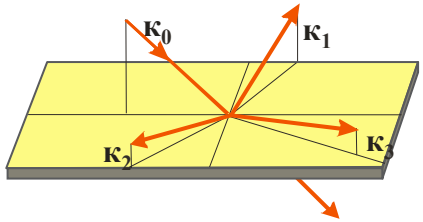


Any non-coplanar diffraction

TER_SL on the Web
X-ray specular reflection from multilayers with rough interfaces at grazing incidence



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



- Calculates multiple Bragg diffraction from perfect plate-shaped crystals including the cases of X-rays grazing along the surface and Bragg angles close to 90° [Stepanov & Ulyanenkov, Acta Cryst. **A50**, 579 (1994)].
- Takes into account specular reflection and refraction of X-rays at crystal surface for grazing X-rays *only*.
- Helps to find multiple diffraction configurations and carry 2D Bragg scans around arbitrary axes
- **Applications**: X-ray optics (multiple diffraction effects including polarization glitches in X-ray monochromators); examples: Sutter, *et.al.* J.Appl.Cryst. **49**, 1209 (2016).
- **Limitations**: may loose precision for thick crystal plates, no instrumental convolutions, no lattice strains or curved crystals.

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X-Server scope: BRL

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

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 →

Web input forms

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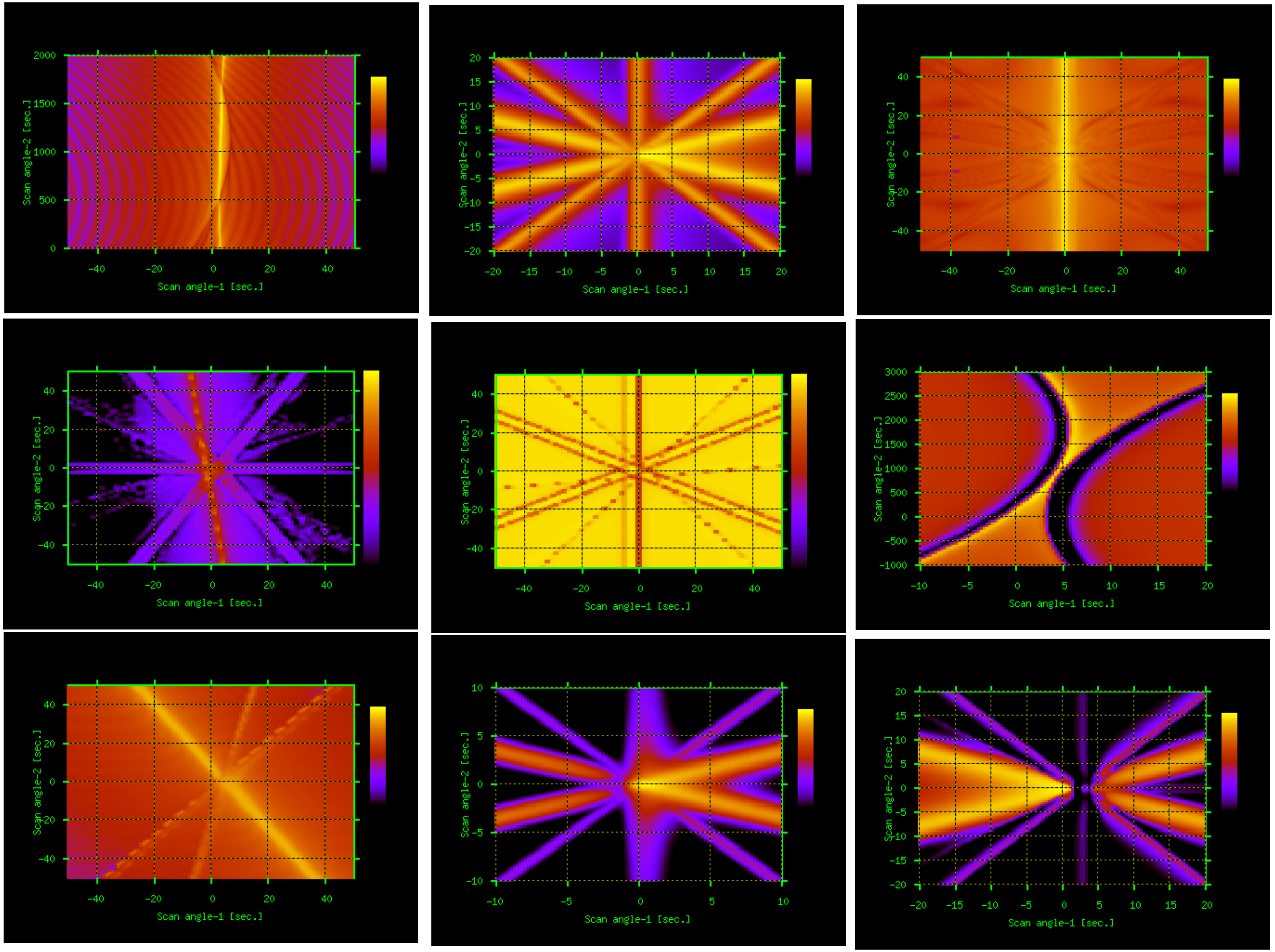
BRL on the Web
X-ray multiple Bragg/Laue diffraction

X-Server scope: BRL



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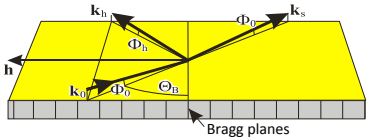
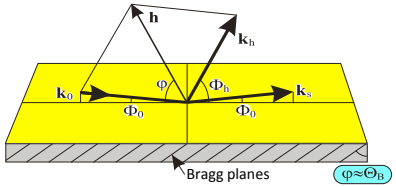
X-Server scope: TRDS_sl (roughness scattering)

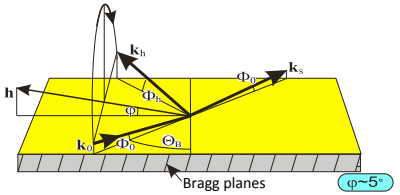
GID_SL on the Web
Dynamical x-ray diffraction from strained crystals, multilayers and superlattices at usual and grazing incidence angles



Grazing incidence diffraction

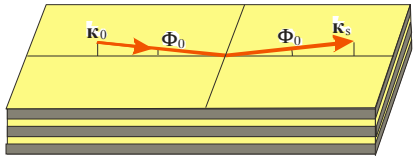


Extremely asymmetric diffraction

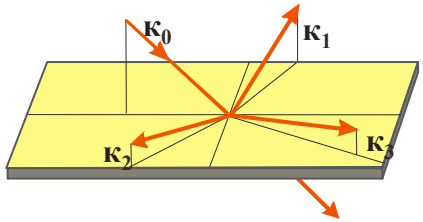


Any non-coplanar diffraction

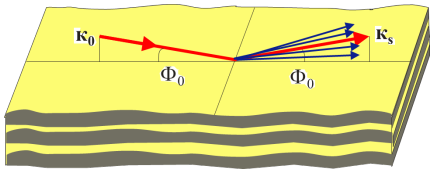
TER_SL on the Web
X-ray specular reflection from multilayers with rough interfaces at grazing incidence



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



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



- Calculates X-ray diffuse scattering from interface roughness in multilayers [Kaganer, Stepanov & Koehler, PRB. **52**, 16369 (1995)].
- Implements modeling for 10 different types of roughness correlations between the layers.
- **Applications**: X-ray optics (X-ray mirrors and multilayer mirrors quality evaluation) and semiconductor material science.

X-Server scope: TRDS_sl

TRDS_SL on the Web

X-ray diffuse scattering at grazing incidence from surface and interface roughness

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/cm^3

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/A

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. A vertical correlation length= A jaggedness= 1.

angle of skew transfer= 0. degr.

Models:	
	Uncorrelated roughness
	Completely correlated roughness
	Ming's model
	Lagally's model — lateral size of vertically correlated roughness= A
	Holy's model
	Spiller's model (*very slow!*)
	Data for all Pukite's models: — miscut angle= degr. Add affine roughness
	Classic Pukite's model
	Smoothed Pukite's model — effective rms height of steps= A
	Pershan's model — terraces size spread= A

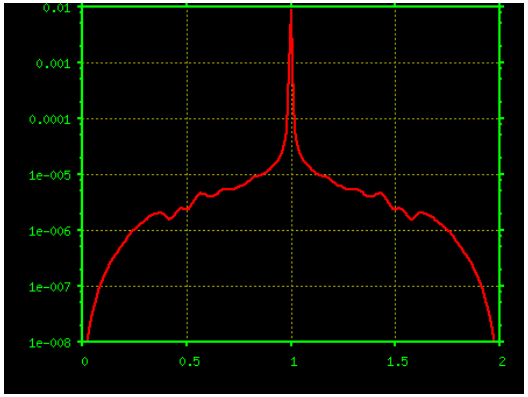
watch progress Submit Query (single click, please!)

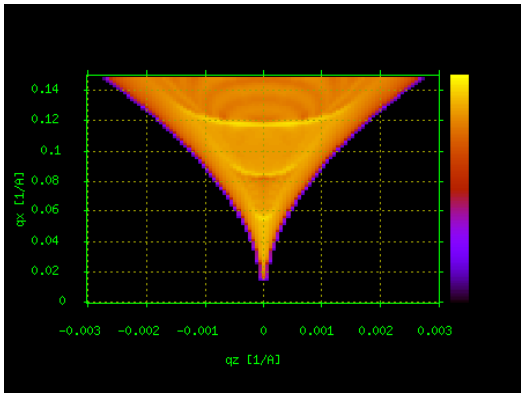
Top layer profile *(optional)*:

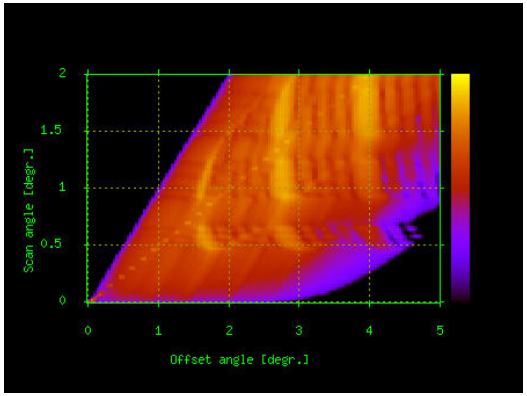
period=
t= sigma= tr= code= rho= x= code2= x2= code3= x3= code4= x0= w0=
end period

Available codes: (use Copy/Paste)

Ac
Ag
Al
Al2O3







Web input form

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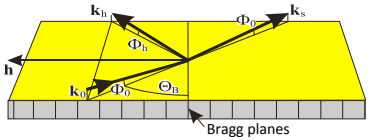
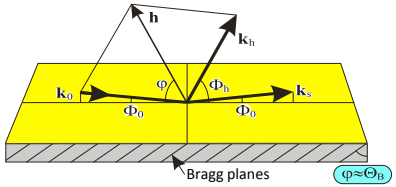
X-Server: MAG_sl (resonance magnetic scattering)

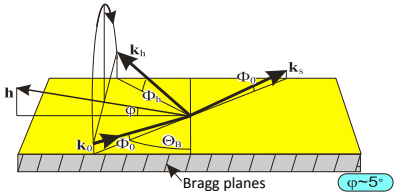
GID_SL on the Web
Dynamical x-ray diffraction from strained crystals, multilayers and superlattices at usual and grazing incidence angles



Grazing incidence diffraction

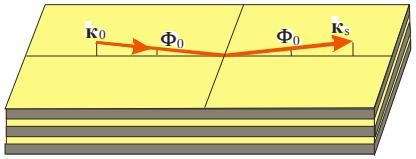


Extremely asymmetric diffraction

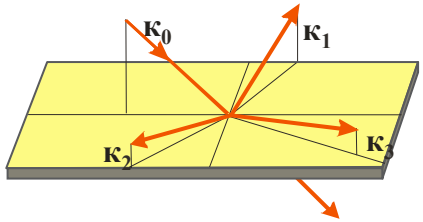


Any non-coplanar diffraction

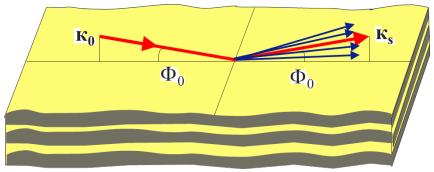
TER_SL on the Web
X-ray specular reflection from multilayers with rough interfaces at grazing incidence



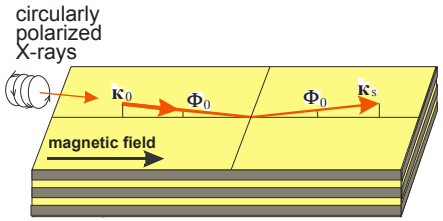
BRL on the Web
X-ray multiple Bragg/Laue diffraction



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



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



Calculates resonant X-ray reflectivity from magnetic multilayers [Stepanov & Sinha, PRB. **61**, 16369 (2000)].

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X-Server: MAG_sl

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

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

Polarization: 4. Circular - angle to Sigma-plane for Option-3 0.

Substrate: Database code: Silicon X0h data (5-25keV; 0.5-2.5A)

Chemical formula: rho= g/cm^3

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 = 0. Angstrom **OR** Transition layer tr = 0. Angstrom

Magnetic atoms share (0.--1.) / density (1/cm^3): 0.

Magnetic orientation X = 0 Y = 0 Z = 0

Magnetic amplitudes F10 = 0., 0. F11 = 0., 0. F1T = 0., 0.

Scan (incidence angle or qz): from 0. to 4. degr. Scan points= 4001

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

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=
                  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
```

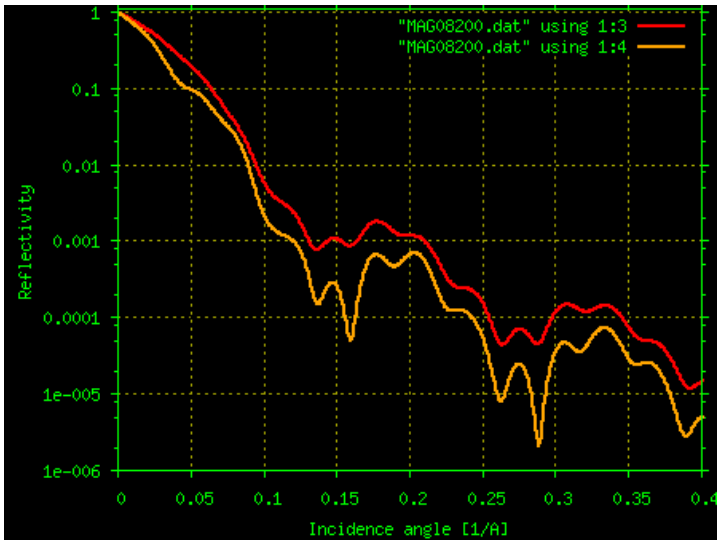
Submit Query (same "Submit" action as above; single click, please!)

Available codes: (use Copy/Paste)

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

More details

Web input form



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

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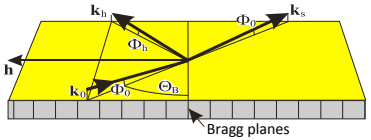
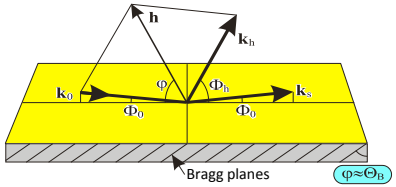
X-Server scope: X0h (structure factors)

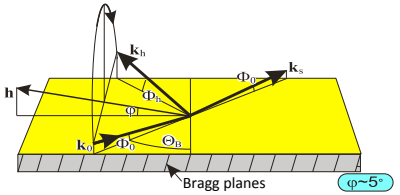
GID_SL on the Web
Dynamical x-ray diffraction from strained crystals, multilayers and superlattices at usual and grazing incidence angles



Grazing incidence diffraction

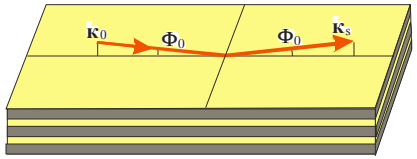


Extremely asymmetric diffraction

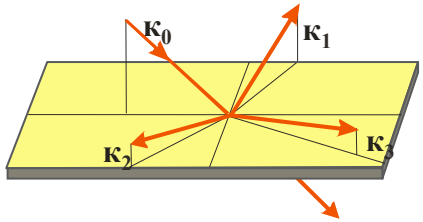


Any non-coplanar diffraction

TER_SL on the Web
X-ray specular reflection from multilayers with rough interfaces at grazing incidence



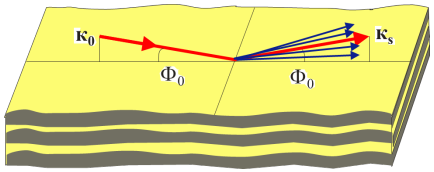
BRL on the Web
X-ray multiple Bragg/Laue diffraction



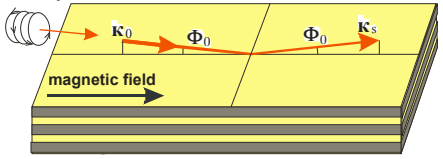
χ_{0h} on the Web !!!

- Provides X-ray scattering factors for all X-Server programs.
- Interpolates data of three different tables with option to compare.

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



circularly polarized X-rays



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

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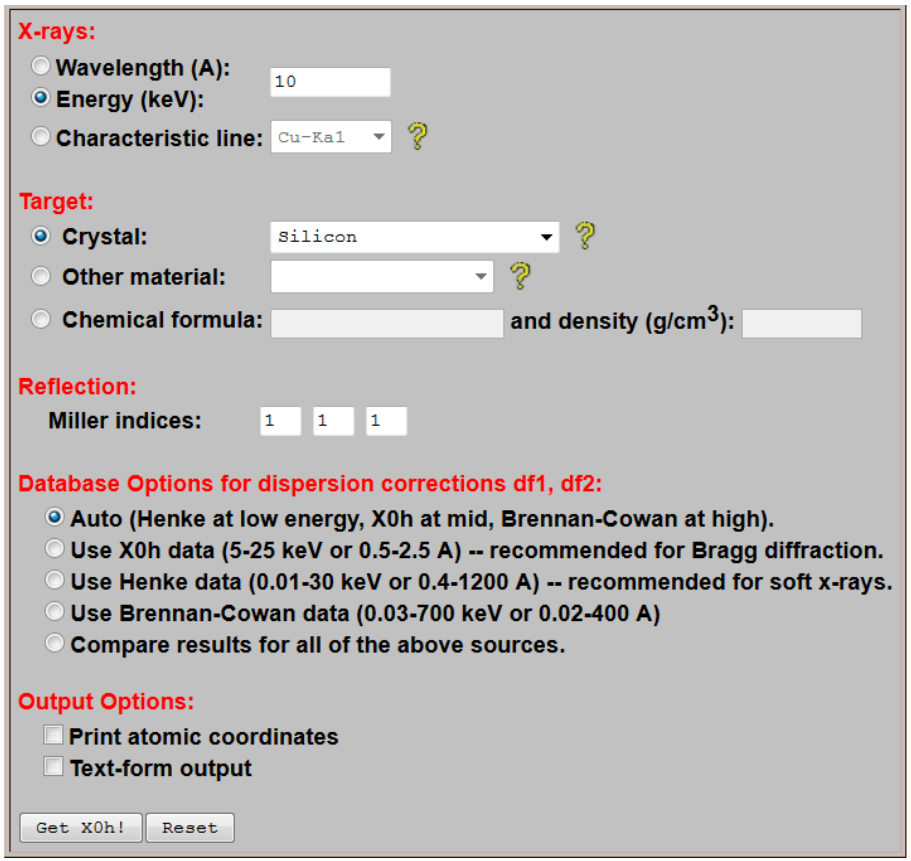
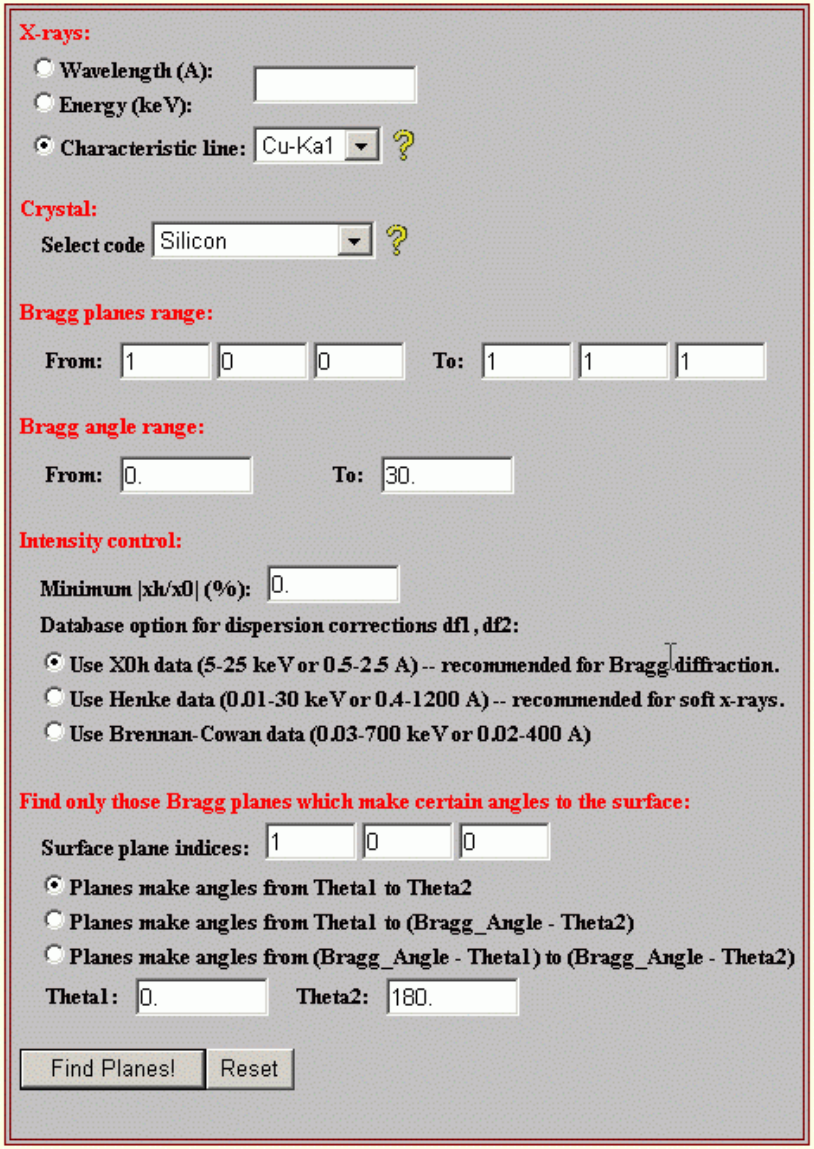
X-Server scope: X0h





Web input forms

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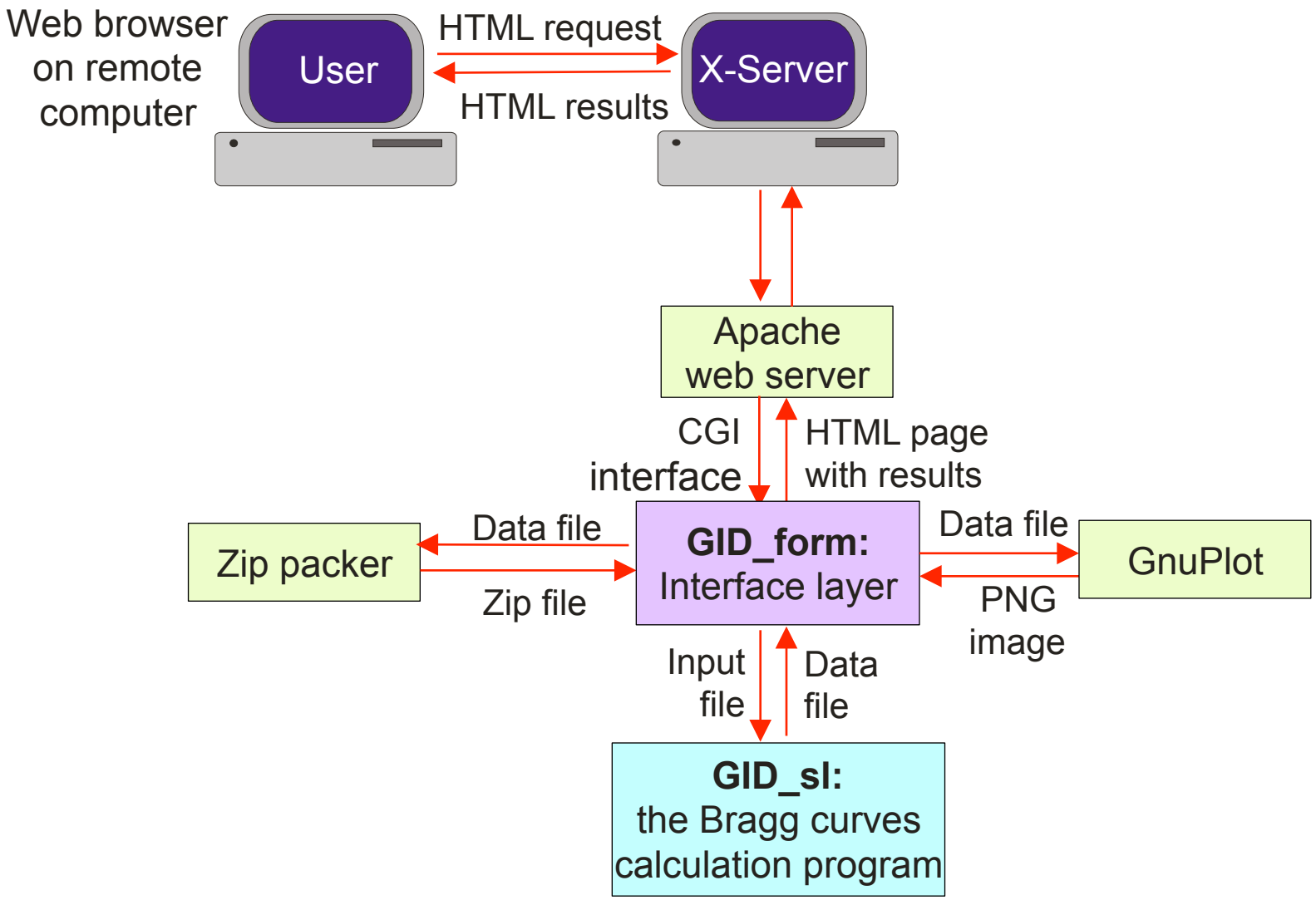
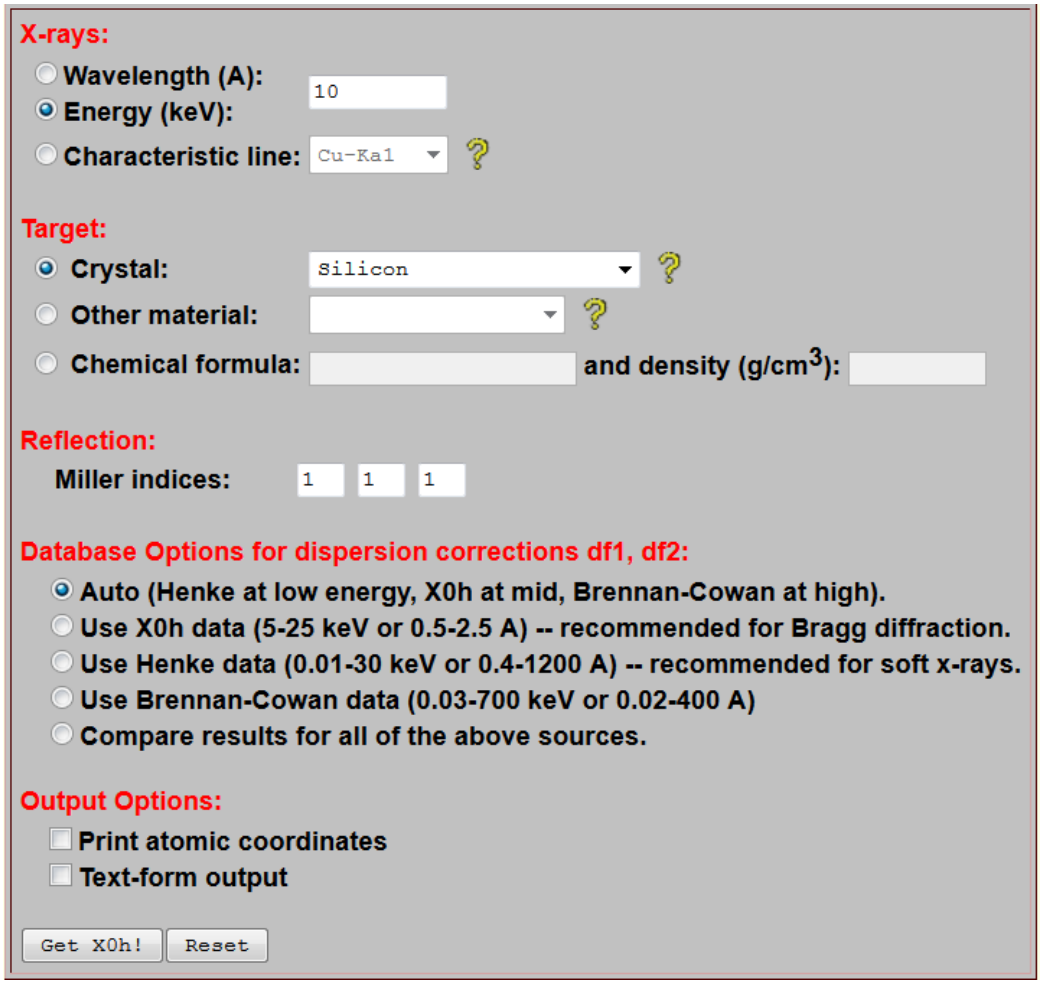
How X-Server works



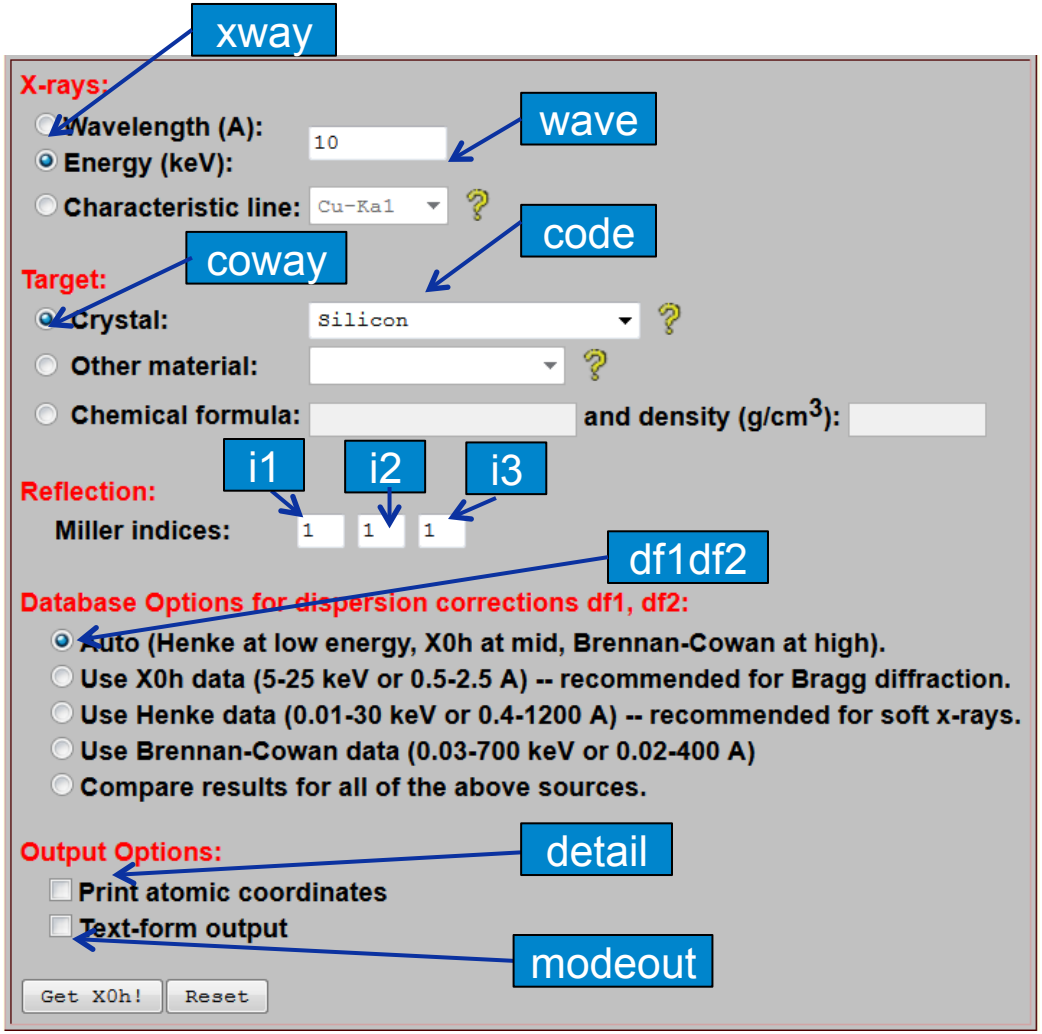
Server access is not limited to web browsers



This is a web browser form of X0h.

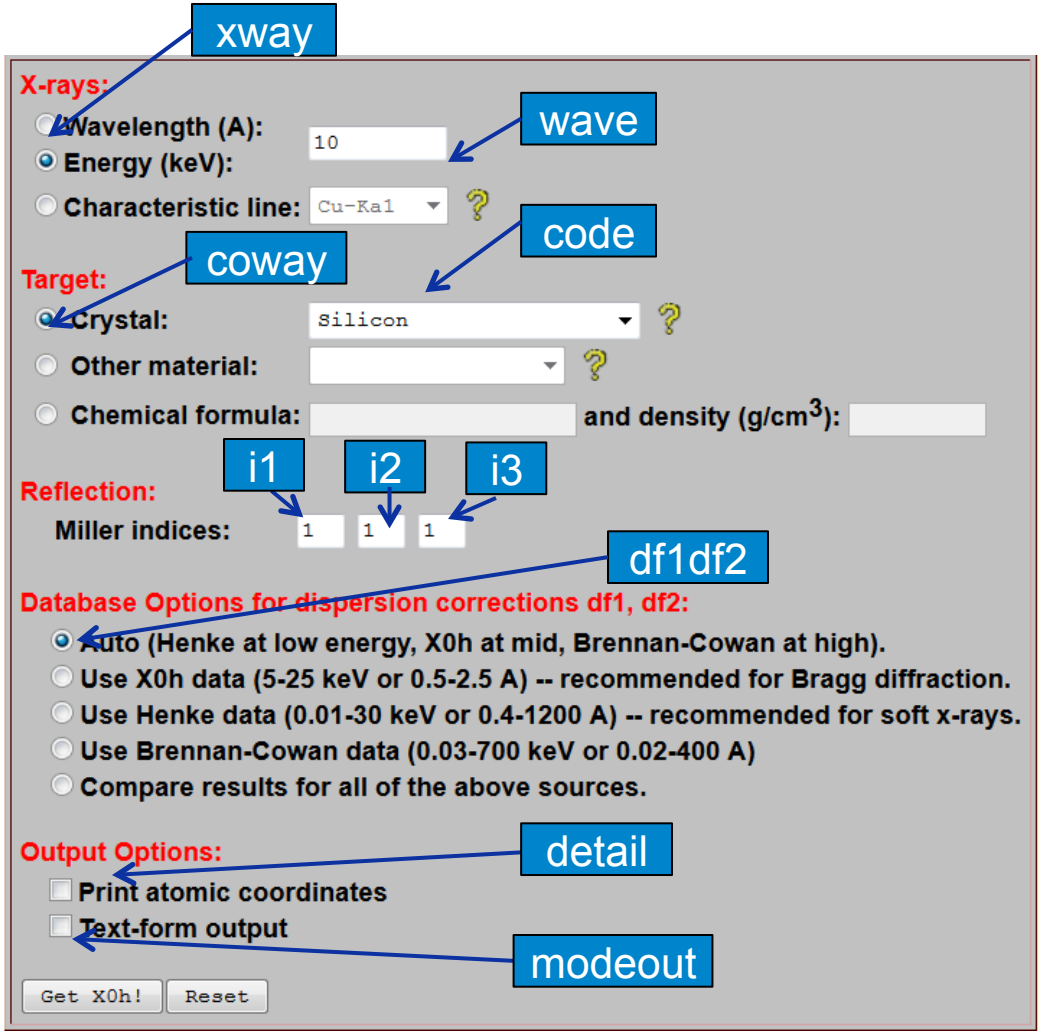
What happens when one clicks the "Get X0h!" button?

Server access is not limited to web browsers



Behind each input on the web browser form there is a named parameter which the browser sends to X-Server upon clicking the "Get X0h!" button.

Server access is not limited to web browsers



Then, one can simply use curl or other command-line program to submit the request:

curl http://x-server.gmca.aps.anl.gov/cgi/x0h_form.exe?**xway**=2\&**wave**=10\&**coway**=0\&**code**=Silicon\&**i1**=1\&**i2**=1\&**i3**=1 > results.file

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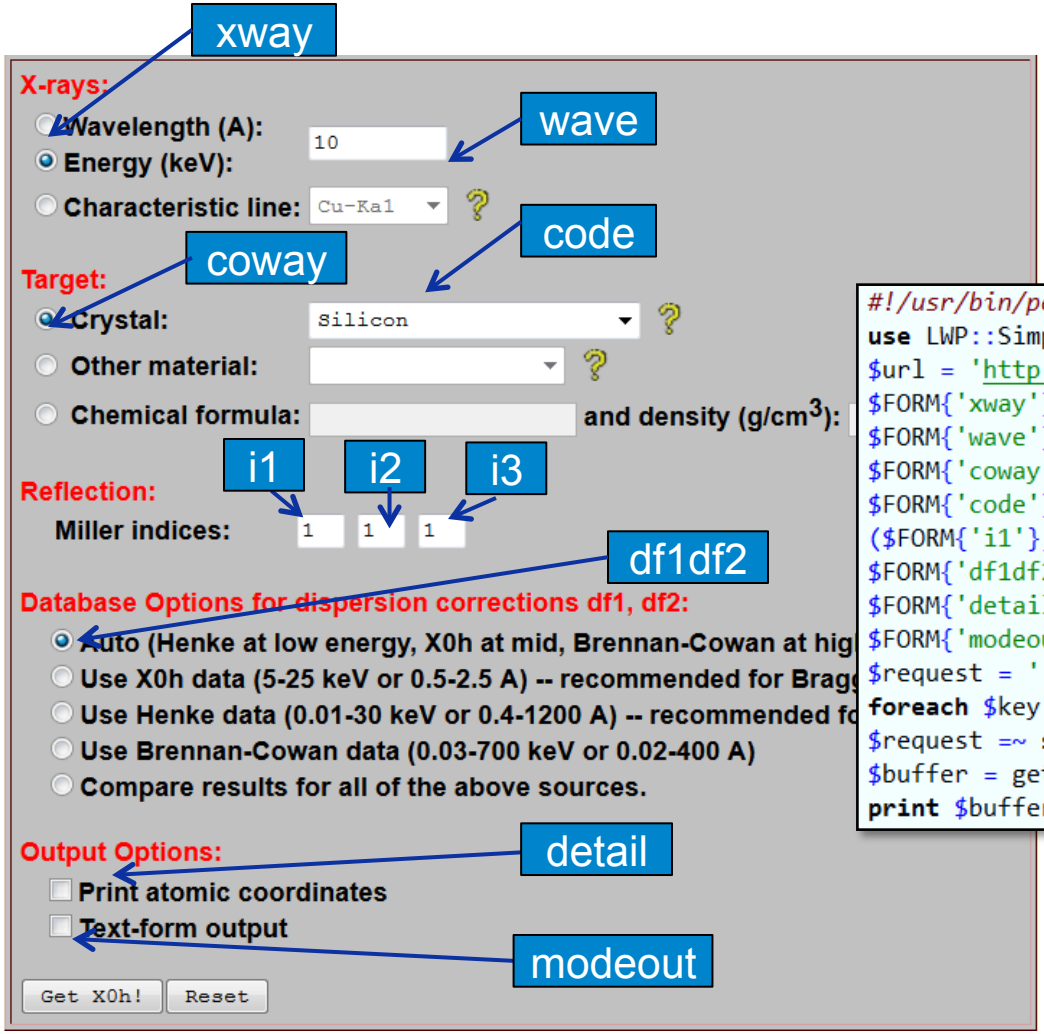
Server access is not limited to web browsers



One can also do the same type of call from almost any scripting or programming language:

```perl
#!/usr/bin/perl
use LWP::Simple;
$url = 'http://x-server.gmca.aps.anl.gov/cgi/x0h_form.exe';
$FORM{'xway'} = 2;
$FORM{'wave'} = 10;
$FORM{'coway'} = 0;
$FORM{'code'} = 'Silicon';
($FORM{'i1'},$FORM{'i2'},$FORM{'i3'}) = (1, 1, 1);
$FORM{'df1df2'} = -1;
$FORM{'detail'}  = 0;
$FORM{'modeout'} = 1;
$request = '';
foreach $key (keys %FORM) {$request .= '&'.$key.'='.$FORM{$key};}
$request =~ s/^\&/\?/;
$buffer = get($url.$request);
print $buffer;
```

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Downloadable examples of X-Server access scripts

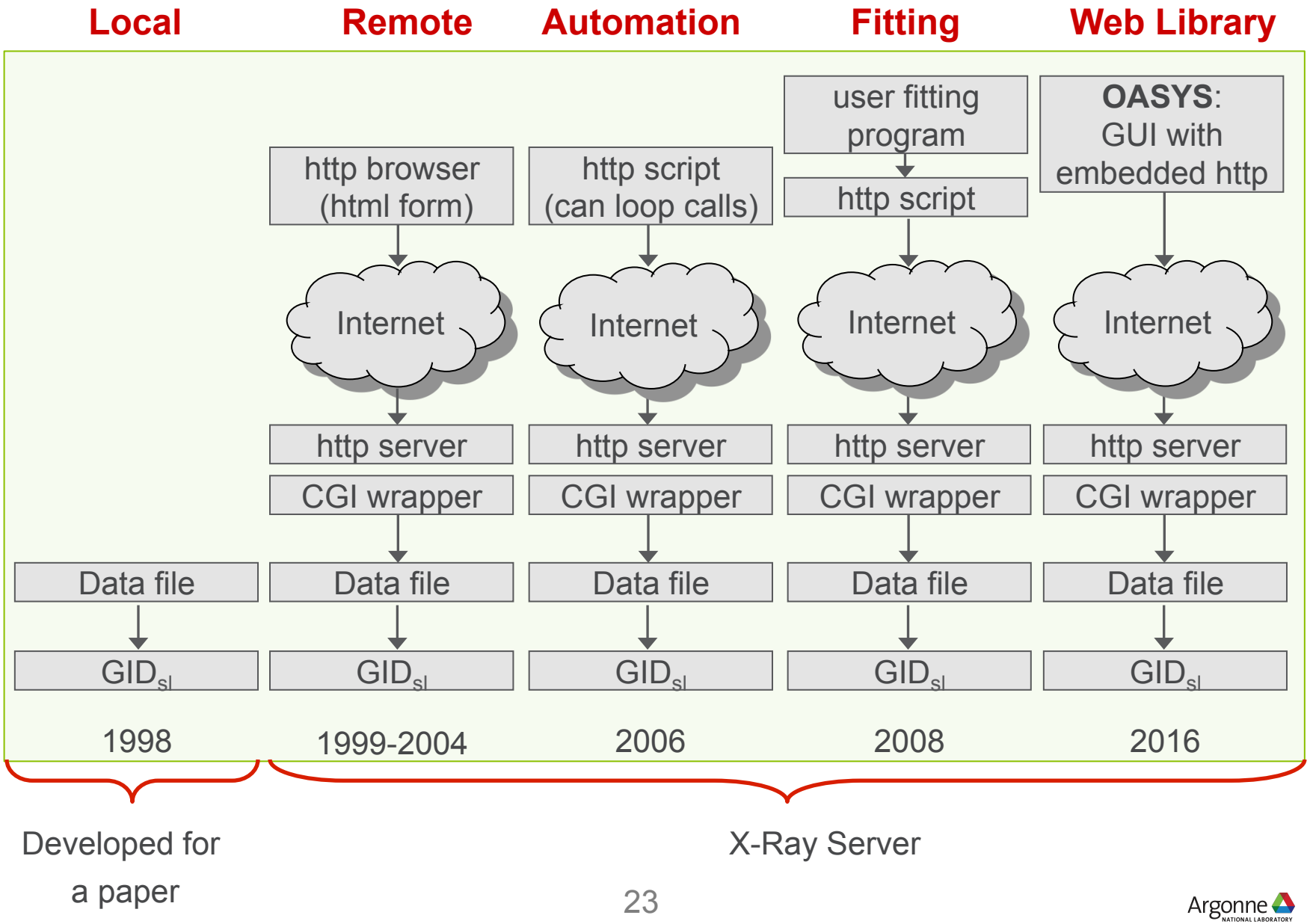
http://x-server.gmca.aps.anl.gov/automation.html

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)

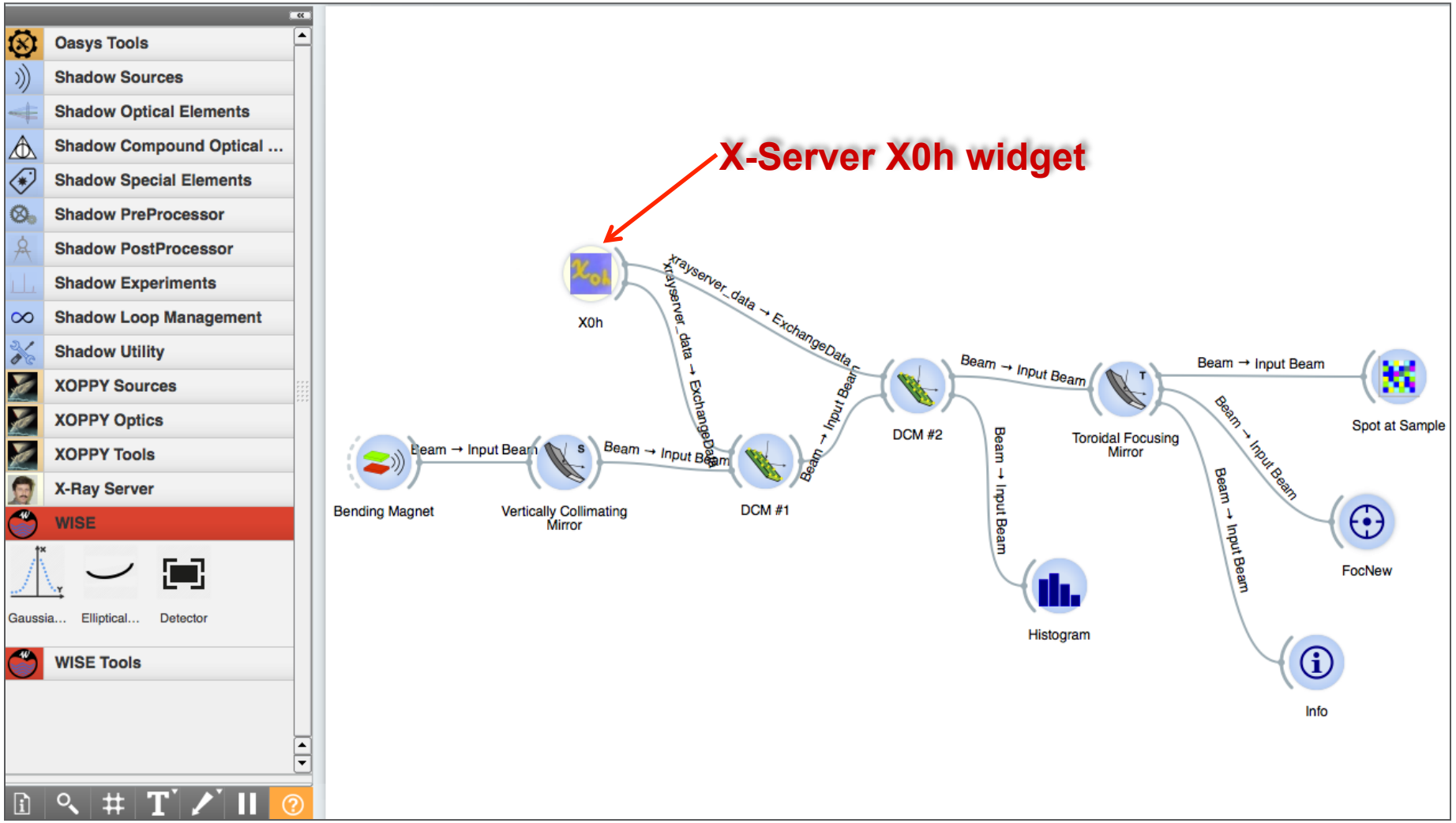
The scripts can be called from user's software written in any language using the **system** function. If one needs to vary a parameter, it can be passed to the script as a command line argument.

These scripts present a practical example of client software accessing the server programs. They are simple, but they **should be simple** to become useful since they address a wide auditory of physicists presumably unexperienced in web interfaces.

X-Server access evolution



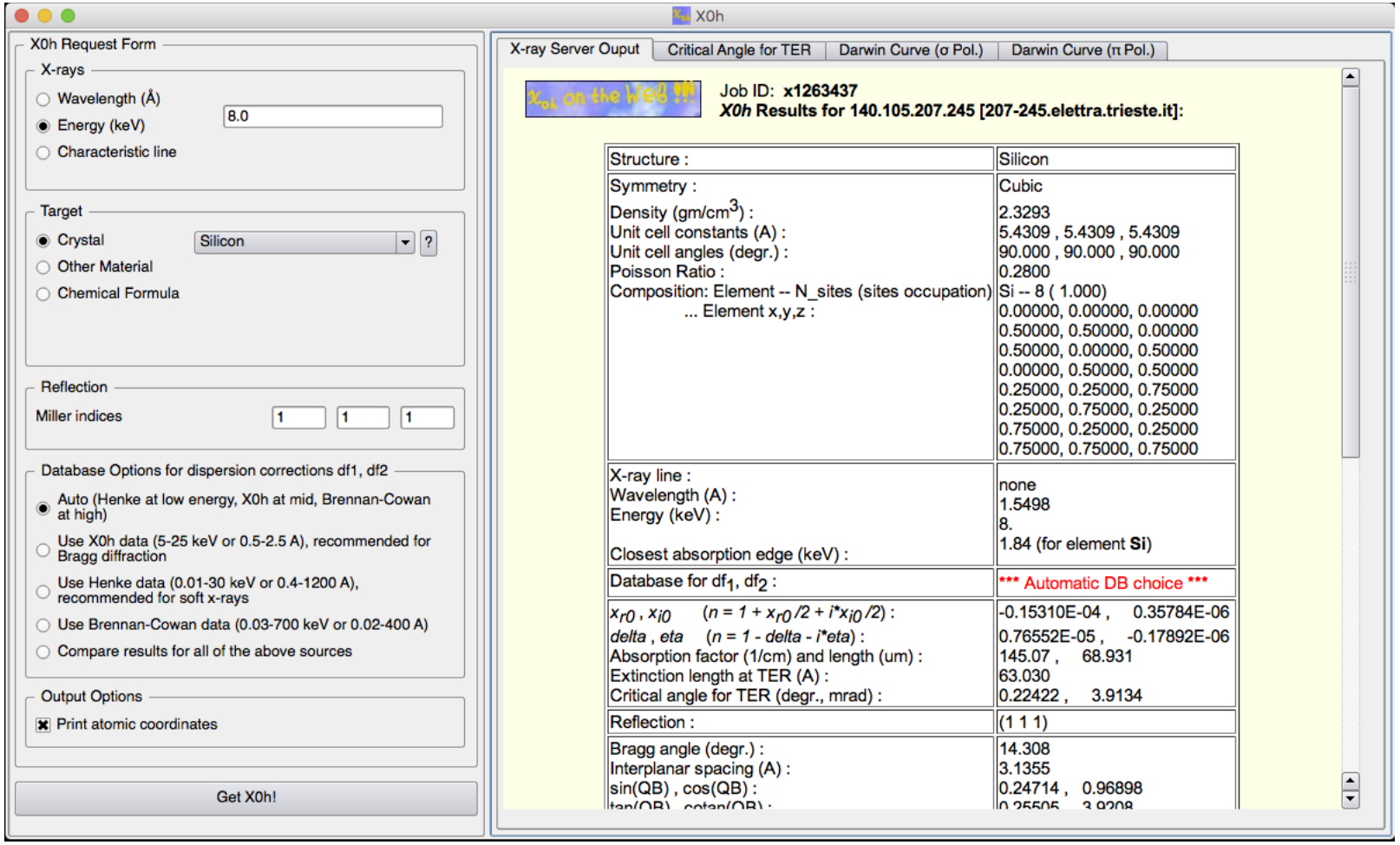
OASYS: new level of interaction with X-Server



X-Server access is embedded into Oasys and user does not need to do any programming; just add the X-Server widgets.

Courtesy: Dr. Luca Rebuffi

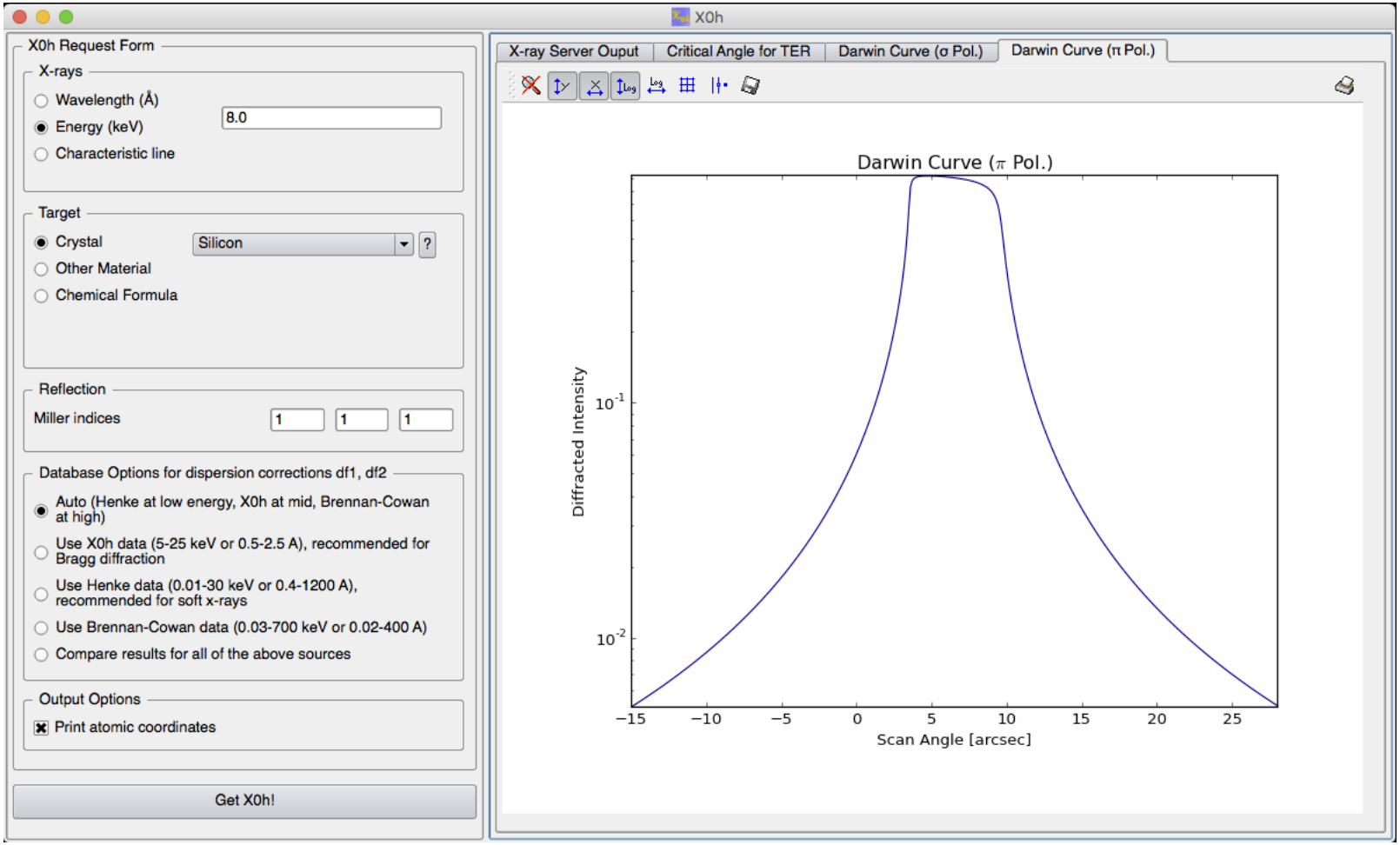
OASYS: new level of interaction with X-Server



Once the widget is added to the Oasys diagram, it allows to retrieve the structure factors …

Courtesy: Dr. Luca Rebuffi

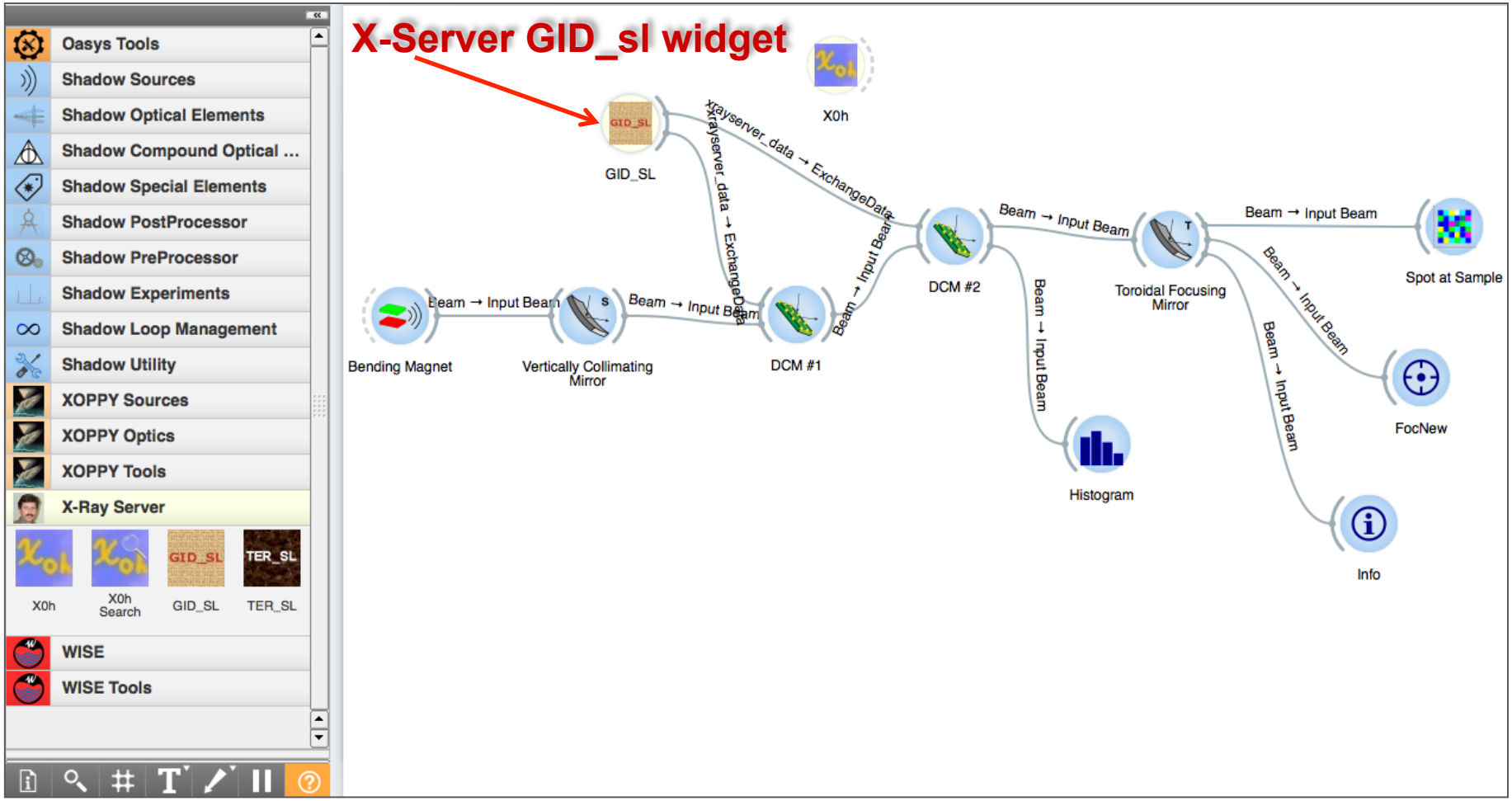
OASYS: new level of interaction with X-Server



… and associated Darwin curves for σ- and π- X-ray polarizations

Courtesy: Dr. Luca Rebuffi

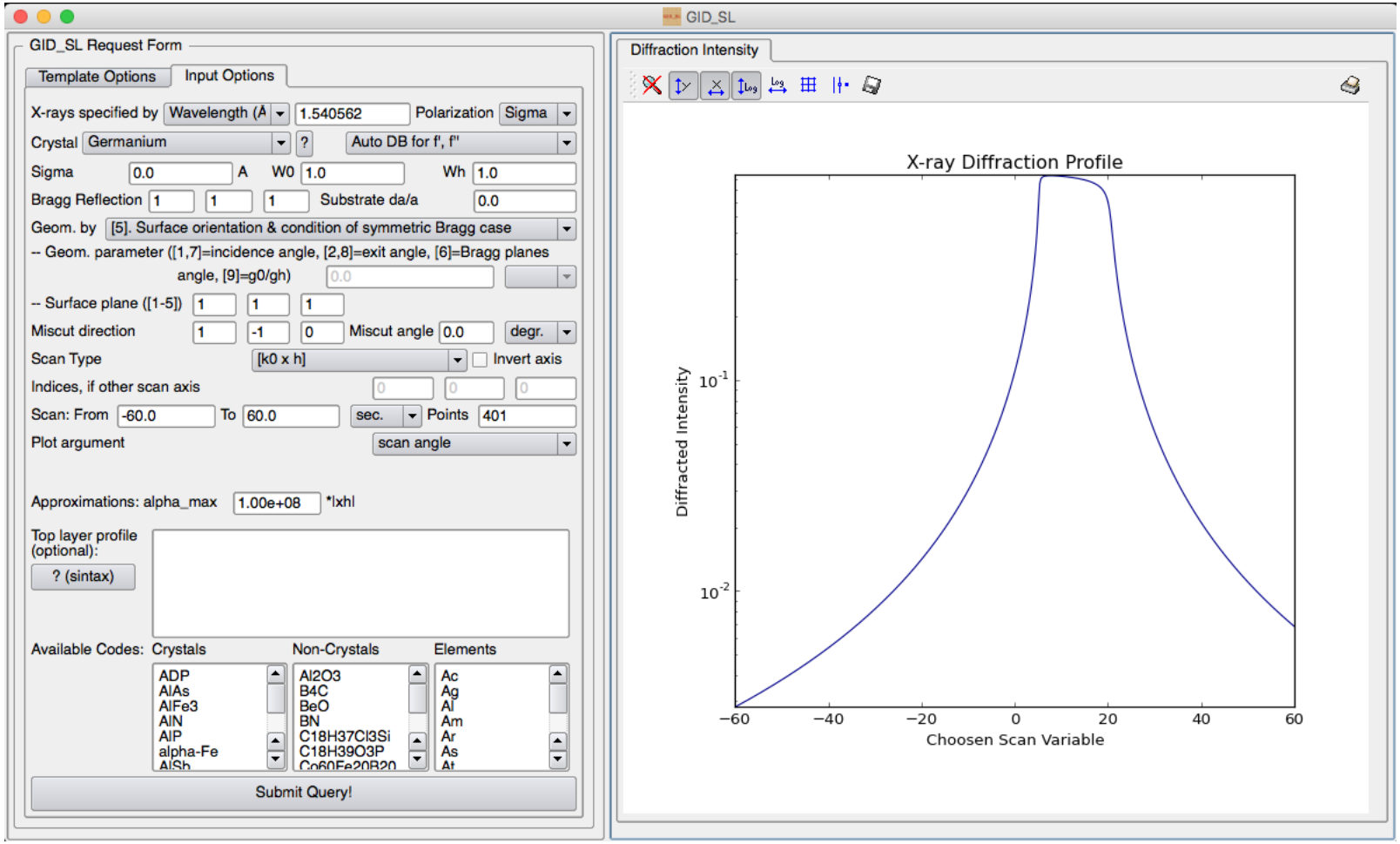
OASYS: new level of interaction with X-Server



Same way one can include the GID_sl and TER_sl widgets

Courtesy: Dr. Luca Rebuffi

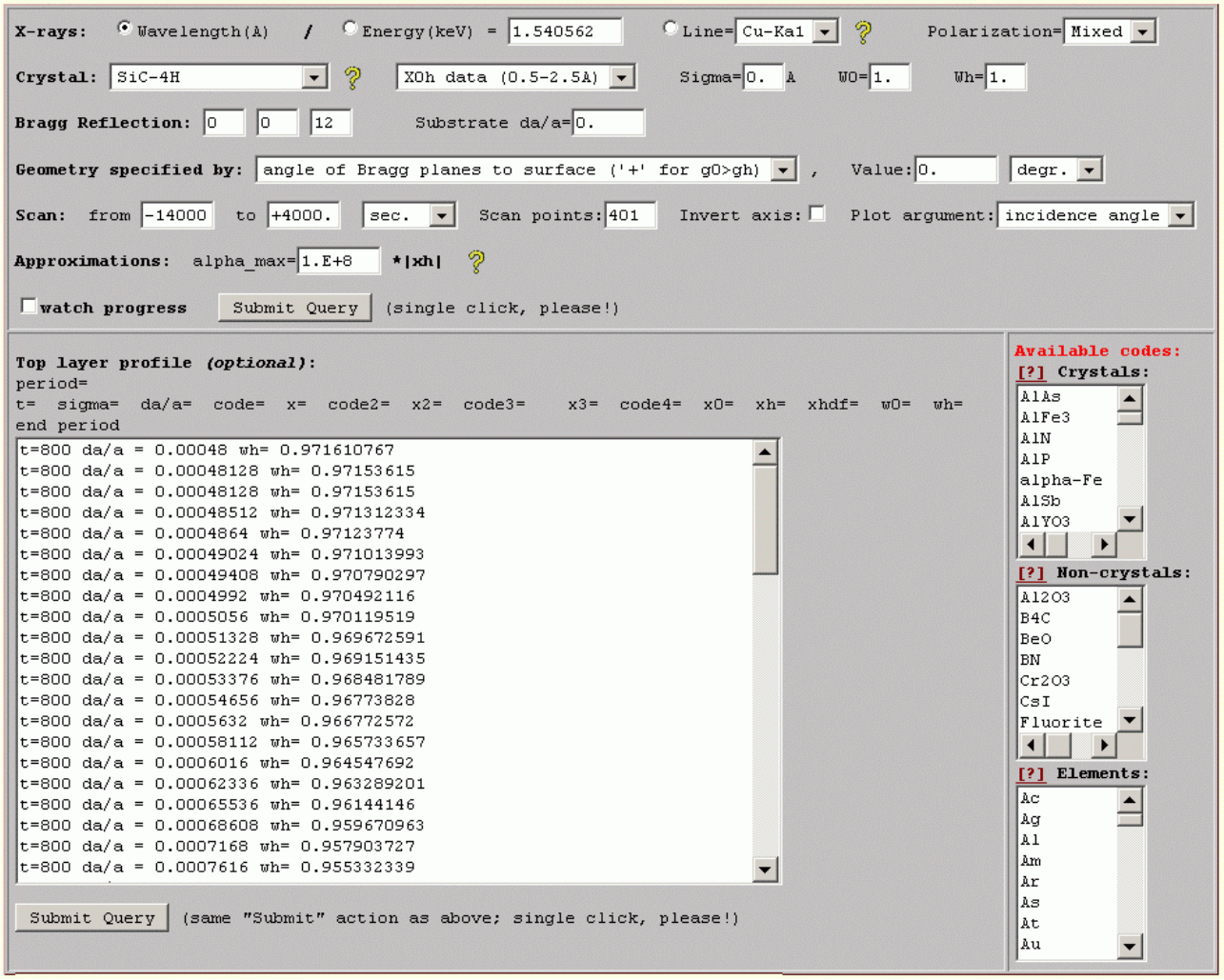
OASYS: new level of interaction with X-Server



… and fetch their data. Note that the surface layer profile can be entered too

Courtesy: Dr. Luca Rebuffi

Why no server-side data fitting & instrument convolution?



Providing Server-side fitting for all cases is non-practical: Too many parameters!

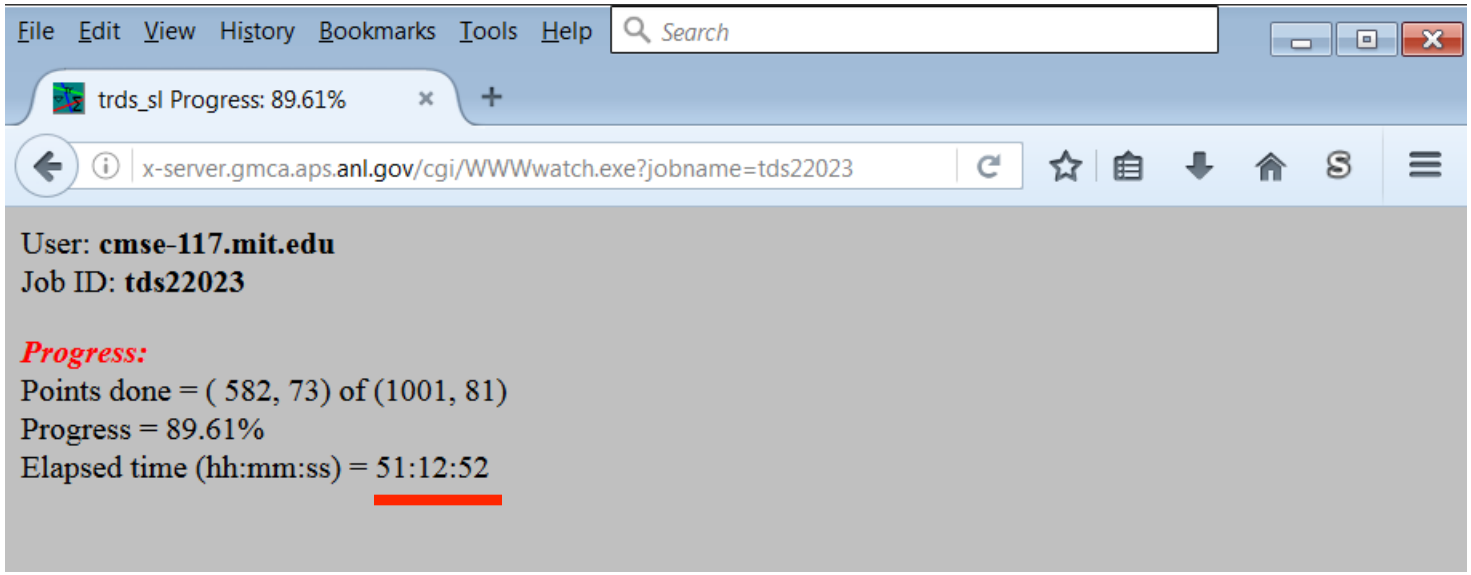
The form at the left is a typical material science application submitted from univ-poitiers.fr. The profile contains 72 lines, i.e. more than 200 parameters.

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

Suggested solution: the Server programs can be used as a library providing Bragg or reflection curves to user's software doing fitting or instrument convolution.

Server overhead & handling of lengthy calculations

- The Server overhead was studied by Stepanov & Forrest, [J. Appl. Cryst. 41, 958 (2008] where X-ray Bragg reflection profiles from superlattices were fitted with the help of X-Server. The observed overhead was 2.9s per request, which in that case corresponded to less than 10%, but the percentage could be less or more depending on the duration of calculation.
- Most of the Server programs return results within several minutes or less. The only exception could be TRDS_sl where the length of calculations is proportional to the 4th power of the number of interfaces. When user submits a job, he can check the "**watch progress**" option. Then, the job ID is returned immediately and user can disconnect and come back later to check the progress and download the results:



Current restrictions & further plans

- GID_sl currently accounts for specular reflection of X-rays in all cases. It needs to do it for grazing X-rays only, which will result in up to 4x faster and digitally more stable calculations.
- GID_sl can be supplied with the printout of X-ray standing waves.
- TER_sl needs to be supplied with energy scans.
- BRL needs an update to the recursion matrix algorithm similar to that used in the other programs for more stable operation on thick crystals.
- Automatic submission of crystal structures is considered, but still questionable. Currently new structures can be added per users submissions (a template is provided at http://x-server.gmca.aps.anl.gov/structure_submission_example.txt). Then, I verify them with the space group generator and typically add to the X0h DB within a day. Unfortunately, the rate of mistakes in users submissions is very high and supplying the user community with mistaken structures does not look as a good idea. Most of calculations can be done by directly specifying the structure factors and thus bypassing the X0h DB, which is simply a convenience.

Conclusions

- We have a well refined resource for the calculations of X-ray dynamical diffraction, specular reflection and diffuse scattering with almost 20 years of online history.
- The main applications are X-ray optics and X-ray material science.
- To get most of this resource, e.g. implement data fitting, one needs to use tools beyond web browser.
- Examples are provided to write such tools on your own, but for some tasks one can use already developed tools like Oasys (to be released soon).
- Users are welcome to share the tools they developed: these tools can be hosted on the server for the benefit of the whole community – same way as any user-submitted structures are available to everyone using the server.

Acknowledgements

X-Ray Server is hosted on a computer of the GM/CA@APS at Argonne National Laboratory. GM/CA@APS has been funded in whole or in part with Federal funds from the National Cancer Institute (ACB-12002) and the National Institute of General Medical Sciences (AGM-12006).

I would like to personally thank the SOS Workshop organizers Dr. Luca Rebuffi, Dr. Marco Zangrando and Dr. Manuel Sanchez del Rio for inviting me to give this presentation.

I also thank many X-Ray Server users for providing their valuable feedback and suggestions and for submitting new structures.