X-RAY SERVER: AN ONLINE RESOURCE FOR SIMULATIONS OF X-RAY DIFFRACTION AND SCATTERING

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This is a status report on the X-ray Server that has been operational at the APS since 1997 and performed more than 80,000 numerical x-ray experiments. X-ray Server is a non-commercial project with the goal to explore novel technologies for establishing scientific collaborations, sharing personal research results, and refining scientific software. The server provides Web-based access to a number of programs developed by the Author for simulating x-ray diffraction and scattering. Unlike similar XOP project by ESRF/APS the software is not shared, but operates directly on the Server. This philosophy brings numerous benefits to both the developer and the users. Currently seven programs are operational. They provide the calculations of:

1. The Bragg curves from strained crystals and multilayers,
2. The specular reflectivity curves from multilayers with interface roughness,
3. The diffuse scattering patterns from correlated interface roughness in multilayers,
4. The resonant x-ray specular reflection from magnetic multilayers,
5. The multiple Bragg diffraction of x-rays in arbitrary diffraction geometries,
6. The dispersion corrections and scattering factors for various materials in the x-rays range,
7. The orientations of the Bragg planes in crystals satisfying given conditions.

The programs (4) and (5) were added in the last year and more additions are on the way.

http://sergey.gmca.aps.anl.gov

X-RAY SERVER

This site has been online since 1997 and has served 81372 x-ray jobs

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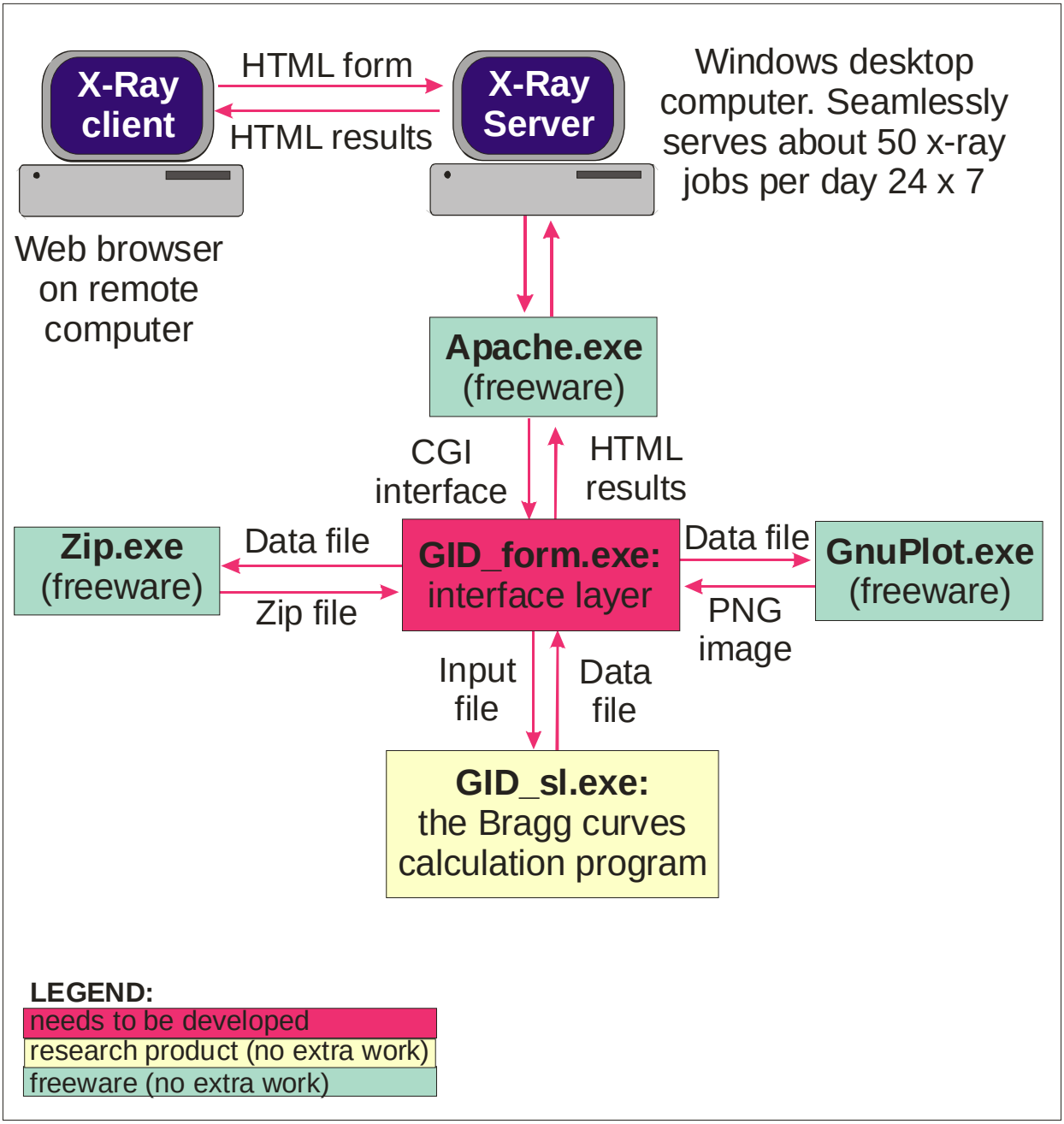
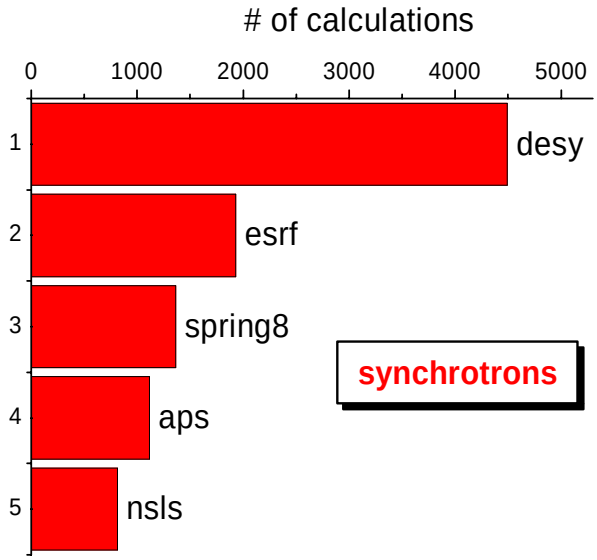
χ_{0h} on the Web !!! χ_{0h} search	***X0h* on the Web** interpolates dielectric susceptibilities χ_0 and χ_h for some crystals and other materials in wide range of x-ray wavelengths with the option to compare the data from different databases [12]. ***X0h-search*** is based on ***X0h*** and it provides tool to search for Bragg planes under various conditions.	39650 jobs
GID_SL on the Web Dynamical x-ray diffraction from strained crystals, multilayers and superlattices at usual and grazing incidence angles	***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 can be used for usual symmetric and asymmetric diffraction, for extremely asymmetric diffraction, as well as for grazing incidence and other non-coplanar cases [16], [19], [20], [21], [31].	20451 jobs
TER_SL on the Web X-ray specular reflection from multilayers with rough interfaces at grazing incidence	***TER_SL* on the Web** calculates x-ray specular reflection from multilayers with interface roughness and transition layers [31], [20].	9011 jobs
TRDS_SL on the Web X-ray diffuse scattering at grazing incidence from surface and interface roughness	***TRDS_SL* on the Web** calculates x-ray diffuse scattering from interface roughness. It implements several different models of roughness and can calculate such effects as skew roughness transfer, dependence of interface-interface roughness correlations on lateral size of roughness and x-ray scattering from atomic steps [23], [24], [26], [29], [32].	4307 jobs
MAG_SL on the Web X-ray resonant specular reflection from magnetic multilayers	***MAG_SL* on the Web** calculates x-ray resonant specular reflection from magnetic multilayers with interface roughness and transition layers [33]. ***NEW, added 07/2003***	7589 jobs
BRL on the Web X-ray multiple Bragg/Laue diffraction	***BRL* on the Web** calculates multiple Bragg diffraction of x-rays by perfect crystals. Can simulate up to 12-wave dynamical Bragg diffraction of x-rays from a plate-shaped crystal including the cases of x-ray waves grazing along the plate surface and Bragg angles being close to 90° [18], [17], [11]. ***NEW, added 07/2003***	364 jobs

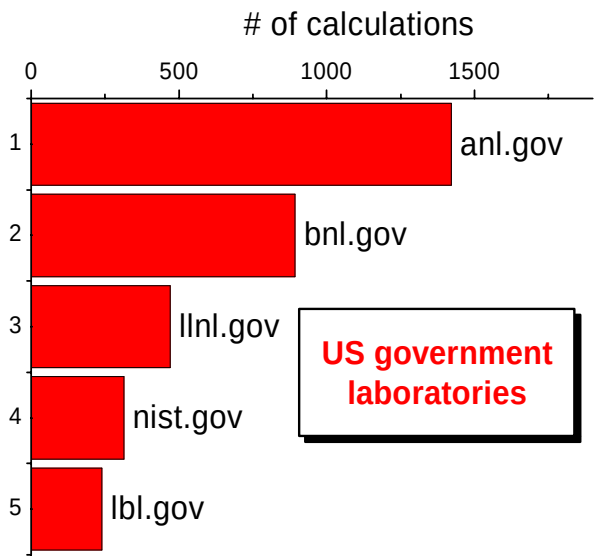
X-Ray Server Technology

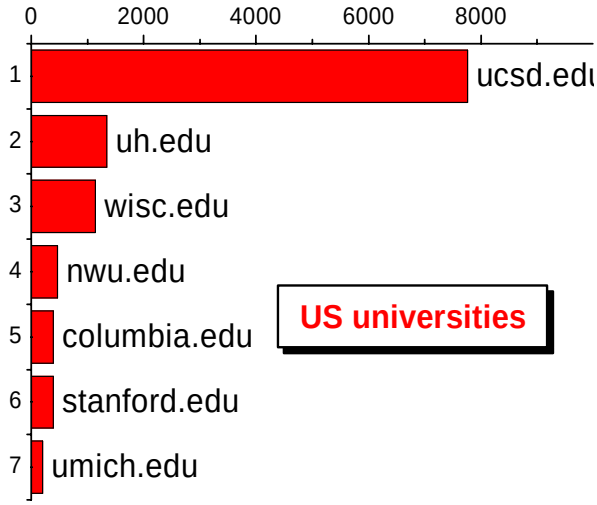


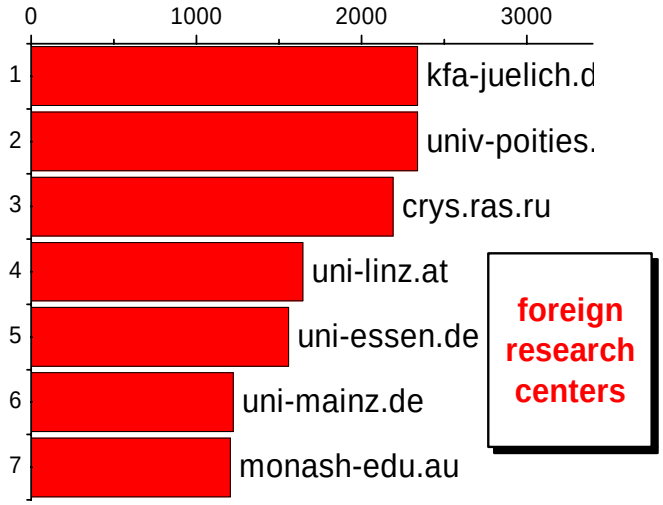
Statistics of X-Ray Server usage as of May 2, 2004

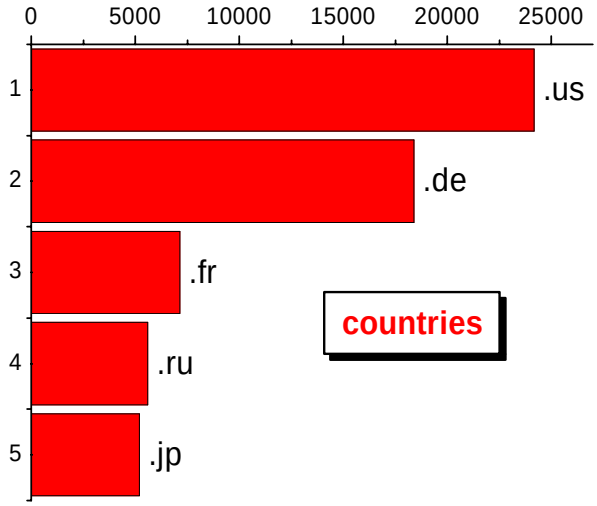
(total number of calculations: 81,372)

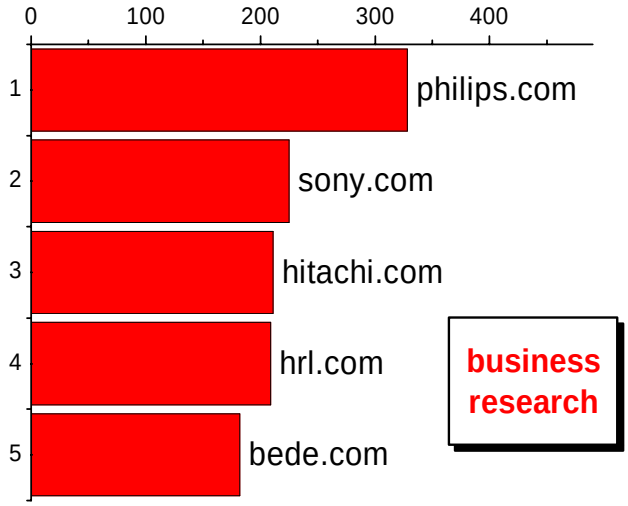












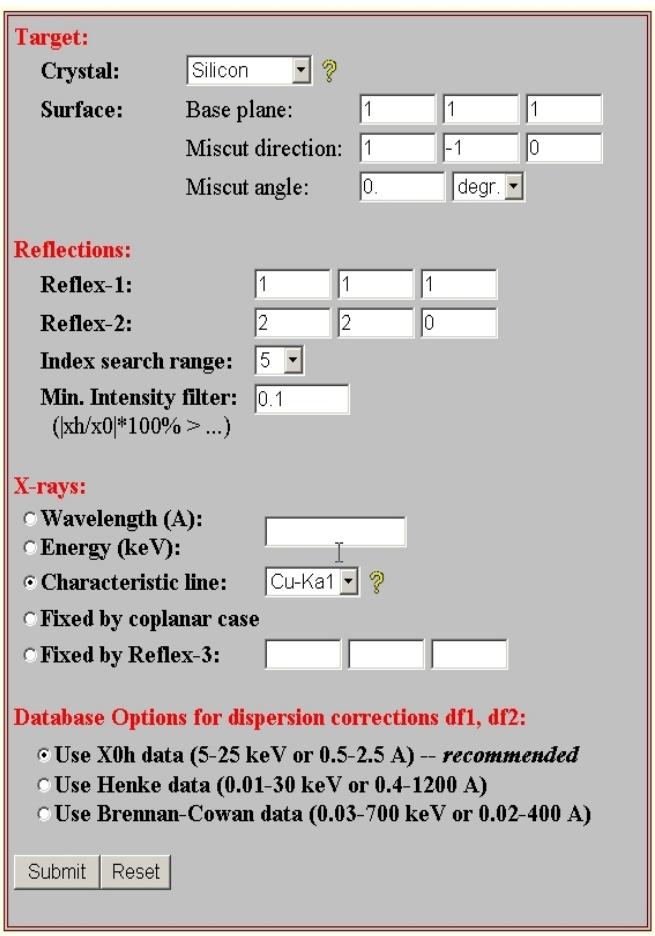
BRL on the Web

X-ray multiple Bragg/Laue diffraction

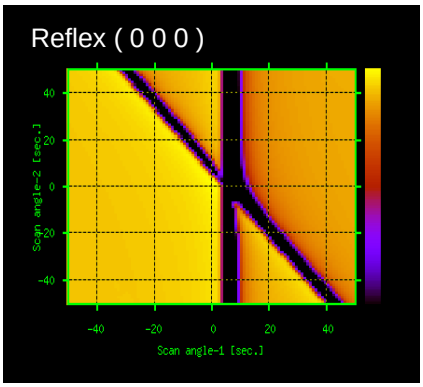
BRL calculates multiple Bragg diffraction of x-rays from crystals. It is based on Ref. [8]. The Web interface provides the possibility to simulate up to 12-wave dynamical Bragg diffraction of x-rays from a plate-shaped crystal including the cases of x-ray waves grazing along the surface and Bragg angles close to 90°.

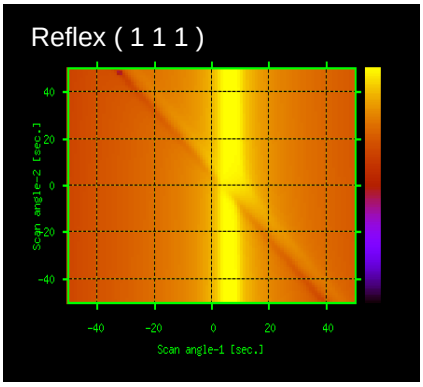
Typically the calculations of multiple Bragg diffraction are reduced to the eigenvalue problem for a scattering matrix. If there are no grazing waves involved into the diffraction geometry so that the specular reflection effects could be neglected, then the size of the scattering matrix is 2N*2N for N-wave diffraction. Here the factor of two appears due to the two polarizations (sigma and pi) of x-rays. However, if the diffraction geometry involves an x-ray wave grazing along the crystal surface, the task becomes more complicated. For this case R.Colella [Acta Cryst. (1974)] suggested a theory where the calculations of multiple Bragg diffraction are reduced to the eigenvalue problem for 4N*4N scattering matrix. This holds even if only one of e.q. 12 waves is grazing. ***BRL*** uses a more effective algorithm and reduces the task to a *generalized* eigenvalue problem for $2(N+N_s)*2(N+N_s)$ scattering matrix where N_s is the number of grazing waves. In some cases like only one of 12 waves is grazing the calculations are reduced dramatically.

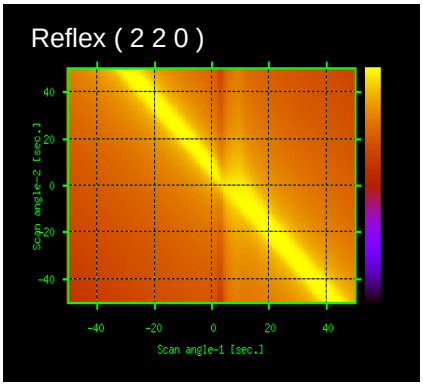
BRL has been successfully used to simulate the applications of Bragg- and Laue-case Renninger effect [9] to x-ray double-plane collimation and the multiple diffraction effect in x-ray surface back diffraction [10].



Example BRL results



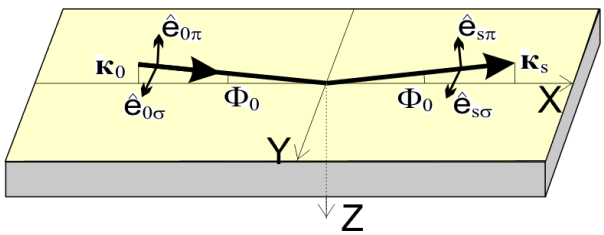


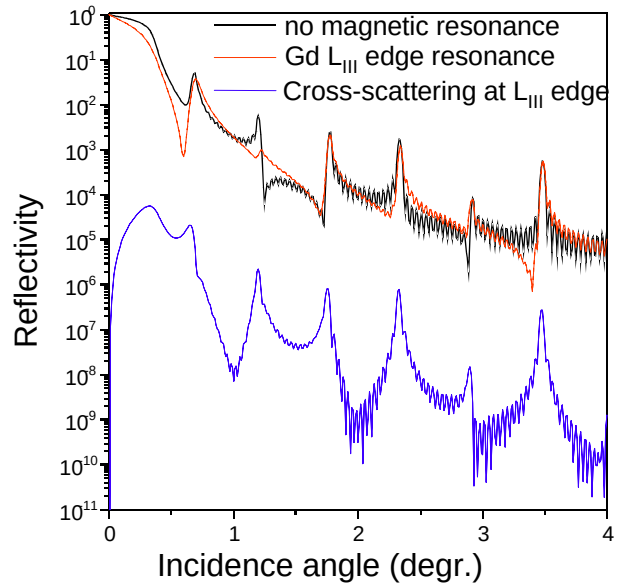


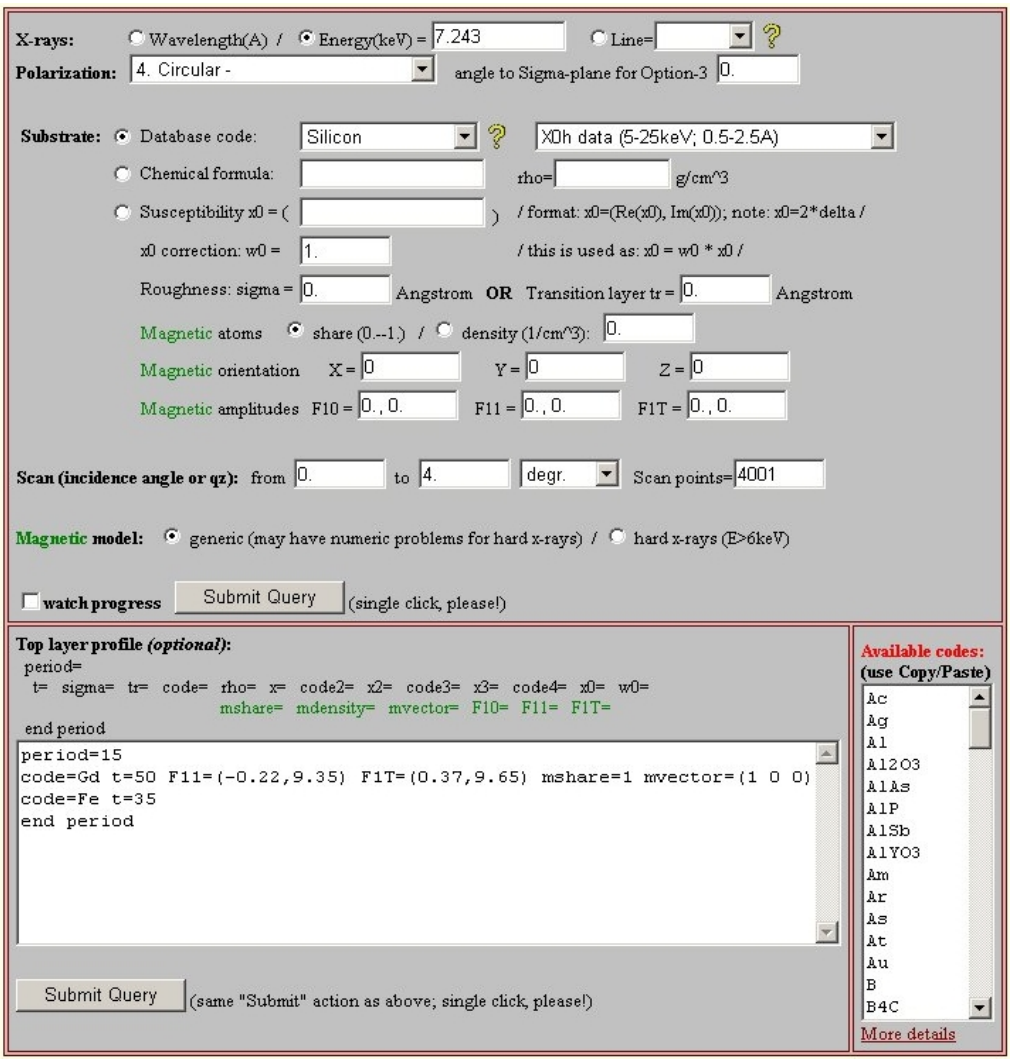
MAG_SL on the Web

X-ray resonant specular reflection from magnetic multilayers

MAG_sl simulates resonant x-ray specular reflection from magnetic multilayers with the account for interface roughness or transition layers. It is based on the recent paper by S. Stepanov and S. Sinha, PRB **61**(2000) 15302.



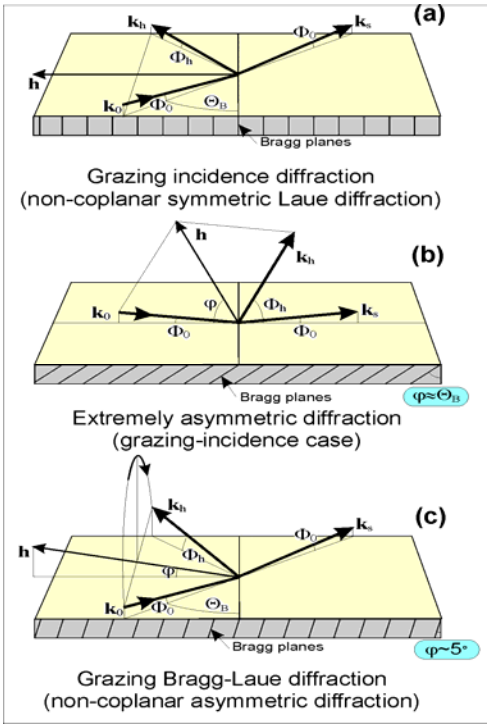




GID_sl (Grazing Incidence Diffraction from Superlattices) was originally developed in [2,4,5] for simulation of GID (Fig.1a) from semiconductor multilayers. In [4] this program was extended to extremely asymmetric diffraction (Fig.1b) and non coplanar asymmetric diffraction (Fig.1c). Finally, in [10] the symmetric Bragg case was also included and the algorithm was made applicable to arbitrary number of layers.

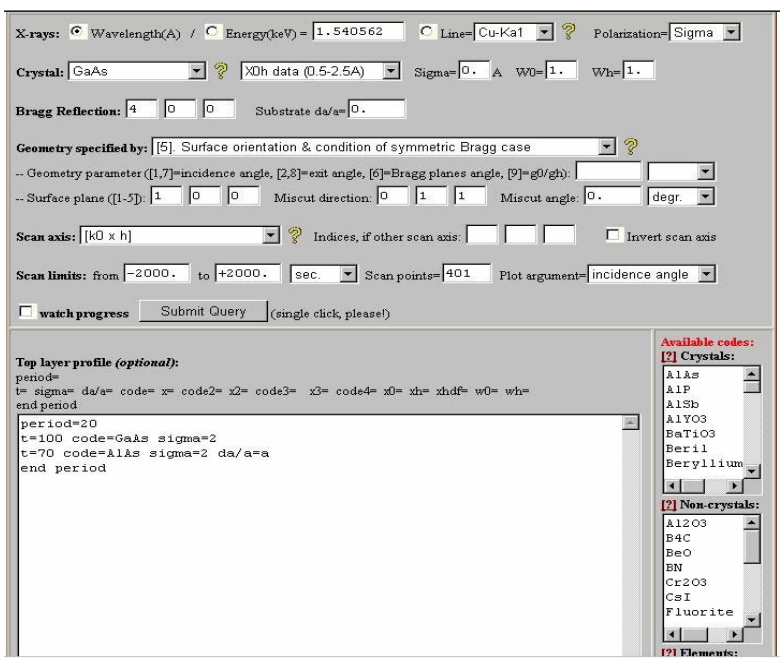
At present the program can simulate the following profiles of structure parameters in multilayers:

1. Normal lattice strains, da(z)/a;
2. Variations of crystal polarizabilities x0(z), xh(z) including the Debye-Waller profiles wh(z), w0(z);
3. The rms height sigma(z) of interface roughness in multilayer.

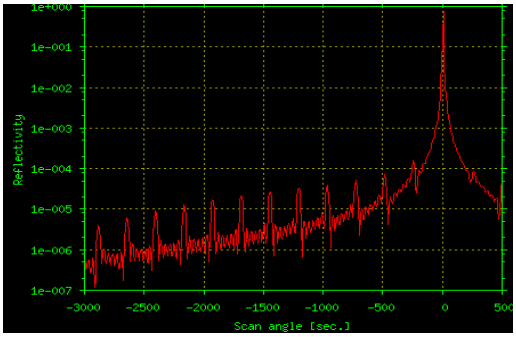


The uniqueness of GID_sl is that it is the only software capable of simulating Bragg diffraction from multilayer in the conditions of total external reflection of x-rays where the x-ray penetration into target reduces to 10nm providing the possibility to study very thin layers. In addition, with GID_sl one can simulate x-ray scans around arbitrary axes. For example, one can design such scans in asymmetric diffraction geometries (Fig.1c) which preserve the small incidence angle.

The program behaves well in usual x-ray diffraction schemes too. As shown in the comparison study by Grundmann & Krost [Phys. Stat. Sol. (b), 218 (2000) 417-423] it turns to be more reliable than some popular commercial software for diffraction curves simuation.



Example GID_sl results



APPLICATIONS OF GID_SL PROGRAM AT ONLINE X-RAY CENTER
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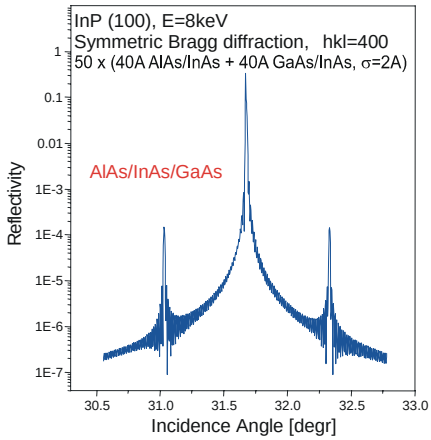

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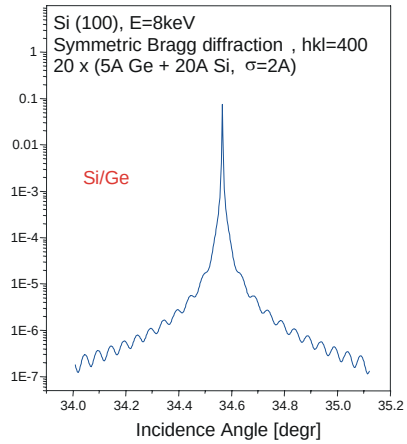

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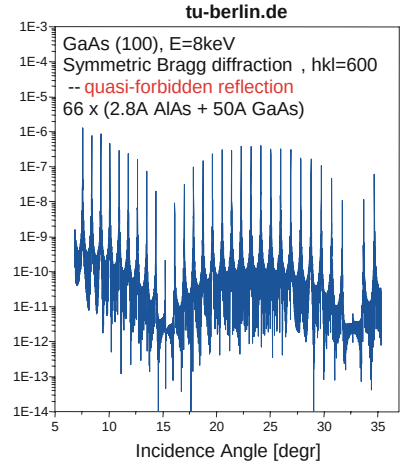

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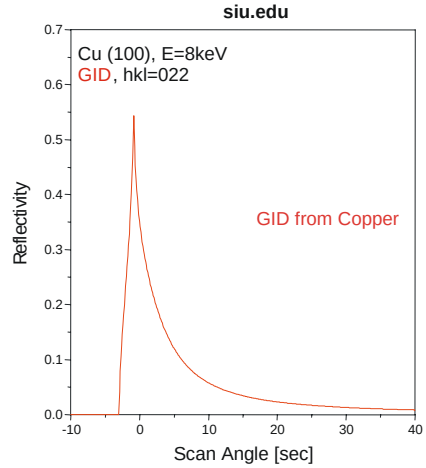

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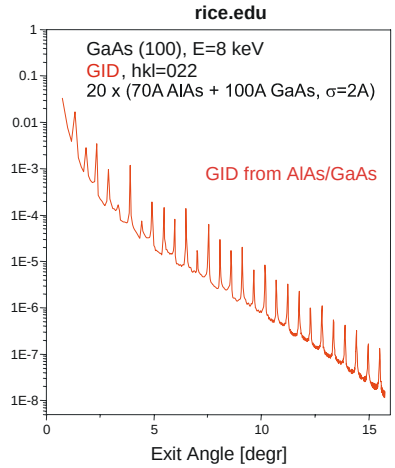

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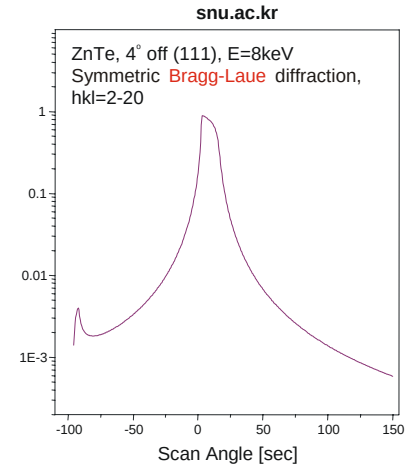

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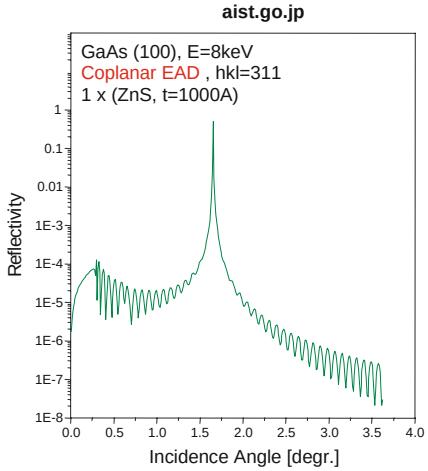

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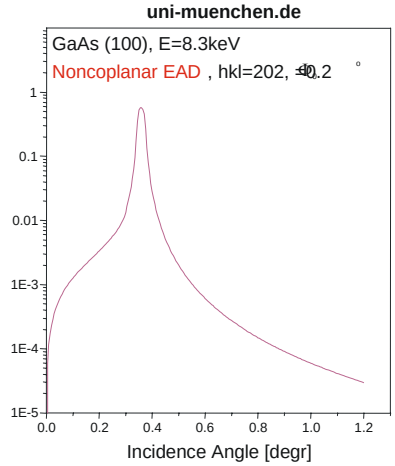

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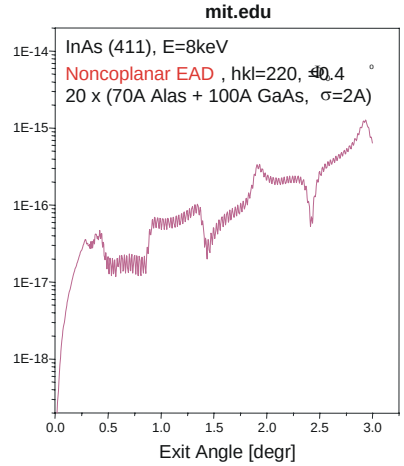
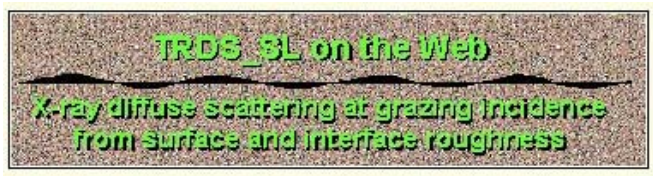




TRDS_sl (Total Reflection Diffuse Scattering from Superlatices) was developed in [6--9] for the simulations of x-ray diffuse scattering from interface roughness in semiconductor multilayers (Fig.1). This program implement a number of different models for interface roughness and for correlations between roughness at different interfaces in multilayers (Fig.2)..Some of these model are suggested in [6--9] and some are due to other authors. Notable is the implementation of model [6] which allows to study the wavelength-dependent inheritance of roughness in layer-by-layer grown multilayers (Fig.3).

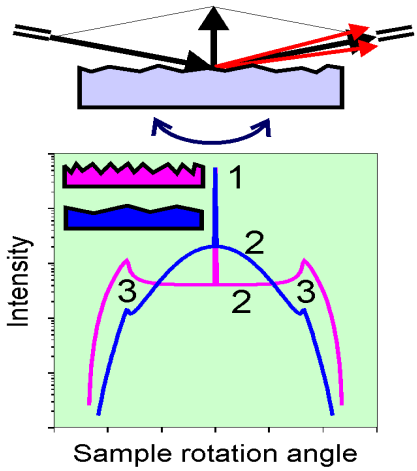


Fig.1. Diffuse scattering of grazing x-rays from surface roughness. 1: specular peak, 2: diffuse scattering for two different lateral scales of roughness, 3: Yoneda peaks at critical angle for total reflection.

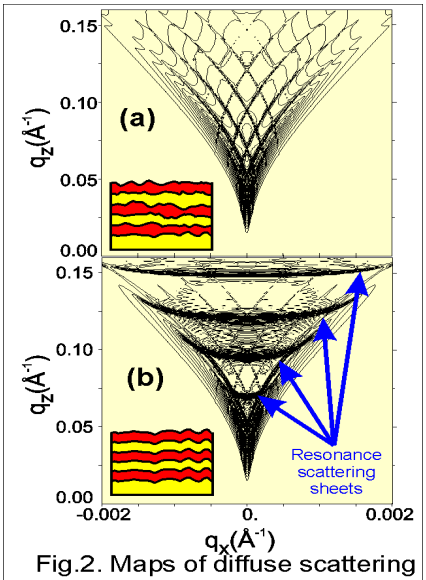


Fig.2. Maps of diffuse scattering from vertically uncorrelated (a) and correlated (b) roughness

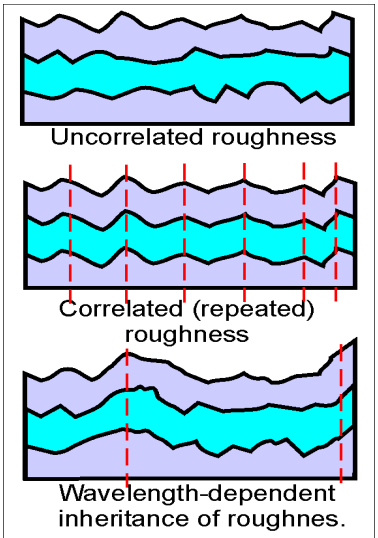


Fig.3. Different models of roughness correlations in multilayers

Another notable feature of TRDS_sl is the implementation of models [6] for x-ray scattering from atomic steps on vicinal interfaces and 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.

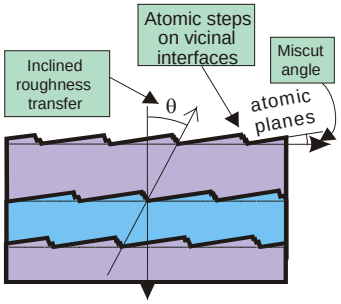


Fig.4. Asymmetric rougness of vicinal interfaces and skew roughness transfer in crystals.

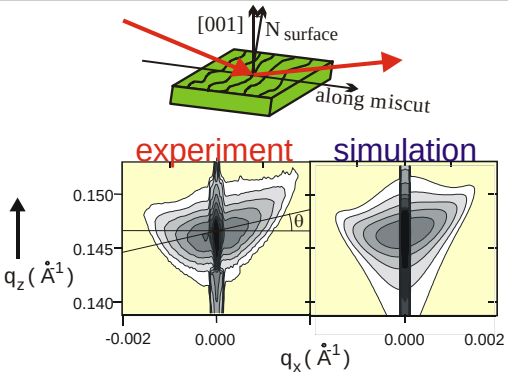
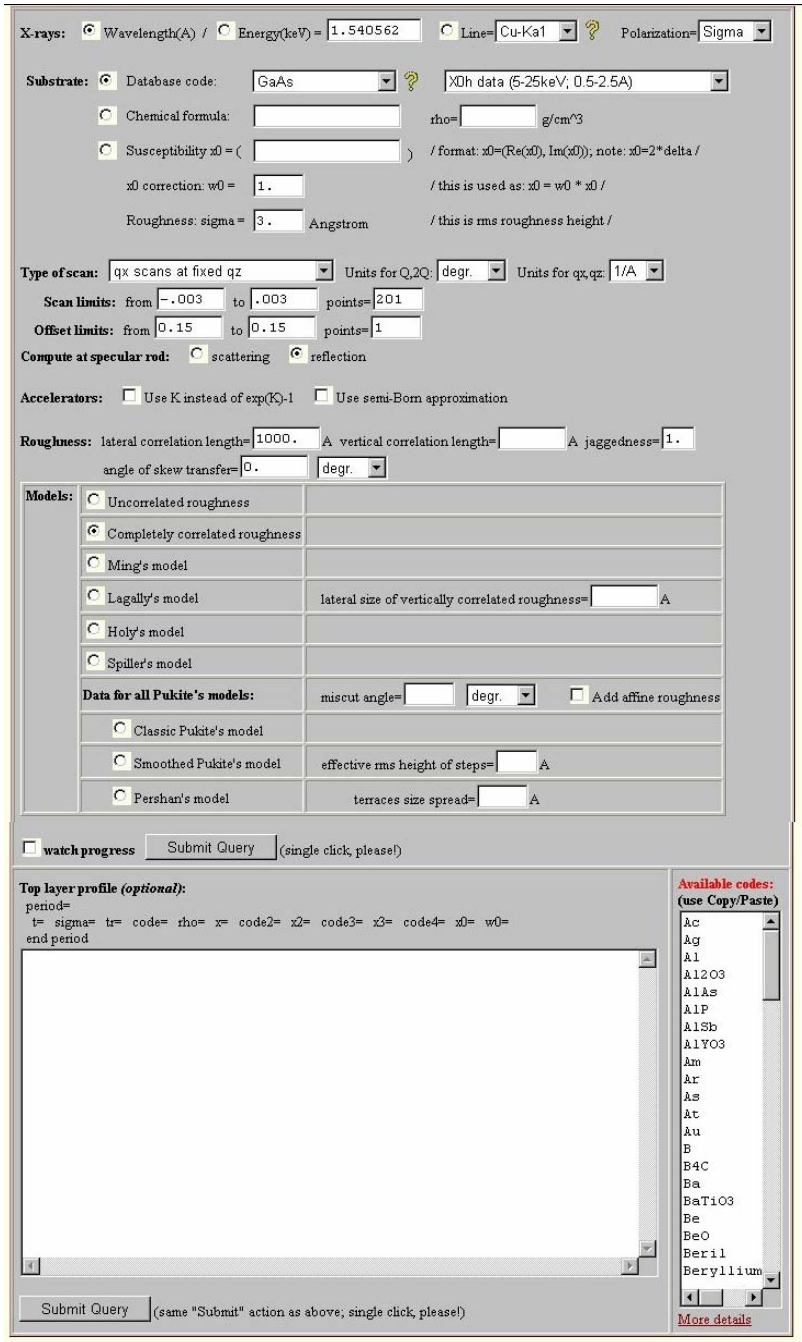


Fig.5. Simulations of inclined roughness transfer in AlAs/GaAs superlattice.

TRDS_SL on the Web

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

TRDS_sl inut form



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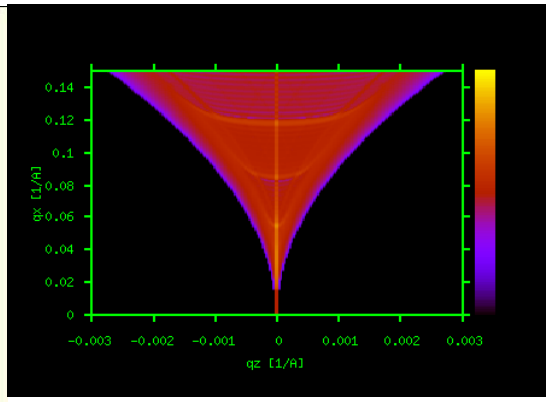

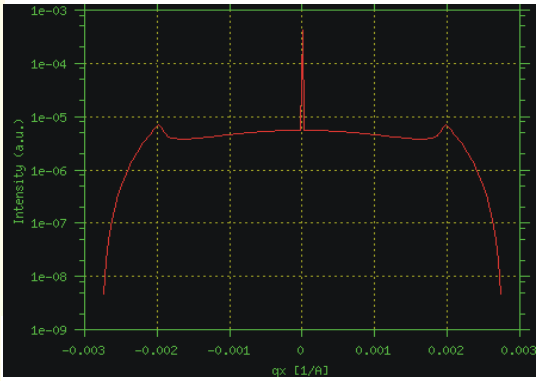

Download ZIPped results: TRDS1942.zip

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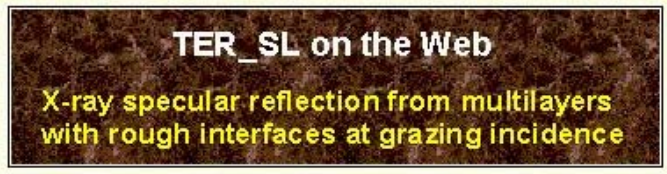
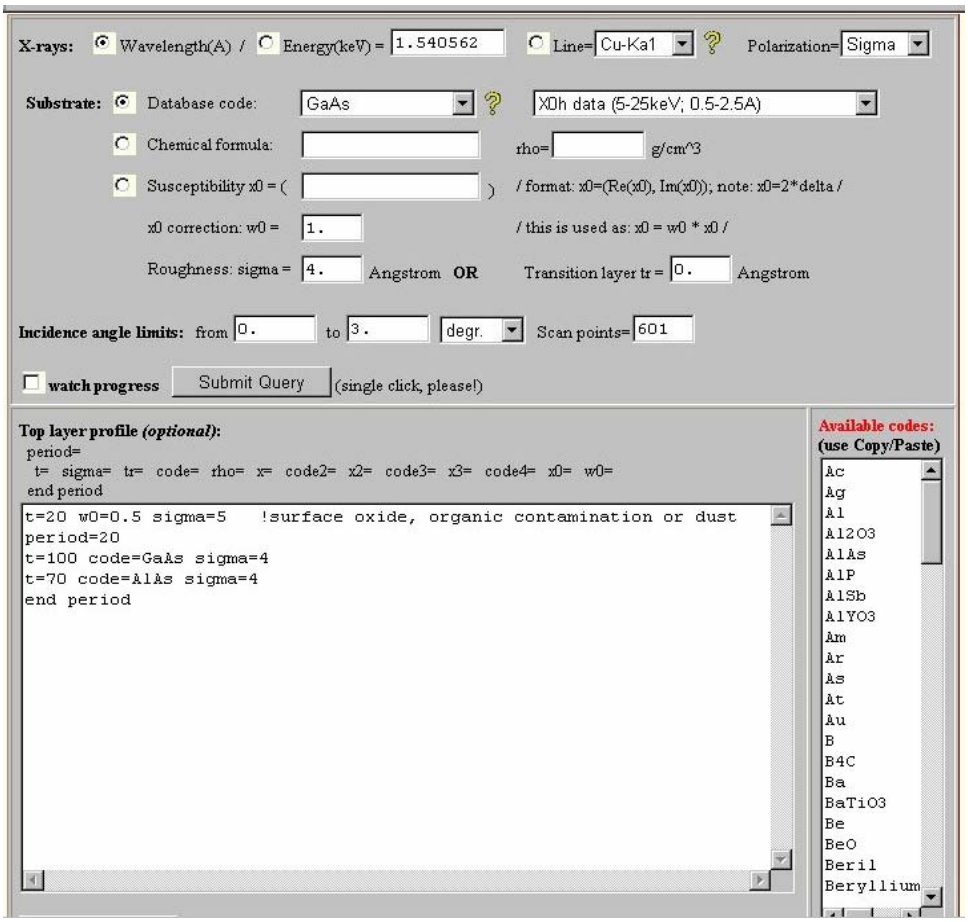
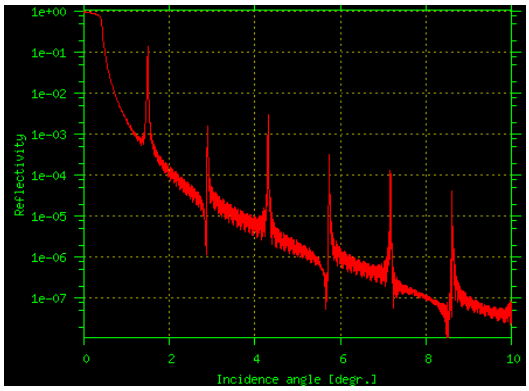
Display INP file: TRDS1942.INP
Display TBL file: TRDS1942.TBL
Display DAT file: TRDS1942.DAT



TER_sl (Total External Reflection from Superlattices) was designed as a by-product in the course of developing GID_sl. It uses the same recursive matrix calculation algorithm as GID_sl and very similar data input. The TER_sl can account for material density profile in multilayers, the interface roughness, or transition layers.



Example TER_sl results



APPLICATIONS OF TRDS_SL PROGRAM AT ONLINE X-RAY CENTER

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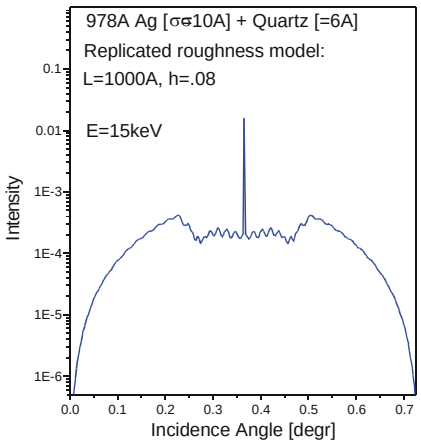

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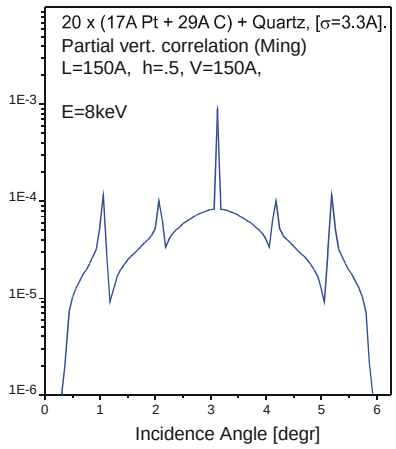

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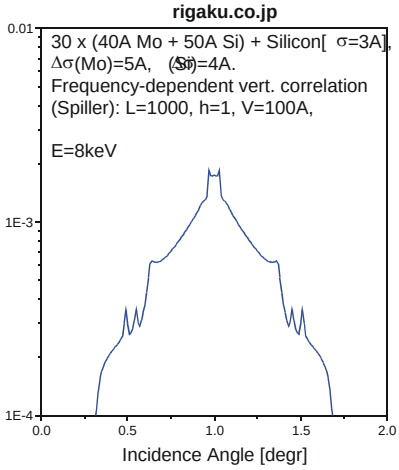

APPLICATIONS OF TER_SL PROGRAM AT ONLINE X-RAY CENTER

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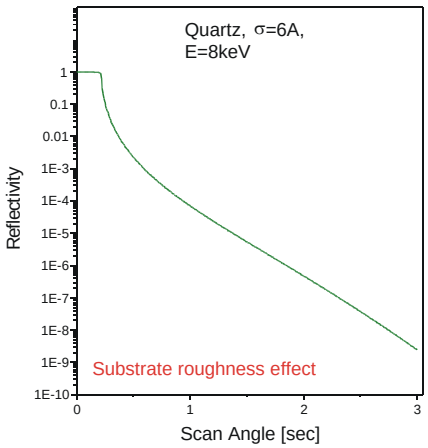

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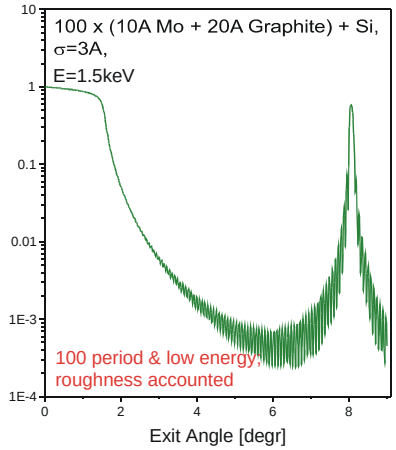

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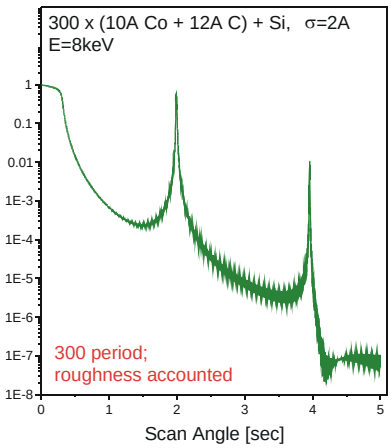
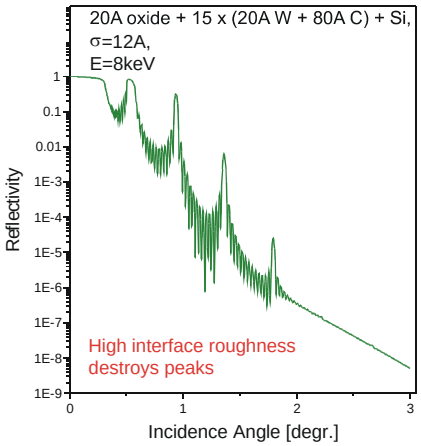


uni-muenchen.de



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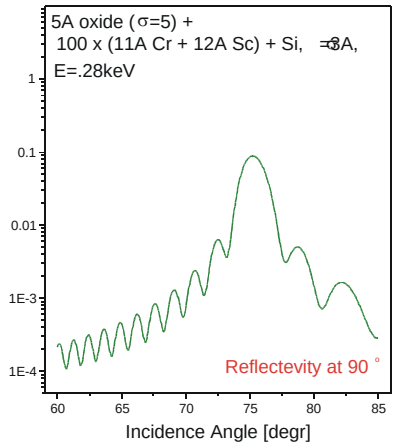

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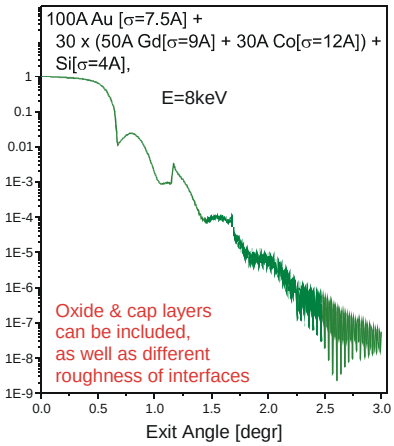


X0h calculates material susceptibilities χ_0 and χ_h for x-ray wavelength range. It was originally developed in [1] for the needs of parametric x-ray radiation studies. Later on it occurred to be a great tool for synchrotron radiation applications. The calculation consists of 5 steps:

1. Calculation of scattering factors *f(s)*.
2. Calculation of dispersion corrections *df'* and *df''*.
3. Calculation of dipole and quadruple absorption cross sections.
4. Calculation of Debye-Waller temperature factors.
5. Calculation of χ_0 and χ_h by summation of atomic scattering over crystal unit cell.

No quantum calculations of atomic wave function are used; basically the algorithm interpolates the data tabulated in the International Tables for X-ray crystallography. There is however the difficulty with Step-2 how to interpolate the dispersion corrections *df'* and *df''* because the International Tables contain *df'* and *df''* for characteristic X-ray lines only (Cr-Ka1, Fe-Ka1, Cu-Ka1, Mo-Ka1, and Ag-Ka1) and any other tables provide the discrete data sets of *df'* and *df''* too. X0h implements the interpolation scheme suggested in [1]. The dispersion corrections can be calculated with the formulae given by Don Cromer [Acta Crystallogr. vol.18 (1965) p.17-23]:

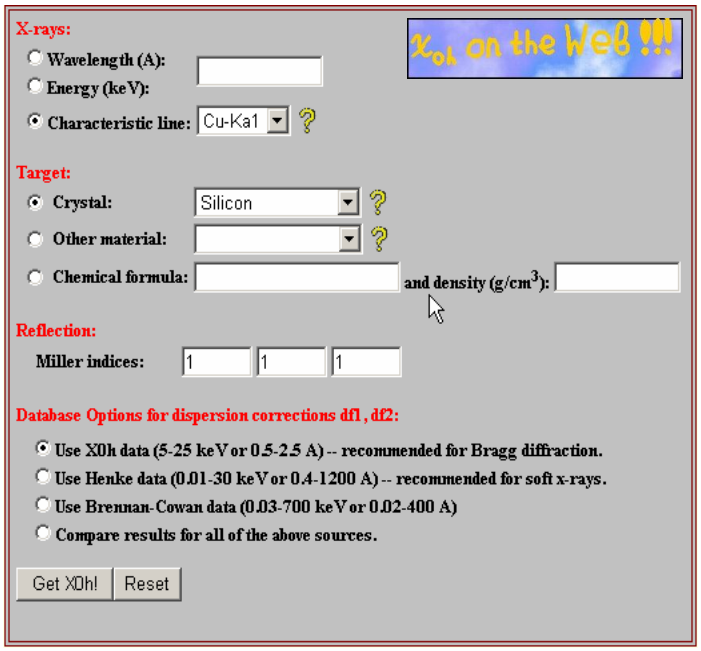
$$df' = \sum_{k=1}^{N_S} g_k P(X_k, N_k)$$

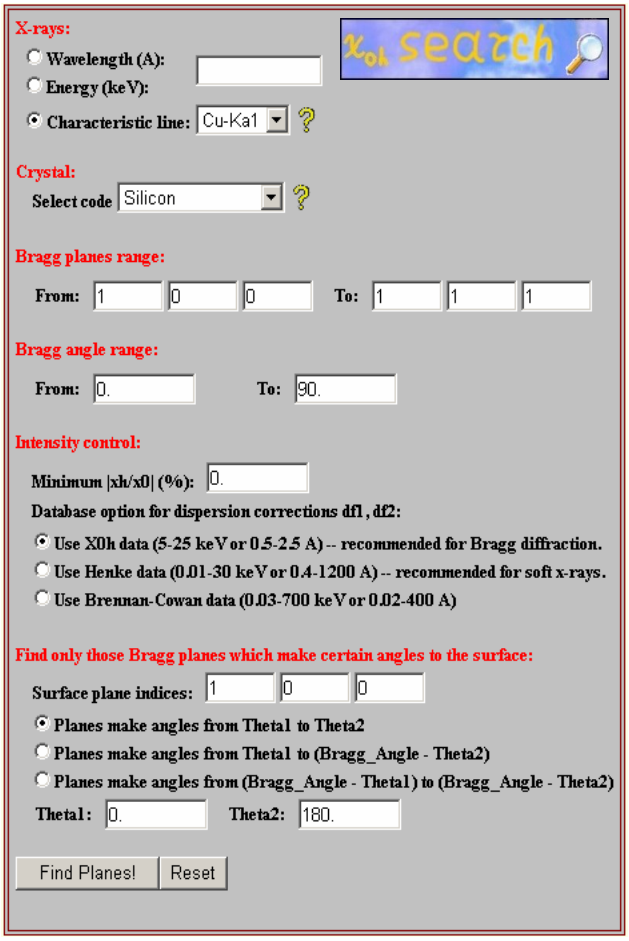
$$df'' = 0.5\pi \sum_{k=1}^{N_S} g_k (N_k - 1) / X_k^{N_k - 1}$$

Here the summation is taken over the absorption edges, N_S is the number of absorption edges taken into account, N_k are known constants for different electron shells, $P(X_k, N_k)$ is the known integral evaluated by Parratt, $X_k = \lambda/\lambda_k$ is the ratio of the x-ray wavelength to that of the absorption edge, and g_k are oscillator strengths at the absorption edges. First, X0h applies the above equations to known tabulated dispersion corrections and evaluates g_k. Then, it uses calculated g_k to find the dispersion corrections of interest.

The above process may work equally well both with the dispersion corrections tabulated in the International tables and with any other source. We found very useful the tables composed by Henke, Gullikson & Davis [Atomic Data and Nuclear Data Tables, vol.54 (1993) p.181-342]
and by Brennan & Cowan [Rev. Sci. Instrum., vol.63 (1992) p.850]. Both of them extend the International Tables data to a much wider wavelength range.

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, etc.





X0h+ Search Results

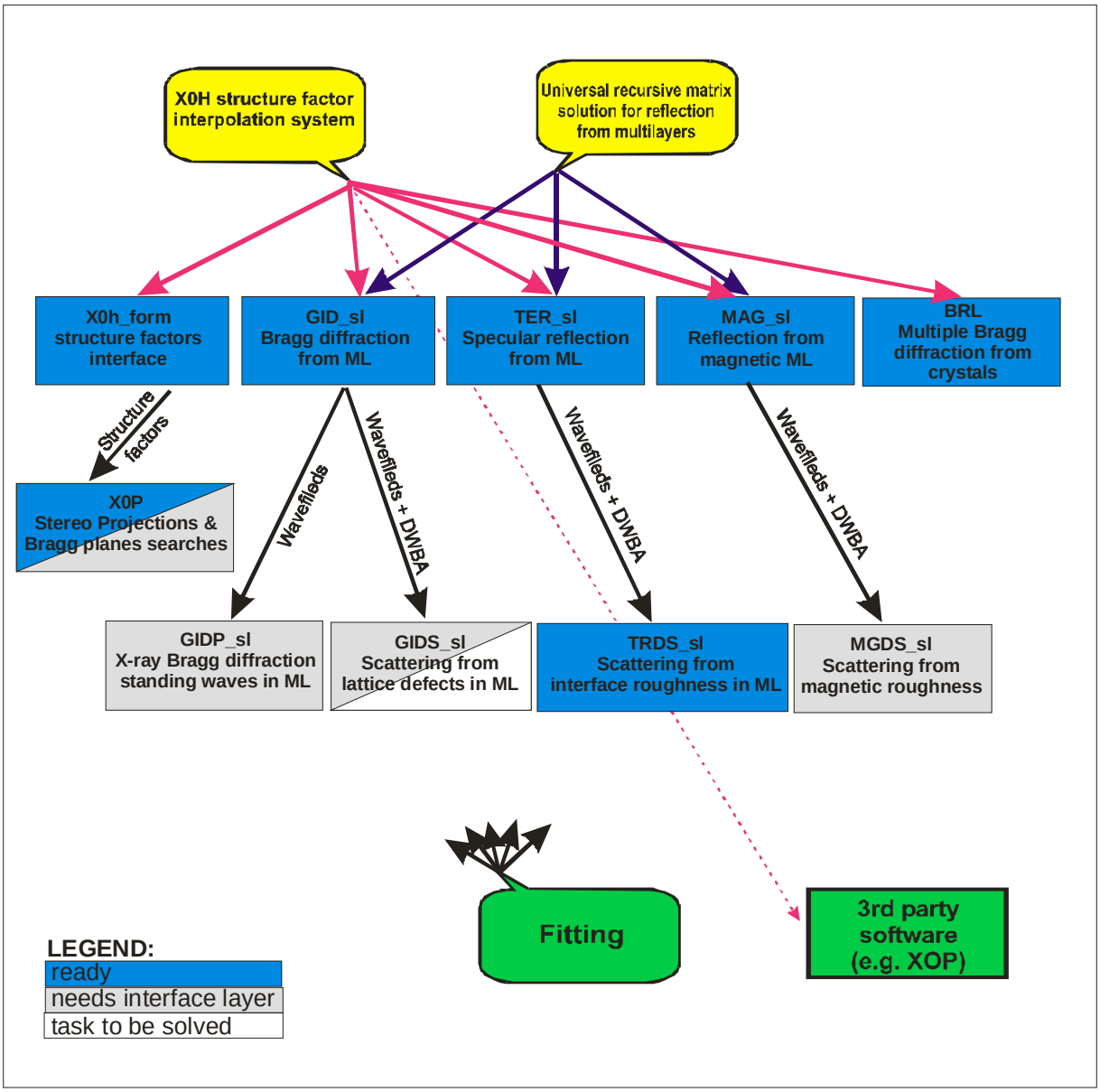
SEARCH CONDITIONS :	
Crystal:	Silicon
Symmetry group:	Cubic
Density (gm/cm^3) :	2.3293
Unit cell constants (A) :	5.4309 , 5.4309 , 5.4309
Unit cell angles (degr.) :	90.000 , 90.000 , 90.000
X-ray wavelength (Angstrom) :	1.540562
X-ray energy (keV) :	8.047777
X-ray characteristic line :	Cu-Ka1
Bragg planes 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

Planned Expansions of X-Ray Server



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