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X-ray server: an online resource for simulations of X-ray diffraction and scattering

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ABSTRACT

X-ray Server is a public project operational at the APS since 1997 with the goals to explore novel network technologies for providing wide scientific community with access to personal research results, establishing scientific collaborations, and refining scientific software. The Server provides Web-based access to a number of programs developed by the author in the field of X-ray diffraction and scattering. The software code operates directly on the Server available for use without downloading. Currently seven programs are accessible that have been used more than 85,000 times. This report discusses the Server philosophy, provides an overview of the physical models and algorithms beneath the codes and demonstrates some applications of the programs. It is shown with examples and statistics how the Server goals are achieved. The plans for further X-ray Server development are outlined.

Keywords: X-ray diffraction, X-ray scattering, X-ray optics, X-ray theory, web-based computations

1. INTRODUCTION

A typical cycle of developing a theory, at least in the X-ray scattering field, is (1) working out a model, (2) deriving respective equations, (3) writing a simulation or data analysis software, (4) comparing numerical data to an experiment, and, provided the above steps were successful, (5) writing a paper. After this cycle is accomplished, the question arises, how to share the software into which a lot of efforts and know-how expertise has been invested? There are several solutions for that. Here we are not considering commercial applications because not all leading-edge studies may be of immediate commercial interest. Then, the most common approach is to give the software away in some way using the principle: use it on your own risk and don't blame the author. Many researchers do it either through their personal web pages or some common repositories like SINCRIS [1]. Some of such scientific X-ray software has been collected under the roof of the XOP project [2] where the programs were supplied with graphical interfaces and ported to multiple operating systems which made them easier to use. However, with any of those approaches, one very important element is commonly missing, namely a link between the developer of code and his users. The developer does not see possible misuses of his software and he has no direct way to learn about attempts to expand his models to new objects or about incorrect software behavior caused by bugs, and etc. Only when some users decide to contact the author, few pieces of such information become available to him. Furthermore, the developer has no direct way to inform the users when a bug is found or the software capabilities are extended, and someone may still keep using an old restricted or incorrect code.
For many years the author of these lines was involved in developing models and software for X-ray scattering and at some point he began thinking how to make the best use of the programs he wrote. It was decided to explore new opportunities given by the Internet. The idea was to make the WWW interface to the software and instead of giving the programs away make them working on a single computer accessible by the WWW. This way the author can immediately see applications of his software as well as tendencies to extend it to certain fields, possible misuses and bugs. The users on their side benefit from the facts that they always run the latest most refined version of the program, do not need to install anything on their computers, and can use software inputs (e.g. crystal databases) expanded by other users. There are also advantages that the codes do not need to be ported to multiple platforms and, last but not least, the HTML provides one of the easiest ways to add Graphical User Interface (GUI) to scientific software [3]. The project began in 1997 and resulted in the X-ray Server currently residing at http://sergey.gmca.aps.anl.gov. For seven

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years of operation it has performed more than 85,000 calculations. The idea of the project was inspired by the WWW interfaces to X-ray reflectivity calculations designed at the Center of X-ray Optics [4] at the LBL.
In the next Section the structure of the Server is described. Then, a brief overview of each of seven programs operational on the Server is given. Section 3 provides some statistics of using the Server and discusses the key components of the Server success. It also outlines the plans for further Server developments.

2. X-RAY SERVER STRUCTURE

The list of software operational on X-ray Server is presented in Table-I. The programs provide simulations of X-ray diffraction, reflectivity, and diffuse scattering curves as well as calculations of scattering factors for the tasks related to X-ray optics and X-ray material science.

No	Name	Description	Usage
1	***X0h***	A program interpolating 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.	40993
2	***X0h+***	A tool based on ***X0h*** that can help to plan X-ray experiments by providing search for Bragg planes in crystals satisfying various conditions.	
3	***GID_sl***	Software that calculates X-ray diffraction curves from strained crystals and multilayers for any Bragg-case diffraction with scans around arbitrary axes. It can be used for usual symmetric and asymmetric diffraction, for extremely asymmetric diffraction, as well as for grazing incidence and other non-coplanar diffraction geometries.	21319
4	***TER_sl***	Software using a new algorithm to calculate X-ray specular reflection from multilayers with interface roughness and transition layers.	9212
5	***MAG_sl***	A program that calculates X-ray resonant specular reflection from magnetic multilayers with interface roughness and transition layers	8139
6	***TRDS_sl***	Software for simulating X-ray diffuse scattering from interface roughness. It implements several different models of roughness and can calculate such effects as skew roughness transfer in multilayers, dependence of interface-interface roughness correlations on lateral size of roughness and X-ray scattering from atomic steps.	6811
7	***BRL***	A program that 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^o.	541

Table I: List of software operational on X-ray Server. The usage statistics is given as of June 25, 2004 (87,015 calls).

The technical details of making the scientific software available through the WWW interface are discussed elsewhere [5]. In a short form, the implementation of the WWW interface is illustrated by Fig. 1. In this example ***GID_sl*** is a program for calculating Bragg curves, i.e. scientific software resulted from a research project. To start the calculations, it expects input data in the form of a file passed as a command line argument. At the end ***GID_sl*** produces a data file containing the dependence of X-ray reflection coefficient on a scan angle. The interface consists of an HTML form for entering the input parameters by a remote user and an additional program ***GID_form*** parsing these parameters and converting them into the input file of ***GID_sl***. The ***GID_form*** receives the data from a web server (e.g. Apache [6]) and calls ***GID_sl***. After the execution of ***GID_sl*** is finished, ***GID_form*** produces an HTML page with the link to the ***GID_sl*** output file. Additionally, ***GID_form*** uses freeware software Gnuplot [7] and InfoZIP [8] to generate a plot for the HTML page and compress the output data, respectively.
All seven programs on X-ray Server are closely linked to each other, as shown by Fig. 2. For example, all the programs use ***X0h*** tool for automatic calculation of X-ray scattering factors. In addition, the programs ***GID_sl*** through ***TRDS_sl*** share the same code for recursive matrix operations when calculating reflections from multilayers. The ***TRDS_sl*** software calculates X-ray diffuse scattering with the help of X-ray wavefields provided by the ***TER_sl*** code. Likewise,

GID_sl is planned to be used in the future expansions of X-ray Server to provide the wavefields for simulations of X-ray standing waves and X-ray diffuse scattering under the conditions of Bragg diffraction.

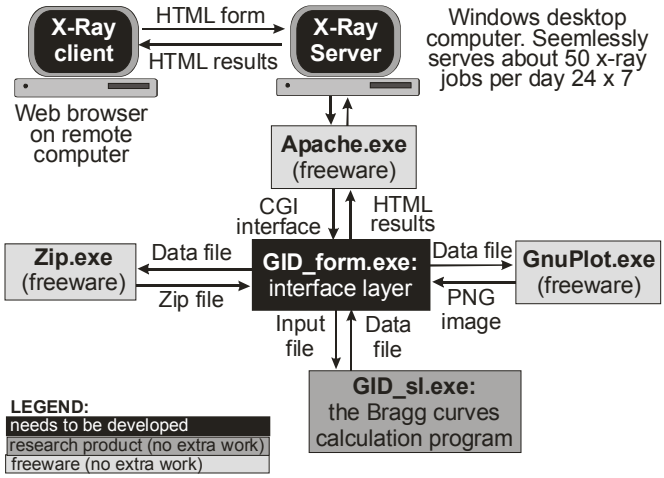

Fig. 1. An illustration how to add WWW interface to scientific software. The only pieces to be developed are the HTML form and the input data parsing layer ***GID_form.exe***.

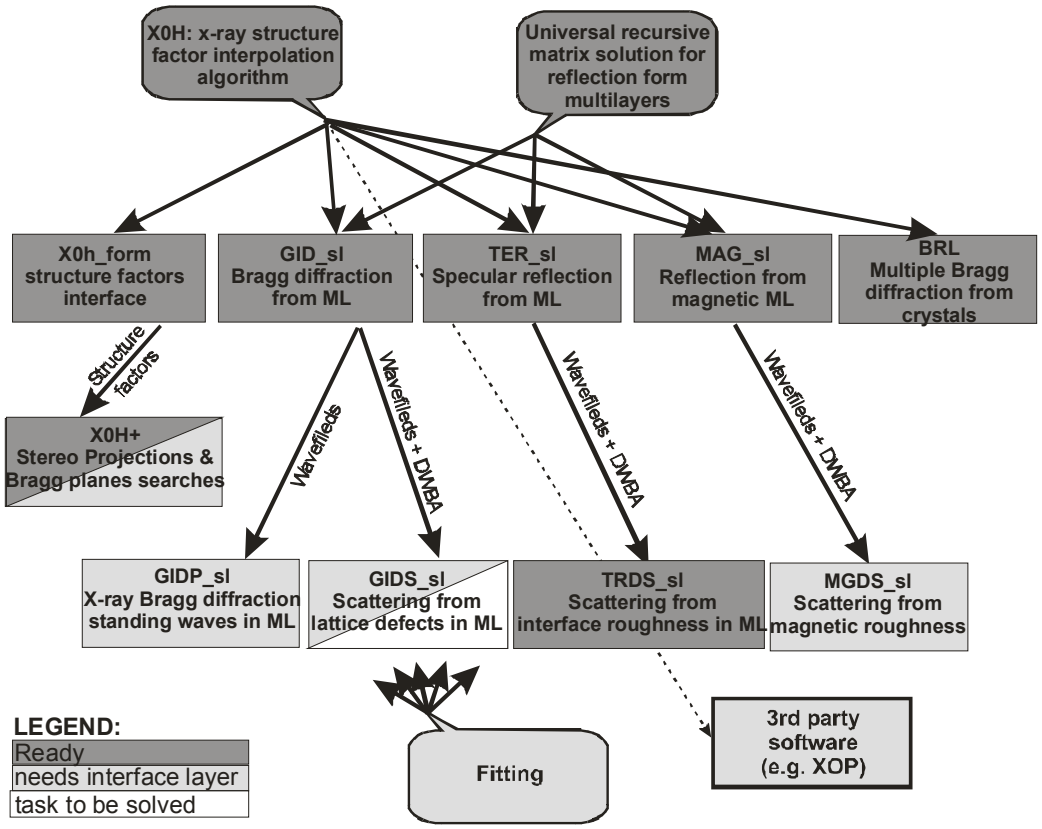

Fig. 2. Relations between programs on X-ray Server. In addition to seven programs that are already available, some more are planned. Fore details see text.

3. X-RAY SERVER APPLICATIONS

3.1 X0h and X0h+ : software for planning X-ray experiments

X0h software calculates dielectric susceptibilities χ_0 and χ_h for crystals and other materials in the X-ray range. Besides, it provides the associated values of the Bragg diffraction peaks HWFM, the extinction and absorption lengths, and other parameters helpful in the analysis of X-ray diffraction and scattering experiments. Originally, this program was developed in [9] in order to facilitate the analysis of the Čerenkov X-ray radiation. The calculations of $\chi_{0,h}$ generally consist of five steps:

1. Calculation of the scattering factors f(s) of individual atoms.
2. Calculation of dispersion corrections df' and df".
3. Calculation of dipole and quadrupole absorption cross sections (the dipole and quadrupole shares in df").
4. Calculation of the Debye-Waller temperature factors.
5. Calculation of $\chi_{0,h}$ by summation over atomic contributions within crystal unit cell.

The initial data for most of these calculations can be found in [10], but in many cases they are incomplete and therefore different algorithms have to be applied in the ***X0h*** program when performing calculations for different materials. The choice of algorithms is stored in the ***X0h*** databases. However, the biggest problem exists with the dispersion corrections that are tabulated for a discrete set of X-ray energies or even for characteristic X-ray lines only. ***X0h*** solves this problem by applying Don Cromer's equations for df' and df" [11]:

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

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 ***k***-th absorption edge, and g_k are the oscillator strengths at the absorption edges. The latter are available for a few elements only and thus have to be determined. The key idea implemented in ***X0h*** is to apply the above equations to known tabulated dispersion corrections and thus evaluate g_k . Then, the calculated g_k are used to find the dispersion corrections at an arbitrary X-ray wavelength or energy. This works equally well not only with the dispersion corrections tabulated in [10], but also with other sources of df' and df". For example, ***X0h*** makes use of the tables [11] and [12] in order to extend the calculations to a wider X-ray energy range.

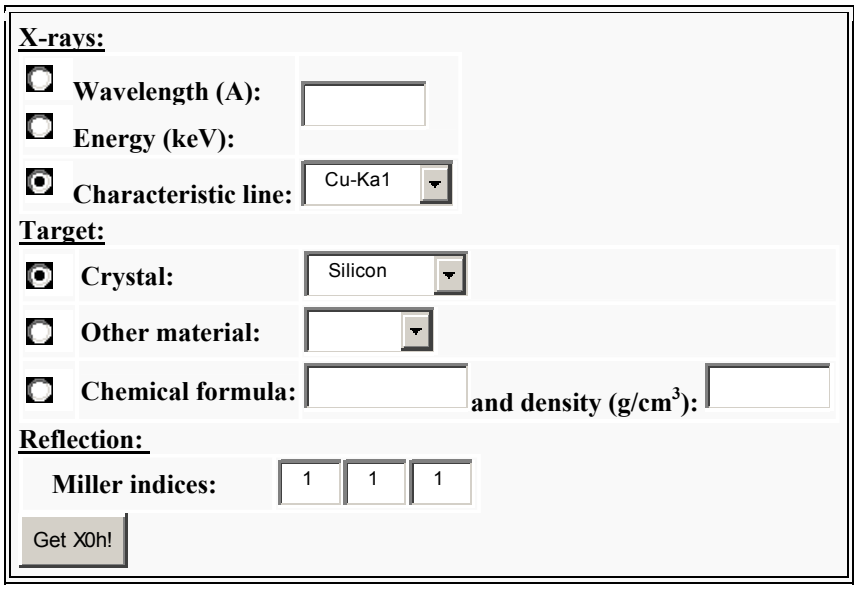

Fig. 3. HTML form for calling ***X0h*** via WWW. The materials database in the form is expandable upon user submissions.

An example HTML form for WWW accessed ***X0h*** is shown of Fig. 3. When users click on the "**Get X0h**" button, their web browsers submit a string with requested parameters to the web server at the X-ray Server location and the web server passes it to parsing software called ***X0h_form***. The latter converts the string into the ***X0h*** input file and calls ***X0h***, i.e. the same scheme takes place as on Fig. 1.

X0h+ is an application built on top of ***X0h***. It allows to search for Bragg planes in crystals satisfying various conditions and thus helps planning X-ray experiments. Possible applications of X0h+ are:

- Find all the reflections from a crystal with the Bragg angles from value-1 to value-2,
- Find all strong Bragg reflections from a crystal,
- Find extremely asymmetric Bragg reflections from a crystal for a given wavelength and surface orientation,
- Find any crystallographic planes in crystal that make angles from value-1 to value-2 with a given plane.

In general ***X0h*** and ***X0h+*** turned out to be very helpful tools for preparing and analyzing X-ray experiments. Their common share in the X-ray Server requests constitutes nearly 50%.

3.2 GID_sl : Bragg curves simulations

GID_sl is a program simulating dynamical X-ray diffraction from strained crystals, multilayers, and superlattices. The name 'GID_sl' comes from the initial version based on Refs.[14-17] that suggested a theory for Grazing Incidence X-ray Diffraction (GID) from multilayered crystals and superlattices (SL). Later on, the theory underlying the ***GID_sl*** code was extended to extremely asymmetric geometries [18] and the standard Bragg case [19]. At present this program is applicable to any coplanar and non-coplanar Bragg-case geometry with diffraction scans round arbitrary axes. Some examples of diffraction geometries where the ***GID_sl*** can be used are shown on Fig. 4.

The key advantage of ***GID_sl*** over the most of other Bragg diffraction simulation software is that it takes into account the specular reflection and refraction of X-rays at crystal surface and interfaces in multilayers. The differential equations by Takagi-Taupin commonly used in the numerical analysis of Bragg diffraction ignore those effects and therefore are not applicable to the cases with X-ray grazing incidence or exit. Instead of the differential equations, ***GID_sl*** implements a "discrete" algorithm, i.e. the crystal is subdivided onto "perfect" sublayers, each one possessing its own X-ray susceptibilities χ_0, χ_h, vertical strain $\Delta a/a$, thickness t, and interface roughness with the rms height σ. After solving the extended dynamical diffraction problem for each "perfect" layer, the reflection from the whole stack is calculated with the help of exact boundary equations taking into account the specular reflection and refraction effects. These equations are reduced to a (2x2) recursive matrix form [19].

Another advantage of ***GID_sl*** is a flexible input that allows for multiple ways to specify the diffraction geometry and define scan axes. For example, one can use either the angle of X-rays to the surface, or the condition of symmetric or vice versa extremely asymmetric diffraction in order to define the geometry. The specification of the profiles of χ_0, χ_h, $\Delta a/a$, t, and σ is also flexible due to the introduction of a simple scripting language. Below is an example script corresponding to a 20-period AlAs/GaAs superlattice:

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

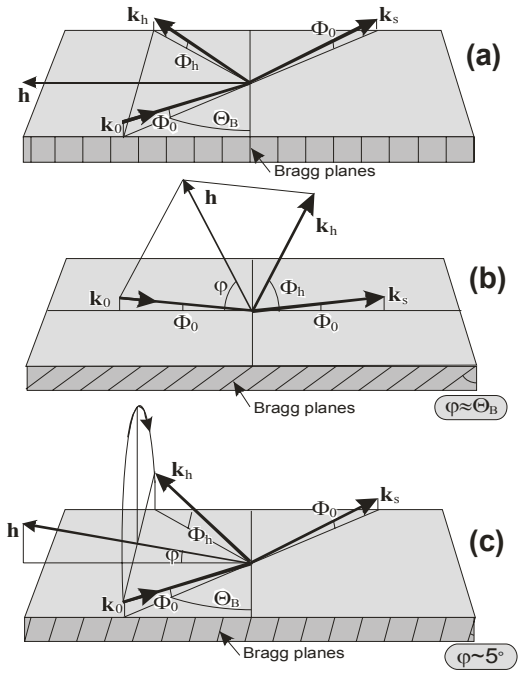

Fig. 4. Some of geometries of X-ray diffraction handled by the ***GID_sl*** program. (a): grazing incidence diffraction, (b): extremely asymmetric diffraction, (c): grazing Bragg-Laue diffraction (non-coplanar asymmetric diffraction)

A combination of the powerful algorithm with the flexible input makes ***GID_sl*** applicable to a wide range of diffraction tasks. As follows from Table 1, ***GID_sl*** is the second most demanded program on X-ray Server. Its applications spawn from simple symmetric Bragg curves of perfect crystals in the evaluations of X-ray optics to complicated GID curves of strained multilayers in data analysis of material science experiments. Several examples are shown on Fig. 5.

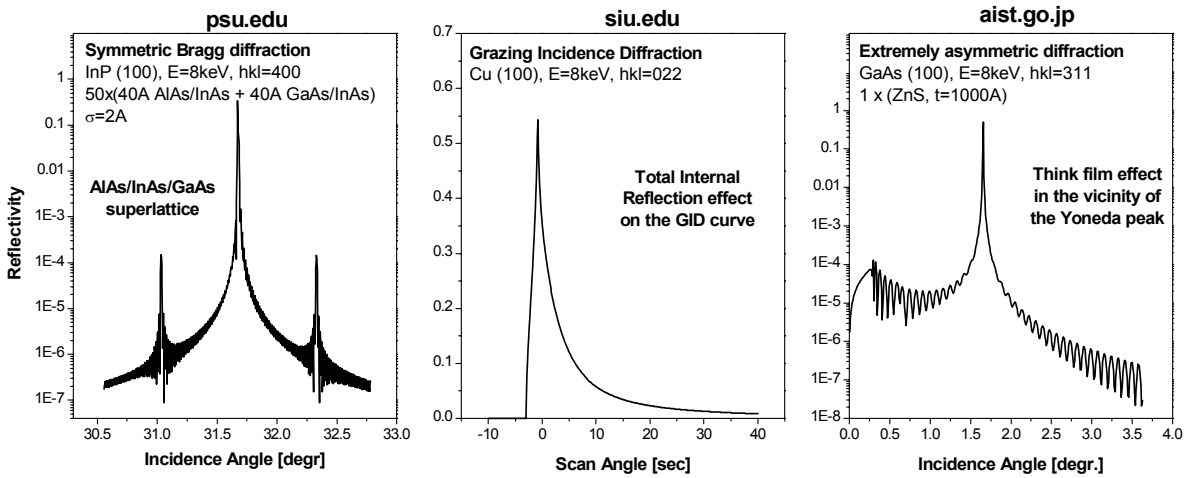

Fig. 5. Examples of ***GID_sl*** applications submitted from different sites. From left to right: symmetric Bragg diffraction from a superlattice, GID from a perfect copper crystal, and extremely asymmetric diffraction from a GaAs crystal with strained ZnS film.

3.3 TER_sl: simulations of X-ray specular reflectivity

The ***TER_sl*** (Total External Reflection) software simulates X-ray specular reflection from multilayers with the account for interface roughness or transition layers. This program shares with ***GID_sl*** the same recursive algorithm for calculating reflections from multilayers, but in the case of ***TER_sl*** the (2x2) matrices are reduced to scalars. The advantage of ***TER_sl*** over the well know Parratt recursive technique [20] 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. The ***TER_sl*** software benefits from the same flexible scripting language for describing multilayers, as in ***GID_sl***.

The most frequent applications of ***TER_sl*** are the simulations of X-ray mirrors in X-ray optics and the studies of multilayers quality in the material science. Some examples are shown in Fig. 6.

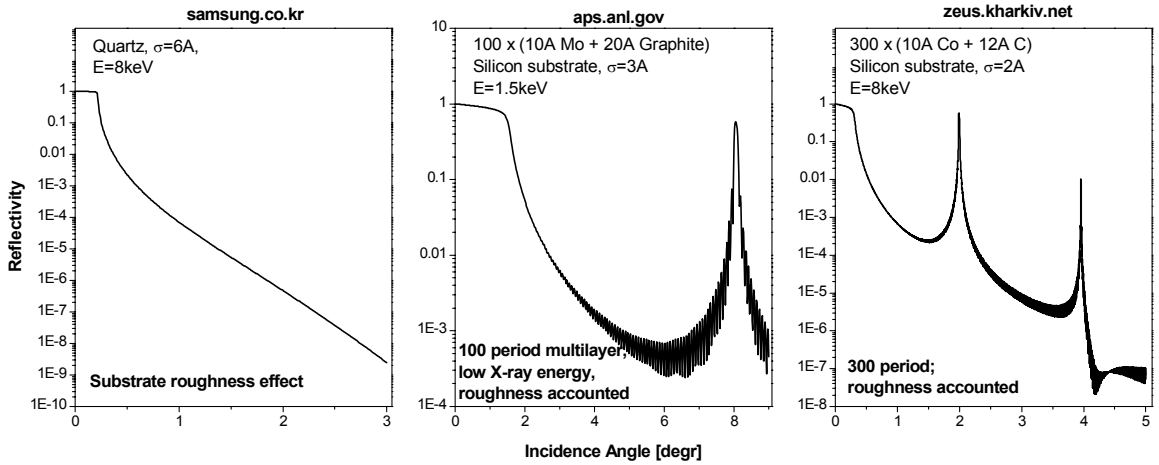

Fig. 6. Examples of ***TER_sl*** applications. From left to right: the effect of surface roughness in Quartz, the reflectivity of 100-period Si/C periodic multilayer with interface roughness, and the reflectivity of 300-period Co/C multilayer.

3.4 MAG_sl: resonance magnetic reflectivity

The ***MAG_sl*** program solves the problem of resonant X-ray reflectivity from magnetic multilayers. It is based on recent results by Stepanov and Sinha [21]. For a number of years magnetic materials were studied with neutrons, while the magnetic scattering of X-rays was not of practical interest because of its weakness as compared to X-ray charge scattering. The situation changed after the discovery of a huge resonant enhancement for the X-ray scattering near some absorption edges [24]. Although this effect is electric by nature (the resonance is caused by multipole electric transitions

in atoms), the scattering amplitude becomes a tensor oriented along the magnetic moment of atom. It occurs due to exchange effects and that is why the resonant scattering is called *magnetic*. The major application of X-ray resonant magnetic scattering is to probe thin magnetic films and magnetic multilayers -- see Figs.7 and 8. This is a hot topic related to studying magnetic heads for computer hard drives. However, since in this case the media susceptibility is a tensor, the conventional Parratt technique [20] 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*** [21]. The ***MAG_sl*** software also uses the same scripting language as in ***GID_sl*** and ***TER_sl*** for flexible input of multilayers parameters.

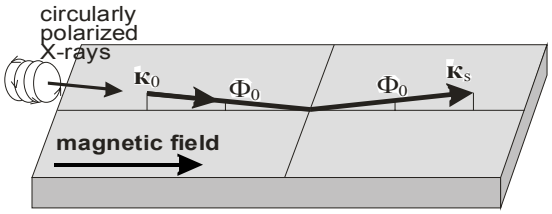

Fig.7. Schematic sketch of X-ray resonant magnetic reflectivity experiment. The effect is the strongest when the magnetic field is applied along the direction of X-ray incidence and the incident X-rays are circularly polarized.

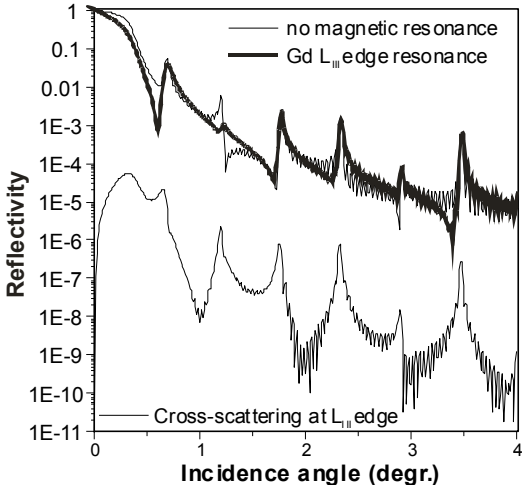

Fig.8. Calculated X-ray magnetic resonant reflectivity for Gd/Fe multilayer [15x(50A Gd + 35A Fe)] at Gd L_{III} edge (E=7.243 keV)

MAG_sl has attracted considerable interest of the community. Having been online for only one year, it became the forth most frequently used program at the X-ray Server (see Table I). Additionally, ***MAG_sl*** can be used to supply the X-ray wavefields for the calculations of X-ray diffuse scattering from magnetic roughness [22-23]. This software is in the Server development plans.

3.5 TRDS_sl: calculations of diffuse scattering from interface roughness

Based on a series of papers [25-27] the ***TRDS_sl*** (Total Reflection Diffuse Scattering) program calculates non-specular scattering of grazing incidence X-rays due interface roughness in multilayers – see Fig. 9. The basic ideas in this field

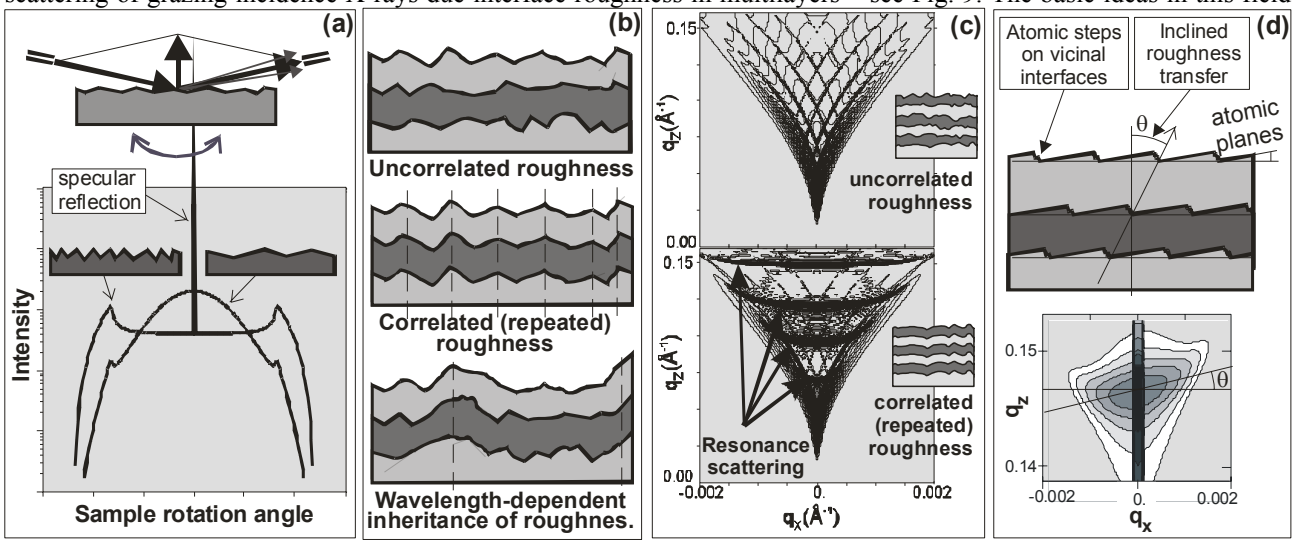

Fig. 9. Models of X-ray diffuse scattering supported by ***TRDS_sl***. (a): effect of affine surface roughness with different lateral correlation length on X-ray diffuse scattering (b): various types of interface-interface roughness correlation in multilayers, (c): respective maps of X-ray diffuse scattering in the reciprocal space, (d): asymmetric roughness at vicinal interfaces and skew interface-to-interface roughness correlations in crystals.

were formulated in the famous work by Sinha *et al* [28] where it was demonstrated that the angular pattern of non-specular X-ray scattering is related to the Fourier transform of the interface roughness spectrum. It gave rise to numerous applications of the technique in material science, especially in microelectronics where the electric properties of devices based on semiconductor multilayers are strongly affected by interface roughness.

The ***TRDS_sl*** software was initially developed for X-ray studies of interface roughness in AlAs/GaAs superlattices. Therefore, the primary goal of this software is to address roughness effects in crystals and interface-to-interface roughness correlations. However, interface roughness in non-crystalline solids is also covered. In the present form ***TRDS_sl*** implements several models for interface roughness spectrum (affine roughness and roughness due to atomic steps) and about 10 models for interface-to-interface roughness correlations in multilayers. Some of these models were suggested in [25-27] and some are due to other authors. Notable are the models for the scattering from:

- interface roughness in multilayers with wavelength-dependent correlations between different interfaces,
- atomic steps at vicinal interfaces in crystals,
- roughness with a skew interface-to-interface correlation in crystalline multilayers.

The calculations are performed using the distorted-wave Born approximation (DWBA) where roughness is considered as a "perturbation" to a plane interface. Within this model the X-ray wavefields corresponding to specular reflection from a multilayer with plane "non-disturbed" interfaces are provided by the ***TER_sl*** program. The input of multilayers parameters is implemented with the help of the same scripting language as in ***GID_sl***, ***TER_sl***, and ***MAG_sl***, and the scattering amplitudes are provided by ***X0h***. This saves the development effort and reduces the software learning period.

3.6 BRL: calculations of multiple Bragg diffraction

The ***BRL*** program is the most recent addition to the X-ray Server. It provides searches for multiple diffraction configurations in crystals and calculates multiple Bragg diffraction patterns with the algorithm [29] based on the extended dynamical diffraction theory (see Fig. 10 for an illustration of multiple Bragg diffraction). 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 can be neglected, then for the N-wave diffraction the size of the scattering matrix is 2N*2N (see e.g. [30]). Here the factor of two appears due to the two polarizations (sigma and pi) of X-rays. However, when the diffraction geometry involves grazing X-ray waves, the task becomes more complicated and for this case Colella suggested a theory where the calculations of multiple Bragg diffraction are reduced to the eigenvalue problem for 4N*4N scattering matrix [31]. This holds even if only one of e.g. 24 waves is grazing which is not effective in terms of calculations. Therefore, ***BRL*** uses a different algorithm suggested in [29] where it was made possible to reduce the calculations of multiple Bragg diffraction 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. 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 like only one of 24 waves is grazing the calculations are reduced dramatically.

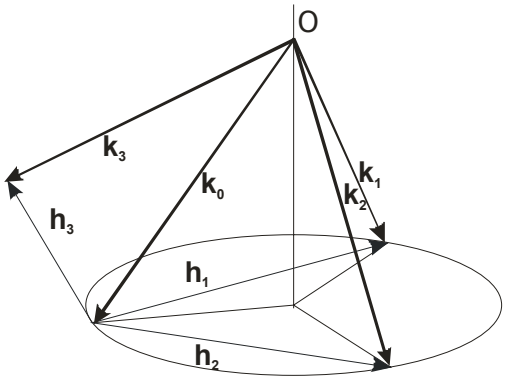

Fig.10. Example geometry of multiple Bragg diffraction (4-wave case). $\mathbf{k}_0$ is the incident wave , $\mathbf{k}_1$ to $\mathbf{k}_3$ are the diffracted waves, $\mathbf{h}_1$ to $\mathbf{h}_3$ are the reciprocal wave vectors simultaneously satisfying the Bragg condition. The Bragg conditions of 4-wave case fix the direction and the wavelength of incident X-rays while the cases with more than four waves can only be due to crystal symmetry. ***BRL*** applies vector constructions for crystals with arbitrary symmetry in order to multiple Bragg diffraction combinations.

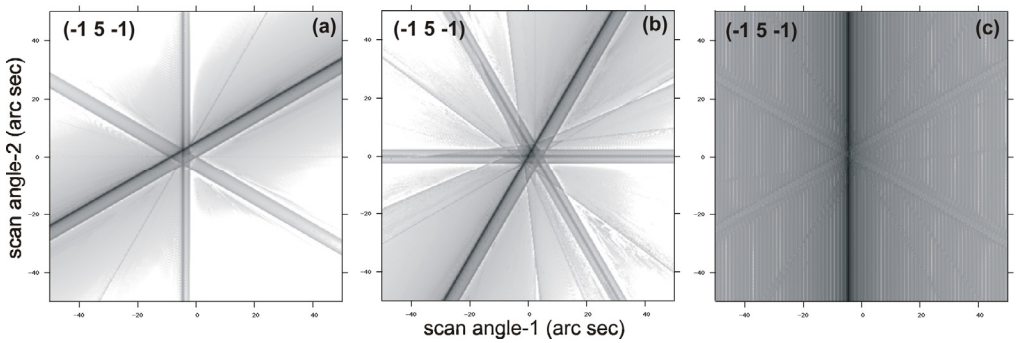

Fig. 11. Calculated intensity maps of multiple Bragg diffraction from Silicon 111 crystal at λ= 0.6968004107Å (tasks submitted from monash.edu.au). The Bragg planes are (3 3 -3), (3 -3 3), (-1 -1 5), (-1 5 -1), (5 -1 -1), (-3 3 3), (2 8 -2), (8 -2 2), and (8 2 -2); all Laue-case. (a): crystal thickness t=10,000μm and 6-wave approximation; (b): t=10,000μm and 10-wave approximation; (c): t=10μm and 10-wave approximation.

The applications of ***BRL*** are the fields of X-ray optics and X-ray crystallography (determination of the phases of X-ray scattering amplitudes, [32]). For example, it can be used to simulate the applications of Bragg- and Laue-case Renninger effect to X-ray double-plane collimation [33] and the multiple diffraction effect in the X-ray surface back diffraction [34]. Some examples of multiple diffraction patterns calculated with ***BRL*** are shown in Fig. 11.

4. DISCUSSION AND CONCLUSIONS

Some statistics of X-ray Server usage presented in Fig. 12 shows that the Server has a wide network of users that geographically covers the whole globe. The majority of requests come from the countries with strong X-ray traditions like USA, Germany, France, and Japan, although the Server log includes calculations originated even from such countries as Vietnam, Algeria, and Indonesia. In terms of applications, the highest Server usage is due to major synchrotrons followed by big research centers worldwide. A significant part of Server users constitute US government laboratories and the presence in this list of the Laurence Livermore National Laboratory (LLNL) and the National Institute of Standards and Technology (NIST) indicates that it is not only due to synchrotrons located in some labs. Many calculations are performed by various universities, especially by students. Finally, there is a considerable demand by research divisions of commercial companies. Thus, the statistics provides a good proof that the technology of sharing research results suggested by the Server works extremely well.

Although a big part of the project success can be attributed to the power of scientific software made available online, the Server demand should also be credited to a number of technological solutions emerged from everyday operations. To mention a few:

- all the programs are supplied with online guides and online access to respective publications,
- the HTML input forms are enhanced with help screens,
- the interfaces to the most of programs offer predefined templates for typical applications so that users can easier learn what parameters to be entered,
- the programs have similar input style (share the same scripting language for describing multiple layers) and use the same database of materials (***X0h***).

Another Server goal, the refining of scientific software, has also worked out extremely well. In 1997 at the beginning of Server operation the author had to fix software bugs weekly, while lately the programs have been running smoothly for many months. Although most of those bugs were due to insufficient input controls causing software misuse, a few problems with physical algorithms were found and fixed too. Then, due to monitoring of users activity the scientific software underwent considerable expansions. For example, ***GID_sl*** was extended to handle larger deviations from the Bragg condition and supplied with a simplified input for routinely used diffraction geometries. ***TER_sl*** was generalized for soft X-rays and large incidence angles up to 90 degrees. ***X0h*** was supplied with an interface to additional structure factor databases that extended it to a broader X-ray energy range, and etc. Most of those modifications were triggered by examining the Server logs and would not be possible if the software was given away instead of running on the Server. Only in a few cases the modifications were due to direct users contacts.

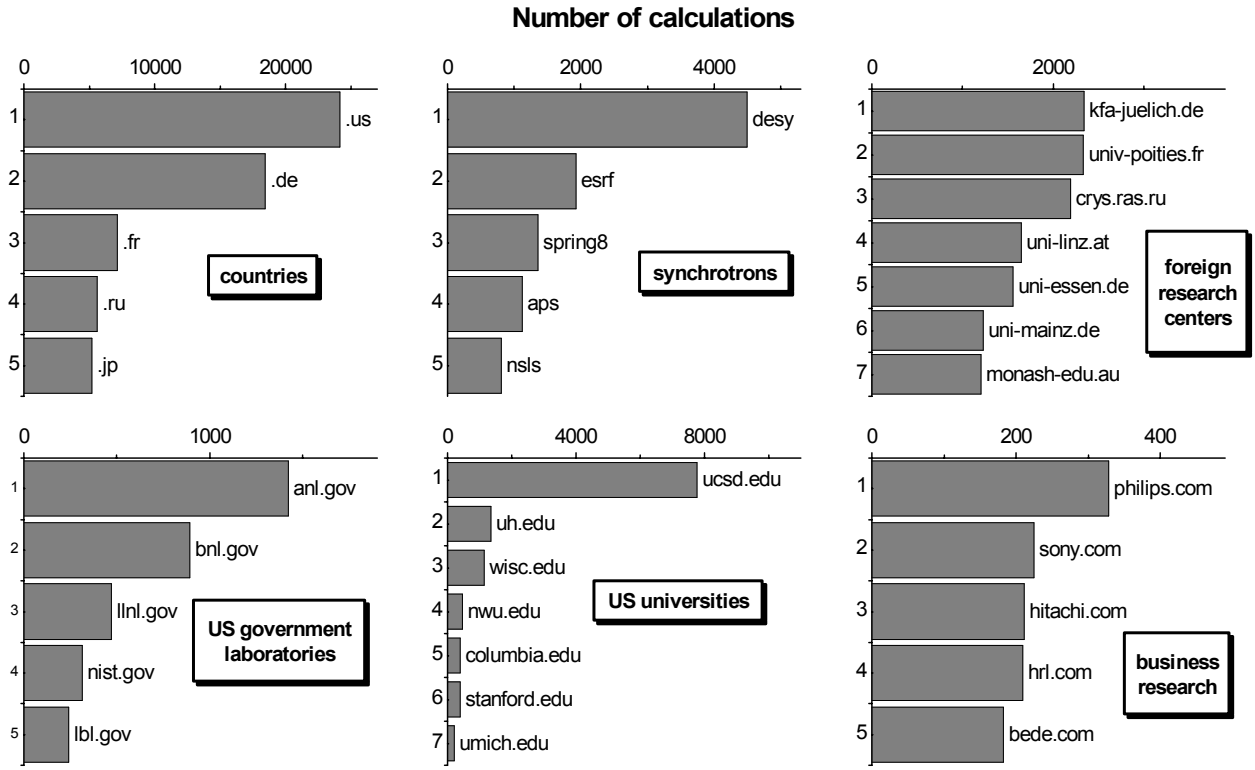

Fig. 12. Some statistics of X-ray Server usage as of May 2, 2004 (total number of calculations requests 81,372).

Additionally, the author has received dozens of submissions of new materials that were added to the ***X0h*** databases used by all the Server programs. With some automation, this process may trigger creating a community jointly expanding the databases of common interest.

The Server mission of establishing scientific collaborations worked less efficiently than the other goals. Although dozens of proposals have been received, the limiting factor has been that the author maintained the project in the background regime to his intensive primary job responsibilities. Therefore, only a small participation in the form of consulting was possible. It resulted in frequent acknowledgements (see e.g. [35,36]) and two research papers [23,37].

In general it is believed that the approach to sharing scientific software implemented in X-ray Server was the right choice resulted in great success. The plans for further Server developments are presented in Fig. 2. Some more interfaces to author's scientific software are planned, including the programs for simulating X-ray standing waves and diffuse scattering under the conditions of Bragg diffraction in crystals, and the software for calculating diffuse scattering from magnetic roughness. Then, it is planned to supply the software with fitting capabilities so that experimental data could be fitted online. Finally, the Server is open for collaborations in providing WWW interfaces for the third party scientific software.

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