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NOP: a new software tool for neutron optics

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Abstract

The neutron optics package (NOP) is a collection of codes for the computation of reactor spectra, neutron reflectivity of crystals, mirrors and multilayers and other quantities as cross-sections, attenuation in materials and refractive index. These calculations rely on the use of a database of materials cross-sections and crystal structures. NOP is freely distributed as an extension of the X-ray package XOP (Sánchez del Río, Dejus, SPIE Proceedings 3448 (1998) 340), from which it inherits the user interface and code structure. The NOP package can be used for estimating the reflectivity of optical elements as crystals and multilayers. The NOP output can also be used as an input for neutron instrument ray-tracing modules.

Keywords: Neutron optics software; Multilayer and crystal reflectivity

0. Introduction

The instrumentation associated with neutron sources includes complex and expensive optical elements. Therefore, it is highly desirable to accurately model and simulate these devices in order to achieve an optimum design in terms of performance and cost. We have developed a new software tool for the simulation of neutron optical elements as multilayers (used for neutron mirrors and guides) and imperfect crystals (used for neutron monochromators and analysers). The Neutron Optics Package (NOP) is a collection of codes to calculate the response of optical elements to neutron beams, in ideal conditions, i.e. monochromatic and collimated pencil beams. In order to include a realistic description of the beams, i.e. polychromaticity, size and divergence, a Monte Carlo method has to be used: as an example we present, in a different paper of these proceedings [1], an original simulation tool for describing Bragg diffraction by a large range of imperfect crystals. NOP is implemented on the top of the X-ray package XOP [2] and is freely distributed as an extension of it [3]. The NOP modules are: NSOURCES for neutron reactor spectra; NMIRROR for cross-sections, refractive index, attenuation and reflectivity by elements and compounds; IMD [4] for multilayer reflectivity; NCRYSTAL for perfect and mosaic crystal reflectivity; MAMON for indexing and computing the intensity of parasitic reflection in crystals. NOP uses a large database (DABAX) of

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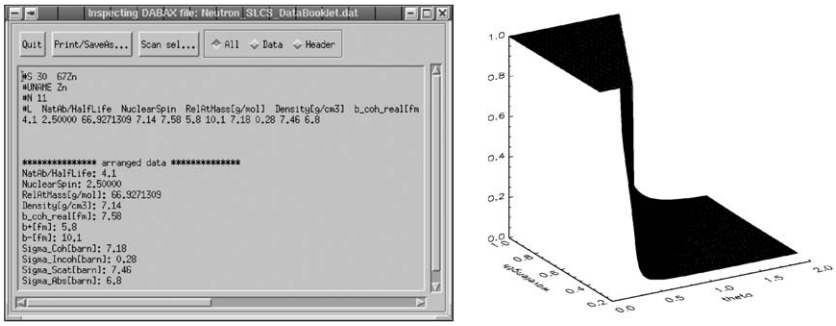

Fig. 1. Browsing the DABAX interface in the case of ^{67}Zn (left). Reflectivity of Fluorite vs. wavelength and angle calculated with NMIRROR (right).

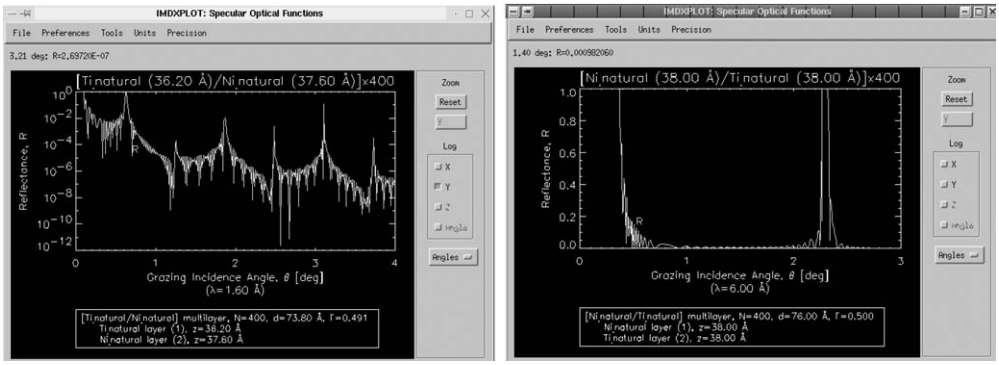

Fig. 2. Reflectivity of Ni/Ti multilayers.

neutron-scattering lengths and cross-sections and standard theories for the computation of attenuation, reflected and transmitted intensity. The cross-sections and scattering length files are the electronic version of the compilations published in the Special Feature section of Neutron News [5] and in the Neutron Data Booklet [6]. These data, together with the crystal structures and cell parameters database (previously present in XOP) are used for computing crystal structure factors. As shown in Fig. 1 the user can browse the complete DABAX database, choose an element and read the data concerning mass, density, neutron-scattering lengths and cross-sections. In the case of compounds, the same quantities, together with the refractive index, are evaluated with the NMIRROR module, which can also be used for computing the material's reflectivity, as shown in the same figure.

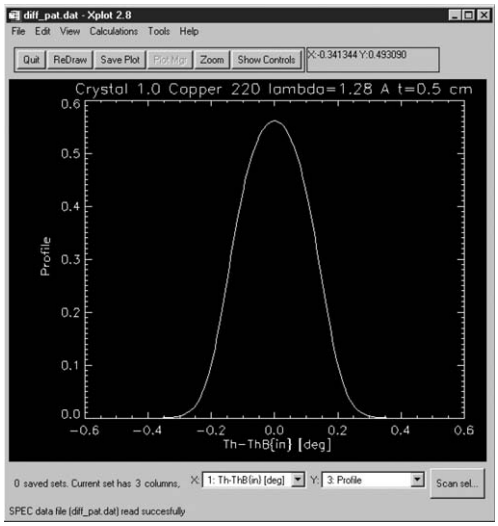

Fig. 3. Reflectivity of a Cu mosaic crystal. The XPLOT interface allows manipulating data, performing simple fit, printing the results. The user can also save the data in a format that can be read by other programs, e.g. for ray-tracing purposes.

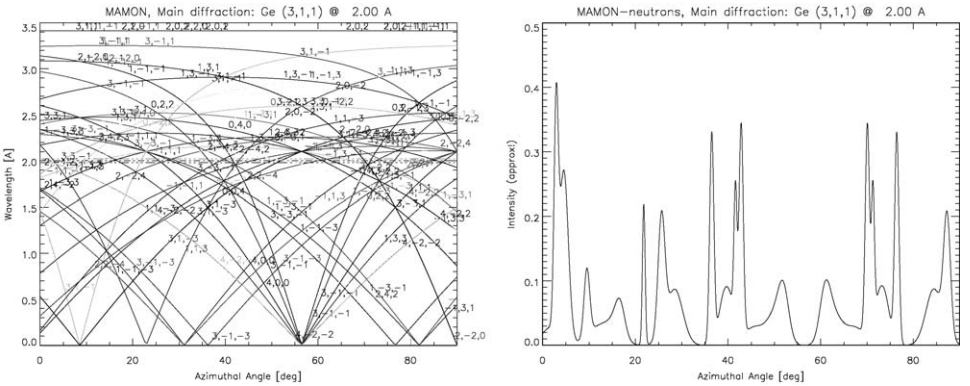

Fig. 4. Parasitic reflections for Ge 311 vs. the azimuthal angle, i.e. rotation of the crystal around the main diffraction vector. The plots represent indexing (left) and intensity (right). The crystal is set to reflect neutrons with $\lambda = 2$ Å.

1. Multilayers

NOP uses IMD [4] for modelling, fitting and plotting the optical properties of multilayers, i.e. systems consisting of any number of layers of any thickness. The original version of IMD works for optical and X-ray photons and is based on the use of a database of refractive index values compiled for many elements in a wide wavelength range. The IMD extension that we have implemented in NOP uses a similar database of neutron refractive indices. The examples in Fig. 2 report the reflectivity of Ni/Ti multilayers (an ultracold neutron filter in the figure on the right).

2. Crystals

The NCRYSTAL application computes the perfect and mosaic crystal reflectivity, according to the theories of Zachariasen [7] and Sears [8]. This NOP module can be used for estimating the reflectivity of crystals used as neutron monochromator and analysers, like Cu 220 in Bragg symmetric geometry shown in Fig. 3. Other interesting quantities, as structure factors, primary and secondary extinction lengths and Q scattering factors, are accessible via the NCRYSTAL interface. We recall that the standard theory describing diffraction by mosaic crystals does not account for effects coming from the non-ideality of the crystal. Primary extinction or inhomogeneities of the mosaic structure can be simulated by applying Monte Carlo techniques. The effect of multiple (or parasitic) Bragg scattering [9] can be estimated with MAMON. Also in this case, the original X-ray module has been interfaced to a neutron cross-section database. The indexing and intensities of multiple reflections for Ge 311 as a function of the azimuthal angle are shown in Fig. 4.

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References

[1] L. Alianelli, M. Sanchez del Rio, R. Felici, K. Andersen, E. Farhi, Phys. B, these Proceedings.
[2] M. Sánchez del Río, R.J. Dejus, SPIE Proc. 3448 (1998) 340.
[3] http://www.esrf.fr/computing/scientific/xop2.1/
[4] D.L. Windt, Comput. Phys. 12 (1998) 360.
[5] V.F. Sears, Neutron News 3 (1992) 29.
[6] H. Rauch, W. Waschkowshi, in: Neutron Data Booklet, Vol. 1.1, OCP Science (2002).
[7] W.H. Zachariasen, Theory of X-ray Diffraction in Crystals, Dover, New York, 1945.
[8] V.F. Sears, Acta Crystall. A 53 (1997) 35.
[9] H. Cole, F.W. Chambers, H.M. Dunn, Acta Crystall. 15 (1962) 138.