

Neutron Optics calculations with NOP

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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 [M. Sánchez del Río and R.J. Dejus, SPIE proceedings 3448, 340, 1998.], 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.

1. INTRODUCTION

We present a software package useful for neutron optics calculations. 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^{1,2}. NOP provides a graphic user interface, a complete cross-section database and programs for performing multilayers calculations (useful for neutron mirrors and guides) and imperfect crystals efficiency (for neutron monochromators and analysers). NOP is implemented on the top of the x-ray package XOP³ and is freely distributed as an extension of it⁴. The NOP modules are:

NSOURCES for neutron reactor spectra;

NMIRROR for cross-sections, refractive index, attenuation and reflectivity by elements and compounds;

IMD⁵ for multilayer reflectivity;

NCRYSTAL for perfect and mosaic crystal reflectivity;

MAMON for indexing and computing the intensity of parasitic reflections in crystals.

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2. CROSS-SECTION DATABASE AND MATERIAL CALCULATIONS

The original XOP DABAX database now includes neutron scattering lengths and cross-sections. These files are the electronic version of the compilations published in the Special Feature section of Neutron News⁶ and in the Neutron Data Booklet⁷. 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. The reflectivity of fluorite, *versus* wavelength and angle, calculated with NMIRROR, is shown in Fig. 1 (right). The optical constants (for instance refractive index as a function of wavelength), calculated by NMIRROR, can be saved in files that are used by IMD for multilayer calculations.

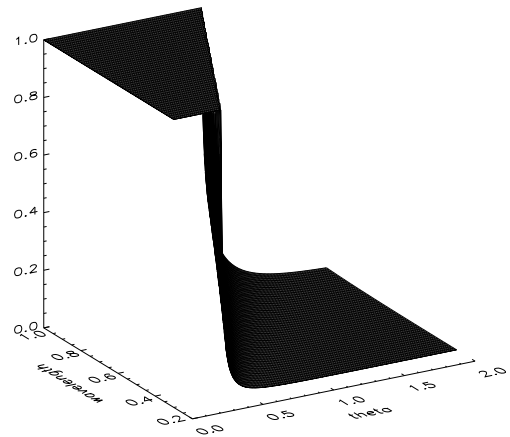
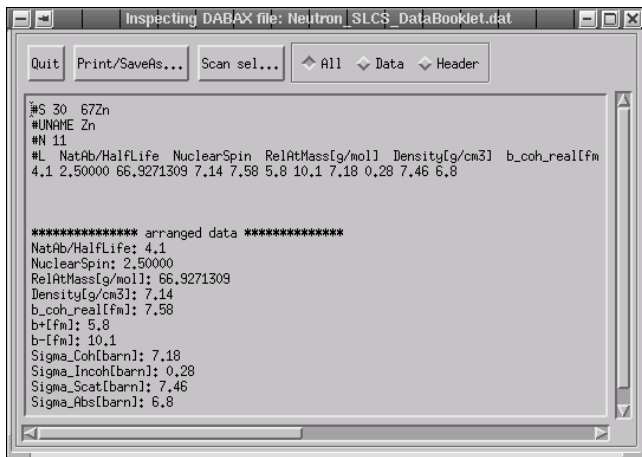


Figure 1. Browsing the DABAX interface in the case of ⁶⁷Zn (left). Reflectivity of Fluorite *versus* wavelength (Å) and angle (deg) calculated with NMIRROR (right).

3. MULTILAYERS

NOP uses IMD⁵ for modelling, fitting and plotting the optical properties of multilayers and supermirrors, *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. This database can be browsed from the IMD interface as shown in Fig. 2. Furthermore, it can be extended by the user by creating refractive index files. This can be useful in the case of magnetic multilayers and can be done with the NMIRROR application. The examples in Fig. 3 report the reflectivity of nickel-titanium multilayers. The plot at the bottom is the reflectivity of an ultracold neutron filter.

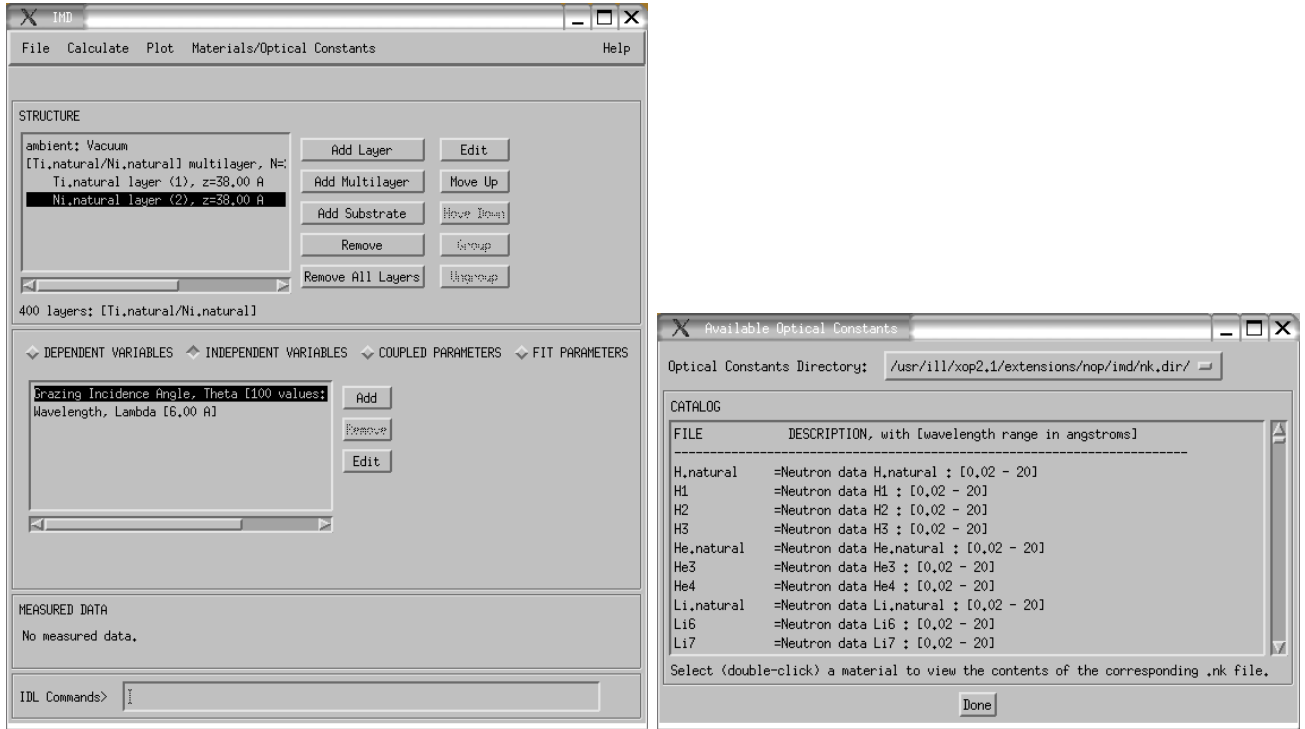


Figure 2. IMD interface. Left: creating the multilayer structure. Right: browsing the neutron refractive index database.

4. CRYSTALS

The NCRYSTAL application computes the perfect and mosaic crystal reflectivity, according to the theories of Zachariasen⁸ (perfect crystal dynamical diffraction or cinematal diffraction depending on the crystal thickness) and Sears⁹ (solutions of the Darwin equations). This NOP module can be used for estimating the reflectivity of a large range of crystals. Silicon, germanium, copper and graphite, which are some of the most commonly used for neutron monochromator and analysers, are included in the NCRYSTAL calculation. The theoretical reflected and transmitted intensity can be calculated with any asymmetry angle between the crystal surface and the Bragg planes. The calculation of transmitted (*i.e.* non diffracted) intensity is also implemented. The example of perfect silicon 111 and mosaic copper 220 in Bragg symmetric geometry are shown in Fig. 4. Other interesting quantities, as structure factors, primary and secondary extinction lengths and scattering factors, are accessible via the NCRYSTAL interface. We recall that the standard theory describing diffraction by mosaic crystals includes secondary extinction and multiple diffraction due to mosaicity, but it does not account for effects coming from the non ideality of the crystal. The effect of primary extinction or inhomogeneities of the mosaic structure cannot be evaluated using NCRYSTAL. However, they can be simulated by applying Monte Carlo techniques^{1,2}.

Multiple (or parasitic) Bragg scattering occurs when a single crystal is orientated in a neutron or x-ray monochromatic beam so that two, or more, sets of planes simultaneously satisfy Bragg law. This can be observed experimentally when the crystal is orientated to diffract from a particular set of Bragg planes, and is rotated slowly around the diffraction vector: changes in the intensity can be observed because the Bragg law can be simultaneously satisfied for a different set of planes¹⁰. In the case of mosaic crystals this effect is observed on a wavelength range larger than that of perfect crystals because of the presence of misoriented blocks. This can have an important role in the decrease of the diffracted intensity, especially at higher neutron energy. The effect of multiple Bragg scattering 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 germanium 311 as a function of the azimuthal angle are shown in Fig. 5.

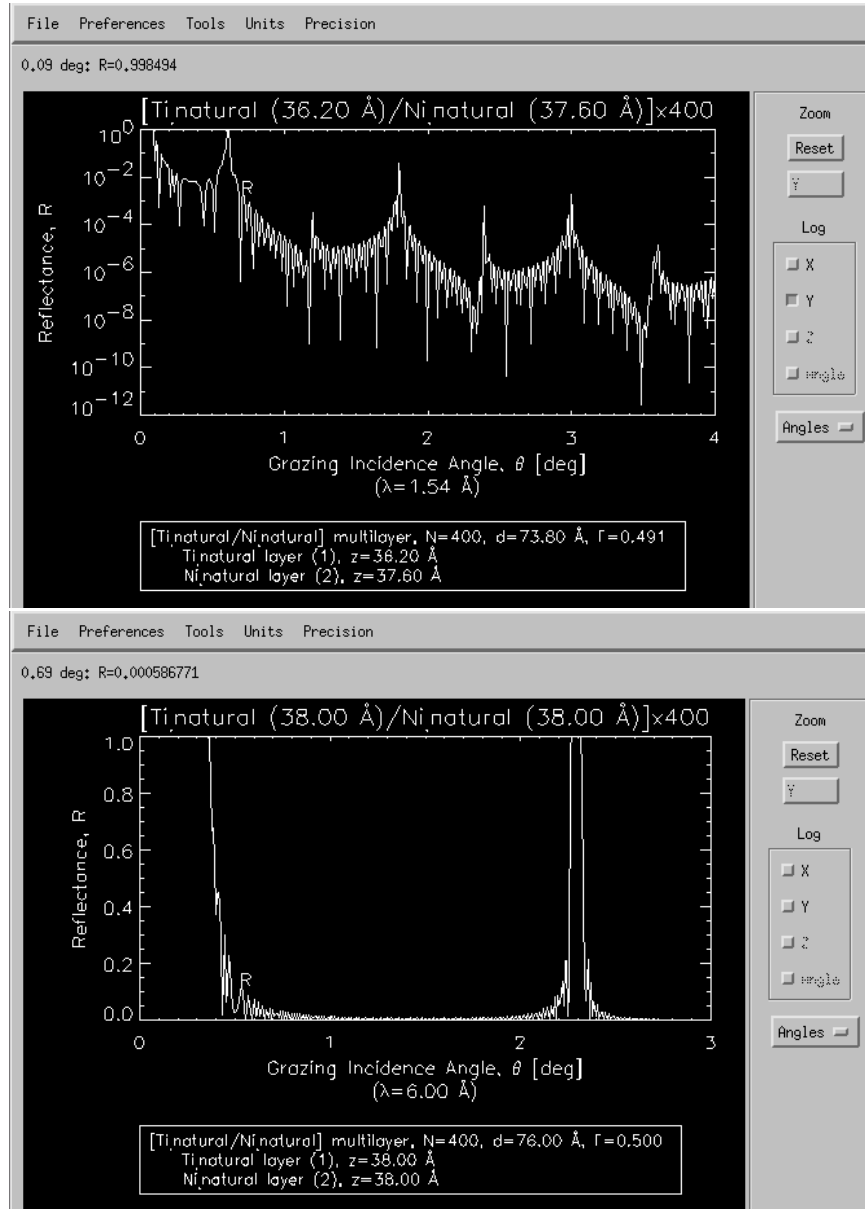


Figure 3. Reflectivity of nickel-titanium multilayers.

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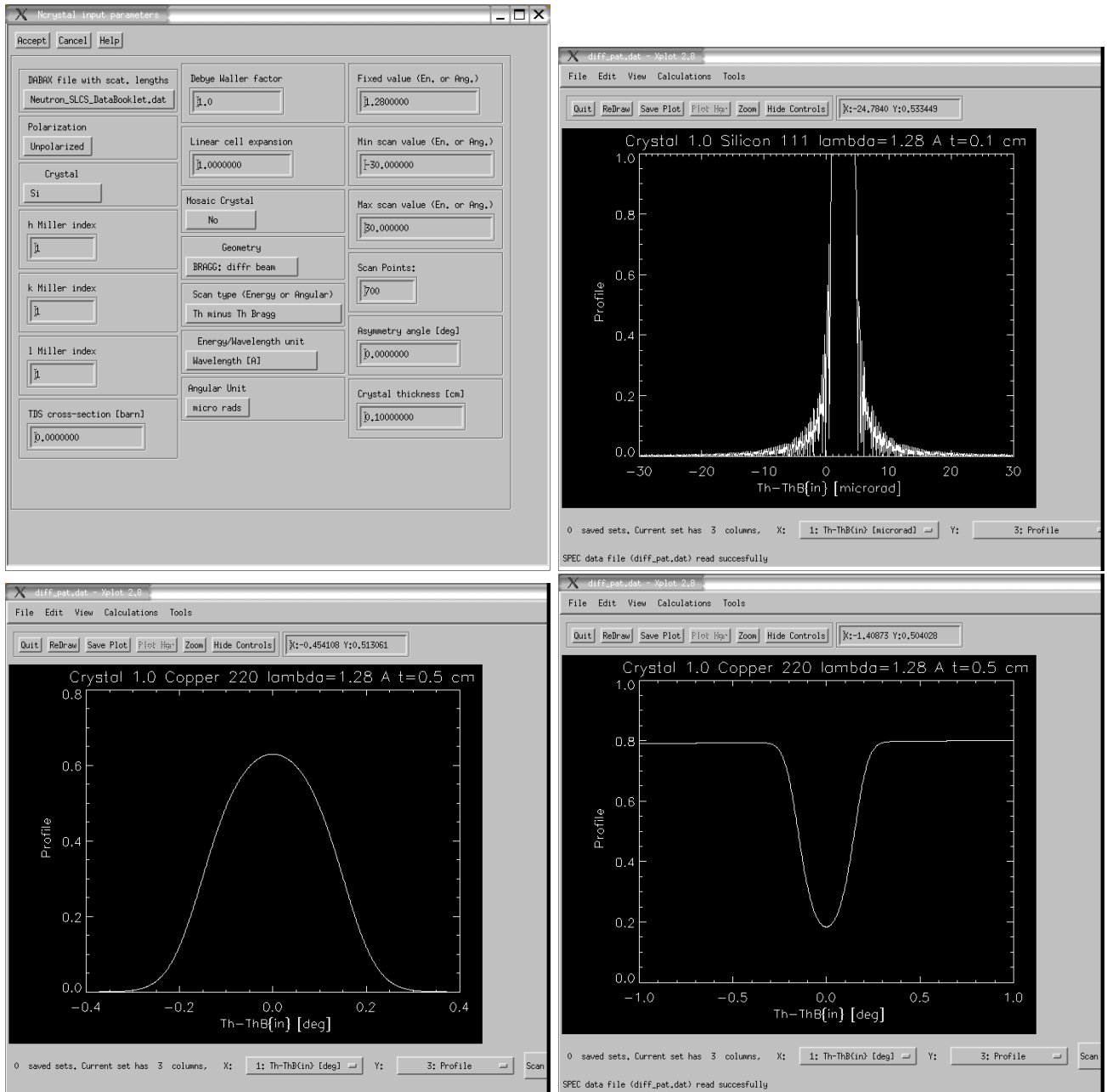


Figure 4. Top: NCRYSTAL interface and perfect silicon 111 reflectivity. Bottom: reflected and transmitted intensity from mosaic copper 220. The XPLOT interface allows manipulating data, performing simple fit, printing the results. The user can also save the data in a format that can be read by other programs, e.g. for ray-tracing purposes.

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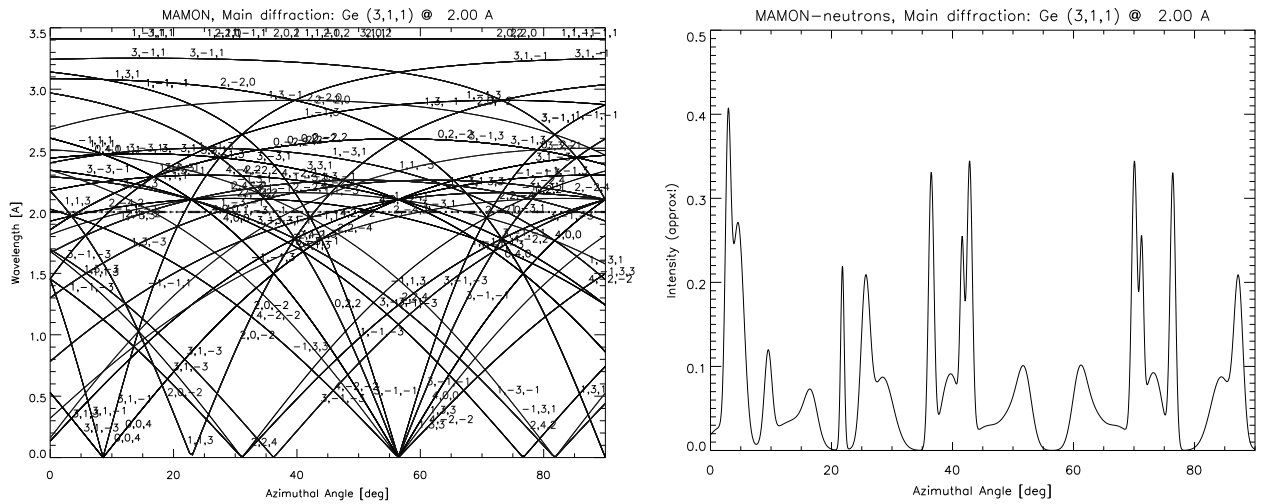
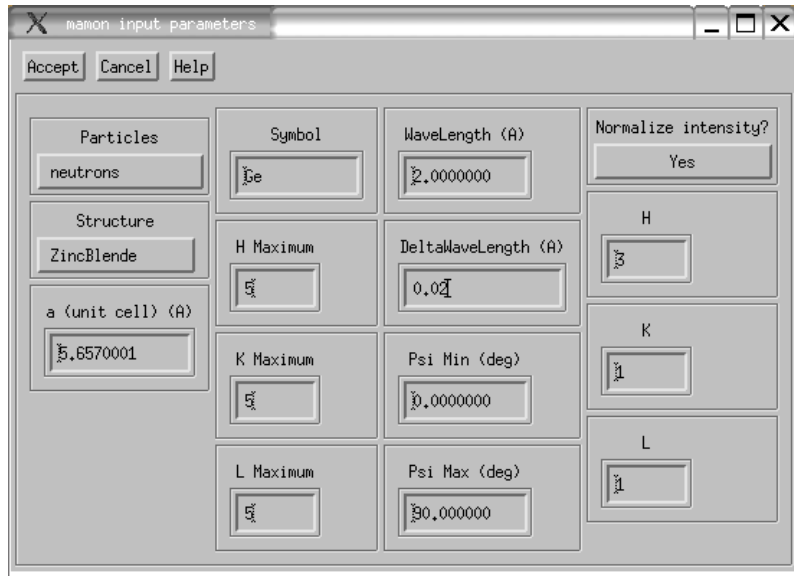


Figure 5. Top: MAMON interface. Bottom: parasitic reflections for germanium 311 *versus* the azimuthal angle, *i.e.* rotation of the crystal around the main diffraction vector. The plots represent indexing (left) and intensity (right). The crystal is set to reflect neutrons with $\lambda = 2 \text{ \AA}$.

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