Evaluation of Synchrotron Based NRS Data

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The discovery of nuclear resonant scattering (NRS) using a synchrotron radiation source by *Gerdau et al.* in 1985 [1] was followed by intense development that was fuelled by availability of third-generation synchrotron facilities: the ESRF in Grenoble, France; the APS in Argonne, USA; the SPring-8 in Hyogo, Japan, and more recently PETRA III in Hamburg. A variety of NRS were explored during the earlier period and some have survived the test of practicality and are in use today for applications such as the study of vibrational and magnetic properties of condensed matter under extreme conditions. In this presentation, specific evaluation software for a selection of NRS techniques is discussed with emphasis on their potential for applicability and availability to users.

The scheme in Figure 1 illustrates how four classes of NRS are distinguished: coherent elastic (I); incoherent elastic (II); incoherent inelastic (III). Each class has seen development of specific tools as shown in Table I that have been used in a variety of applications, and superior brightness and focused spectral flux density of third-generation synchrotron radiation facilities has permitted scientists to develop applications with ever smaller samples under increasingly extreme conditions.

Early nuclear resonant scattering studies showed that synchrotron radiation experiments with nuclear resonances greatly benefitted from a new, translational approach: time resolved instead of energy resolved measurements, the latter familiar to traditional Mössbauer spectroscopy. This advance resulted from the time structure of synchrotron radiation, which is emitted as a sequence of very short x-ray pulses of typically less than 100 ps duration. Energy spectroscopy in the μeV to neV range is possible by analysis of the time-decay pattern of x-rays scattered off or transmitted through samples containing a suitable nuclear resonant isotope. The measurement and analysis of such time spectra constitutes the main part of the NFS/SMS, GINRS, NBS/NLS, NLE, and SRPAC methods. NRIXS on the other hand, integrates time spectra but nevertheless requires time discrimination.

Nuclear resonant scattering science continues to evolve with enhanced instrumentation, improvement of synchrotron radiation sources, development of nuclear resonant methods, and new applications. Almost always scientific results rely critically on tested and easily accessible evaluation software, such as the CONUSS and PHOENIX programs [3]. Continuous maintenance of software and proper hands-on training to potential users are very important to optimize user experience.

Table I: Nuclear resonant scattering tools and classes. Abbreviations: Nuclear Resonant Inelastic X-ray Scattering (NRIXS); Nuclear Resonant Vibrational Spectroscopy (NRVS); Nuclear Forward Scattering (NFS); Synchrotron Mössbauer Spectroscopy (SMS); Grazing Incidence Nuclear Resonant Scattering (GINRS); Nuclear Bragg/Laue Scattering (NBS/NLS); Nuclear Lighthouse Effect (NLE); Synchrotron Radiation Perturbed Angular Correlation (SRPAC); traditional Mössbauer Spectroscopy (MS).

tool	I	II	III
NRIXS/NRVS	-	-	X
NFS/SMS	X	-	-
GINRS	X	-	-
NBS/NLS	X	-	-
NLE	X	-	-
SRPAC	-	X	X
MS	-	X	X

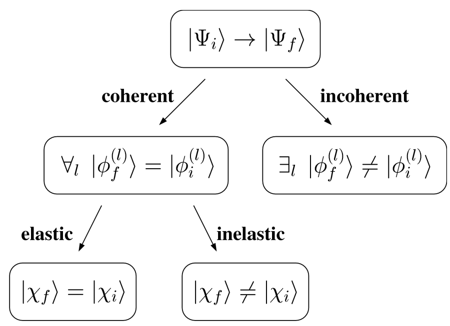

Figure 1. Classification of scattering processes. The quantum state of the scatterer $|\Psi\rangle$ is factorized into quantum states of the atom cores $|\phi\rangle$ and vibrations $|\chi\rangle$. (adapted from [2])

1 E. Gerdau et al., Phys. Rev. Lett. 54, 835-838 (1985).
2 W. Sturhahn, J. Phys.: Condens. Matter 16, S497-S530 (2004).
3 https://www.nrixs.com