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INELASTIC X-RAY SCATTERING FROM COLLECTIVE ATOM DYNAMICS

F. SETTE - M. KRISCH
European Synchrotron Radiation Facility, Grenoble, France

1. INTRODUCTION

The study of atomic dynamics in condensed matter at momentum transfer, $\boldsymbol{Q}$, and energy, E, characteristic of collective motions is, traditionally, the domain of neutron spectroscopy. The experimental observable is the dynamic structure factor $S(\boldsymbol{Q},E)$, which is the space and time Fourier transform of the density-density correlation function. Neutrons as probing particle are particularly suitable, since

- the neutron-nucleus scattering cross-section is sufficiently weak to allow for a large penetration depth,
- the energy of neutrons with wavelengths of the order of inter-particle distances is about 100 meV, and therefore comparable to the energy of collective excitations associated with density fluctuations such as phonons, and
- the momentum of the neutron may be used to probe the whole dispersion scheme out to several $Å^{-1}$.

This is in contrast to inelastic light scattering techniques such as Brillouin and Raman scattering, which can only determine acoustic and optic modes, respectively, at very small momentum transfers.

While it has been pointed out in several text books [1,2] that X-rays can in principle be utilized as well to determine the $S(\boldsymbol{Q},E)$, it was stressed that this would represent a formidable experimental challenge, mainly owing to the fact that an X-ray instrument would have to provide an extremely high energy resolution. This is understood considering that photons with a wavelength of $\lambda = 0.1$ nm have an energy of about 12 keV. Therefore, the study of phonon excitations in condensed matter, which are in the meV region, requires a relative energy resolution of at least

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$\Delta E/E \approx 10^{-7}$. On the other hand, there are situations where the use of photons has important advantages over neutrons. A specific case is based on the general consideration that it is not possible to study acoustic excitations propagating with the speed of sound v_s using a probe particle with a speed v smaller than v_s. This limitation is not particularly relevant in neutron spectroscopy studies of crystalline samples. Here, the translation invariance allows one to study the acoustic excitations in high order Brillouin zones, thus overcoming the above-mentioned kinematic limit on phonon branches with steep dispersions. On the contrary, the situation is very different for topologically disordered systems such as liquids, glasses and gases. In these systems, in fact, the absence of periodicity imposes that the acoustic excitations must be measured at small momentum transfers. Thermal neutrons have a velocity in the range of 1000 m/s, and only in disordered materials with a speed of sound smaller than this value (mainly fluids of heavy atoms and low density gases) the acoustic dynamics can be effectively investigated [3]. Another advantage of the inelastic X-ray technique arises from the fact that very small beam sizes of the order of a few tens of micrometers can presently be obtained at third generation synchrotron sources. This opens the possibility to study systems available only in small quantities down to a few 10^{-6} mm^3 and/or their investigation in extreme thermodynamic conditions, such as very high pressure. These differences with respect to inelastic neutron scattering motivated the development of the very high resolution inelastic X-ray scattering (IXS) technique, and following the pioneering experiments in 1986 [4,5], the IXS technique rapidly evolved. To date there are four instruments operational at the ESRF (2), APS (1) and Spring-8 (1), and several more under construction.

The aim of the present article is to give the reader an introduction to the IXS technique, where the similarities and differences with respect to coherent inelastic neutron scattering (INS) shall be highlighted, therefore providing a natural link to other chapters of volume *V*. The present capabilities of the IXS technique are illustrated by discussing two representative experiments in some detail.

2. *SCATTERING KINEMATICS AND INELASTIC X-RAY SCATTERING CROSS-SECTION*

The inelastic scattering process is depicted schematically in figure 1. The momentum and energy conservation impose that

$$\boldsymbol{Q} = \boldsymbol{k}_i - \boldsymbol{k}_f \qquad \{1a\}$$