APPLICATIONS OF PHONON EXTINCTION RULES FOR INELASTIC NEUTRON SCATTERING AND THERMAL DIFFUSE SCATTERING EXPERIMENTS

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The determination of crystal phonon frequencies through experiments of coherent inelastic neutron scattering is now a rather standard technique in solid state physics which, in principle, allow the determination of the phonon spectra. However, a proper interpretation of the results and/or an unambiguous comparison with theoretical predictions requires in many cases additional information on the symmetry of the phonon modes. Usually only partial symmetry assignments are achieved either by comparison with other spectroscopic results or complex lattice dynamic model calculations. It is a quite widespread belief that inelastic neutron scattering experiments do not obey any particular systematic symmetry extinction rules except for the obvious ones coming from the transverse or longitudinal character of their polarization vectors. Recently, it has been demonstrated the existence of general selection rules which are of considerable help in identifying the symmetries of the measured phonon branches[1]: the resulting restrictive phonon absences depend only on the mode symmetry and the scattering vector, and not on the specific atomic positions in the crystal structures.

The aim of the present contribution is the development of the above-mentioned theoretical results into a systematic procedure. One of its essential steps is the distribution of the reciprocal-space vectors (Brillouin zones) into orbits with respect to a point group describing the symmetry properties of the scattering vector. It is possible to show that Brillouin zones belonging to the same orbit are characterized by the same selection rules, which is of essential importance for the analysis and the optimization of the inelastic neutron scattering experiments.

In addition, we discuss the straightforward extension of the selection-rules procedure to thermal diffuse scattering studies (including those with X-rays). The corresponding extinction rules allow a quantitative account for the phonon induced scattering (dynamic disorder) which proves to be very useful, *e.g.* in phase-transition problems.

The simplicity and the importance of the phonon extinction rules are demonstrated by their application on several examples. In the analysis of the phase transition in K_2SnCl_6[2] it is possible to characterize symmetrically not only the mode driving the phase transition, but also a low lying dispersion branch of symmetry compatible with that of the critical mode. In cristobalite[3] the dynamically disordered nature of the high temperature phase is accessed. The application of the extiction rules in the leucite case[4] permits the identification of the corresponding active modes.

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