

13.1-4 NEUTRON SINGLE-CRYSTAL DIFFRACTOMETRY WITH AN AREA DETECTOR. By G.J. McIntyre, R.F.D. Stansfield, S.A. Mason and M. Thomas, Institut Laue-Langevin, 156X, 38042 Grenoble Cédex, France.

In principle the combination of an Eulerian cradle with which to orient a single-crystal sample and a large two-dimensional position sensitive detector allows a nearly free choice of rotation axis about which to scan each reflection, and a wide choice of where the reflection strikes the detector. In practice the optimum choice of scan geometry and data-collection strategy for a particular sample will be determined by the shape and the permissible motion of the detector, by the instrumental resolution function and by the ratios of the unit cell dimensions to the wavelength.

For the specific case of the narrow ($4^\circ \times 64^\circ$), vertically curved detector on the D19 diffractometer at the ILL, there are three obvious scan geometries: i) equatorial-plane; ii) normal-beam; and iii) flat-cone. For each geometry the accessible regions of reciprocal space and the smallest scanned regions necessary to include a complete set of independent reflections (if possible) are discussed. A simple formalism for the resolution function and its influence on the scan geometry are also presented. In particular the differences in reflection size and motion between conventional four-circle geometry and the non-equatorial geometries are emphasized. Suitable strategies for data collection are prescribed for crystals of different symmetry and unit cell dimensions. In some cases a combination of geometries is necessary. The conclusions are illustrated by results from measurements on samples of greatly different unit cell dimensions. These include several small molecules and a protein.

13.2-1 STUDY ON ACOUSTICAL ACTIVITY OF $\text{Bi}_{12}\text{GeO}_{20}$ BY NEUTRON INELASTIC SCATTERING.

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Acoustical activity of $\text{Bi}_{12}\text{GeO}_{20}$ has been studied by measuring a splitting of the degeneracy of transverse acoustical waves propagating along the directions corresponding to acoustic axes, [100] and [111], by using neutron inelastic scattering. A comparison with the experimental results of quartz and NaClO_3 (C. Joffrin, et, J. Physique-Lettes 41 (1980) L-391-L-395) has been done. Three striking features of acoustical activity could be obtained from present study.

Firstly, specific rotary power φ/l is directly proportional to q^2 (where q is the reduced wave vector of transverse acoustical wave) for small q , named square law here, as a prediction of a phenomenological theory on acoustical activity based on the concept "first-order spatial dispersion" (Portugal, D.L., et, Phys. Rev. 170 (1968) 673). And its validity also has been proved by the results of neutron scattering (C. Joffrin, et, mentioned above), ultrasonic measurements and Brillouin scattering (Pine, A.S., Phys. Rev. B2 (1970) 2049). But the q limit within which the square law holds is shown to be different for different kinds of crystals. And it has nothing to do with what kind of point group the crystal belongs to, which is unexpected preliminarily.

Secondly, the eigen modes of transverse-acoustical vibration propagating along higher symmetrical axes in acoustically active crystals are right and left circularly polarized acoustical modes (RCPAM and LCPAM). The present results show the integral intensities of neutron scattering of RCPAM and LCPAM still obey the law of $1/\omega \cdot (1 - \exp(-\hbar\omega/KT))$ within the limit of our experimental error, the same as the linearly polarized modes in normal crystals. It means that this law is more fundamental.

Thirdly, RCPAM and LCPAM have different propagating velocities along the acoustical axes, as shown before. Now the present results show that they have a remarkably different attenuation also, and the attenuation of the faster one is larger. That is, the attenuation of LCPAM is larger in a left-hand crystal and vice versa. Some results on $\text{Bi}_{12}\text{SiO}_{20}$ are present here and a comparison with $\text{Bi}_{12}\text{GeO}_{20}$ has been done also.

At end of the paper the relations between acoustical activity and optical activity are also mentioned briefly.

13.2-2 SPECTROSCOPIC DATA, LATTICE DYNAMICS AND DISCRETE QUANTUM STATES OF SOLIDS. By V.I. Muromtsev, Yu.N. Venevtsev, Karpov Institute of Physical Chemistry, Moscow, USSR

Spectroscopic data can be interpreted either in terms of frequencies or quantum states (QS). A quantum approach involves already at an early stage the problem of relative location of QS and then brings forth an even more difficult task of systematizing the QS. Using such an approach to analyse spectral data on lattice dynamics for a number of different solids (Muromtsev et al., DAN SSSR (1976) 227, 1405), we have discovered for them an identical subsystem of discrete QS, described by the empiric relation

$$E = B [J(J+1) - \lambda^2], \text{ where } B = 8.7 \text{ cm}^{-1}; \\ J = 1, 2, 3, \dots; \lambda = 0, \pm 1, \pm 2, \dots; |\lambda| \leq J.$$

In this report, the applicability of this relation is demonstrated by analysing neutron, Raman and Brillouin scattering spectra for SrTiO_3 (Muromtsev et al., Fizika i khimiya tverdogo tela. NIFI, Moscow (1978), vyp. 9, p.4) and solid He (Muromtsev, Safronov, Spektroskopiya atomov i ionov v rentgenovskoi i ultravioletovoi oblastiakh. AN SSSR, Nauchnyi Sovet po spektroskopii, Moscow (1982), p. 206).

It is concluded that the temperature changes in spectra of solids, including those related to the presence of soft modes, and the discovered multiplicities of critical temperature points in solids can be interpreted in terms of corresponding QS by studying temperature dependences of their population and possible transitions between them (Venevtsev et al., DAN SSSR (1976) 230, 121).