

## 4.1. THERMAL DIFFUSE SCATTERING OF X-RAYS AND NEUTRONS

elastic constants are represented by  $c_{ij}$  with  $i, j = 1, \dots, 6$ . Applying the principle of conservation of energy gives

$$c_{ij} = c_{ji}$$

and the number of constants is reduced further to 21. Crystal symmetry effects yet a further reduction. For cubic crystals there are just three independent constants ( $c_{11}$ ,  $c_{12}$ ,  $c_{44}$ ) and the  $6 \times 6$  matrix of elastic constants is

$$\begin{pmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0 \\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & c_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & c_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & c_{44} \end{pmatrix}.$$

In principle, the elastic constants can be derived from static measurements of the four quantities – compressibility, Poisson's ratio, Young's modulus and rigidity modulus. The measurements are made along different directions in the crystal: at least six directions are needed for the orthorhombic system. The accuracy of the static method is limited by the difficulty of measuring small strains.

Dynamic methods are more accurate as they depend on measuring a frequency or velocity. For a cubic crystal, the three elastic constants can be derived from the three sound velocities propagating along the single direction [110]; for non-cubic crystals the velocities must be measured along a number of non-equivalent directions.

Sound velocities can be determined in a number of ways. In the ultrasonic pulse technique, a quartz transducer sends a pulse through the crystal; the pulse is reflected from the rear surface back to the transducer, and the elapsed time for the round trip of several cm is measured. Brillouin scattering of laser light is also used (Vacher & Boyer, 1972). Fluctuations in dielectric constant caused by (thermally excited) sound waves give rise to a Doppler shift of the light frequency. The sound velocity is readily calculated from this shift, and the elastic constants are then obtained from the velocities along several directions, using the Christoffel relations (Hearmon, 1956). The Brillouin method is restricted to transparent materials. This restriction does not apply to neutron diffraction methods, which employ the inelastic scattering of neutrons (Willis, 1986; Schofield & Willis, 1987; Popa & Willis, 1994).

Tables of elastic constants of cubic and non-cubic crystals have been compiled by Hearmon (1946, 1956) and by Huntingdon (1958).

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