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DETERMINATION OF THE ELASTIC CONSTANTS OF GALLIUM BY MEASUREMENT OF X-RAY DIFFUSE SCATTERING

V. P. Glagoleva, A. P. Zvyagina, and Fung Van Tkhom

M. V. Lomonosov Moscow State University

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The measurement of the intensity of x-ray diffuse scattering to determine the elastic constants of crystals was described in detail in [1-3]. The intensity of x radiation scattered by the crystal can be represented as a sum $I = I_0 + I_{d_1} + I_{d_2} + \ldots$, where I_0 is the intensity of the interference maximum, I_{d_1} is the intensity of the first order diffuse scattering (single-phonon scattering), and the subsequent terms are defined respectively as the intensity of scattering with participation of two, three and more phonons. Close to the reciprocal lattice points the diffuse scattering of second and higher orders can be neglected and one can assume that the main contribution to the intensity is given by single-phonon processes.

Using the results of the classical theory of elasticity and the theory of x-ray scattering, Jahn [4] and later Prasad and Wooster [5] showed that the intensity of the diffuse scattering close to reciprocal-lattice point can be represented in the form

$$I_{d_1} = \frac{kT}{\tau} |F_T|^2 \frac{H^{*2}}{K^{*2}} \mathcal{K}[f]_g,$$

where F_T is the structure amplitude at the temperature T, τ is the volume of the unit cell, H* is a reciprocal lattice vector, K* is the wave vector of the elastic wave, $\mathcal{K}[f]_g$ is a function defined by the value of the elastic constants and the direction cosines of the wave vector f and the vector g of the nearest reciprocal lattice point.

In a small interval one can assume that the function $I_{d_1} = I(1/K^{*2})$ is a straight line, and, determining the angle of the inclination to the axis $(1/K^{*2})$, one can find the value of $\mathcal{K}[f]_g$ for definite values of f and g. Having a set of equations for $\mathcal{K}[f]_g$ for different combinations of f and g, one can obtain the values of the elastic constants of the crystal.

In our investigation this method was used to find the elastic constants of gallium. In the case of gallium the x-ray method is to be preferred since gallium is very plastic and has a low melting point (~30°C).

Gallium single crystals were grown from the melt by the seed crystal method. The seed crystals were chosen from Laue diffraction patterns so that one of the faces was the plane with indices (001). The gallium was melted in an electric furnace held at the temperature of 45°C, and was then slowly cooled to 30°C. Then it was poured into a collapsible form made of quartz laminas, to one of which the seed crystal was attached. An almost cubic crystal was obtained with an edge of about 1 cm, bounded along the planes {100}.

The orientation of the samples was refined using epigrams. Then on the instrument URS-50I with monochromated Cu Kα radiation a series of measurements was made of the intensity of the x-ray diffuse scattering close to the (400), (040), and (006) reciprocal lattice points.

Gallium has a rhombic lattice with $a = 4.5107 \pm 0.0001$ Å, $b = 4.5167 \pm 0.0001$ Å, $c = 7.6448 \pm 0.0002$ Å and belongs to the space group D^{18}_{2h} [6]. In the cell there are eight atoms which are unique in their structural relationship which leads to the appearance of optical vibrations in such a lattice. However, the intensity of x-ray scattering due to high-frequency optical vibrations close to podes is considerably smaller than the intensity due to low-frequency acoustic vibrations and we can therefore neglect the optical contribution to the intensity.