05.2-14
ELASTIC CONSTANTS OF m-DINITROBENZENE FROM DIFFUSE REFLECTION OF X-RAYS. By S.B. Sarkar and S.K. Talapatra, X-ray Laboratory, Molecular Physics Division, Dept. of Physics, Jadavpur University, Calcutta - 700 032, India.

All the nine elastic constants of orthorhombic (Pbn 2_1) m-dinitrobenzene $C_6H_4N_2O_4$ (J. Trotter, Acta. Cryst. 18(1961) 244) have been determined at room temperature (293K - 298K) from the measurement of intensities of thermal diffuse scattering (TDS) of X-rays using photographic-photometric method (S.C. Chakraborty & R.K. Sen, Bull. Natl. Inst. Sci. (India), 14(1958) 20). The method is best suited for small single crystals compared to other methods where large single crystals are needed. A series of Laue photographs were taken with a monochromatic CuK_α radiation obtained by reflection from a Fluorite crystal. The direct beam was reduced photo-graphically after being absorbed through Nickel foils of known thickness, its intensity being reduced to a factor of 10^6. Diffuse scattering domains near the reciprocal lattice nodes 600, 040, 081, 101 & 520 were extensively studied. The average time of exposure varied from 20-40 hours depending on the structure factors of the plane considered. The intensity of the observed diffuse reflection was corrected for skew, polarisation, divergence, mosaicity and background correction following G.N. Ramachandran & W.A. Wooster (Acta. Cryst, 4(1951a) 335 and Acta. Cryst 4(1951b) 431), J.L. Amorós & M. Amorós (Molecular Crystals, New York, John Wiley (1968). The absorption correction was determined graphically following G. Albrecht (Rev. Sci. Instrum, 10 (1930) 221). The correction due to second-order TDS was made for all constants by the method of successive-approximation following Ramachandran & Wooster (1951 (a,b) and B.W. Lucas (Acta. Cryst A 24 (1968) 336). The values of elastic constants in units of 10^9 Nm^{-2} are :-

C_{11} = 10.70 (05), C_{22} = 11.30(03), C_{33} = 20.27 (19), C_{44} = 4.37 (04), C_{55} = 2.04(05), C_{66} = 5.31 (03), C_{12} = 6.30 (18), C_{13} = 1.95 (14) C_{23} = 3.19 (16) (From Ph.D. Dissertation of S.B. Sarkar). The accuracy of the experimentally determined values of the constants will be discussed.

05.2-15   KNOOP HARDNESS ANISOTROPY OF SINGLE CRYSTALS WITH HEXAGONAL STRUCTURE. By R. Nowak, Institute of Physics and Nuclear Techniques, University of Mining and Metallurgy, Cracow, Poland

The significant changes in Knoop Hardness Number (KHN) for different Knoop penetrator positions on the indentation plane of crystal were observed by several authors. The relationship: KHN versus indenter orientation with reference to index direction, is plotted as a hardness anisotropy curve (HAC). Since the anisotropy of Knoop hardness is firmly established for years, some theoretical approach, claiming to predict the shape of HAC, had already been proposed. Two of them: Daniels and Dunn model (1949) and its further modification by Brookes et al. (1971) are widely accepted up to now. Nevertheless, neither the first model nor the second one were able to predict the experimental HAC shape for any hexagonal material.

The objective of the present paper was to propose more comprehensive model based on Pospiech and Gryziecki considerations (J.Pospiech, J.Gryziecki, Arch. Hut., 1970, XV,268-283) for cubic crystals, predicting HAC shape for a range of materials including crystals with hexagonal structure. In addition, some combinations of the elements of the three models mentioned above were taken into calculations in order to find the best approach.

The basic assumptions of the new, proposed model were, that:
- the anisotropy of the deformation imposed by a Knoop indenter results from a relationship between the geometry of the penetrator, the initial orientations of all the slip and twinning systems and the orientation of the crystal free surface (indentation plane);
- the directions of the acting forces are perpendicular to the respective indenter facets;
- the activation of a chosen slip system depends on the position (μ) of the penetrator on the surface;
- the probability of activation of i-th slip system (T_i) is proportional to the resolved shear stress value $(\mathcal{T}_i)$ and to the factor estimating the tendency of the movement of the material towards the surface (Λ), and is inversely proportional to the critical stress of the slip system $(\mathcal{T}_{CRi})$:

$$T_i(\mu) \propto \frac{\mathcal{T}_i}{\mathcal{T}_{CRi}} \Lambda \quad \dots (1)$$

- the theoretically established hardness value (H) is considered as a reciprocal of the mean value of T_i:

$$(2) \dots \qquad H(\mu) \propto \left(\sum_{j=1}^{4} \max_i T_i(\mu) \right)^{-1}$$

- the considerations deal with the early stages of crystal deformation, i.e. the work hardening and friction effects are disregarded.

The H(μ) values were calculated for a number of materials. The indentation process on the (0001),(1$\bar{1}$00) and (14$\bar{5}$0) crystallographic planes was considered. The slip systems most likely to be activated at a given indenter position, were determined graphically (eq. 1). The most of experimental results (HAC), were taken from the data published by the other authors. The shape of the calculated hardness anisotropy curves was in very good agreement with that of HAC obtained experimentally. The proposed new model provides satisfying results for hexagonal, as well as for cubic crystal structure, thus proving that the simplifying assumptions mentioned above do not undermine its usefulness and validity.