boundaries (Petritz *et al* 1956). The height of the potential barrier depends upon the number of electrons trapped at the grain boundary which in turn depend upon the two competing processes viz.. (1) release of trapped electrons from the traps at the barrier, and (2) capture of free electrons into the same traps. Since both these processes are thermally assisted, we propose that ΔE may increase or decrease depending upon the new equilibrium values of the processes (1) and (2) at the temperature of heat treatment. This may lead to the observed variation of c_r with T_A. Since c_r is directly related to the absorption coefficient, the spectral response of the ceramic CdS samples may vary with different heat treatment temperature. In fact, the shifting of the absorption edge towards both higher and lowerr energy sides of the normal vaue has already been observed for Ge films for different annealing temperatures (Masatava *et al* 1974). Such an optimisation of the optical properties of ceramic CdS by prior heat treatment may be useful for the fabrication of LDR and solar cell.

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K-surface and diffuse X-ray reflections from 1,8-dihydroxianthraquinone

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The variation of diffuse scattering intensity of X-rays from points round a reciprocal lattice node is conveniently expressed as a surface known as *K*-surface,

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and this was first used by Jahn (1942) in the case of cubic crystals. Such surface show large deviation from spherical character for substances with high elastic anisotropy. The use of K-surface in interpreting diffuse spots on a photograph have been elaborated by Prasad and Wooster (1956a, 1956b, 1956c). Apart from its application to divergence correction, it can also reveal anomalies in the diffuse X-ray scattering due to diffuse reciprocal plates such as occur with β-tin. While studying the K-surfaces of cubic and tetragonal system of crystals, Wooster (1962) suggested that the same could be calculated for any system of lower symmetry, but in that case the labour of computation would increase. It was, therefore, of interest to see how the K-surface could be readily drawn and interpreted in all the non-cubic cases. Accordingly, a programme for IBM 1130 has been written to evaluate K from eqs. (1) and (2) noted below, and a few cases of tetragonal, orthorhombic and monoclinic crystals are being studied. In this communication stereograms of only one tetragonal crystal (1,8-Dihydroxinanthraquinone) drawn on (100), (001) and (110) faces have been presented. The corresponding nodes are $h00$, $00l$ and $hh0$

Along any wave vector through a reciprocal lattice point the K-factor is expressed as

$$K[f]_{hkl} = g_1{}^2(A^{-1})_{11} + g_2{}^2(A^{-1})_{22} + g_3{}^2(A^{-1})_{33} + 2g_1g_2(A^{-1})_{12}$$
$$+ 2g_2g_3(A^{-1})_{23} + 2g_3g_1(A^{-1})_{31} \qquad \dots \ (1)$$

where $f_1 \ f_2 \ f_3$ are the direction cosines of the thermal wave vector and $g_1 \ g_2 \ g_3$ are the direction cosines of the reciprocal lattice vector corresponding to the point hkl with respect to the orthogonal elastic axes of the crystal and $(A^{-1})_{11}$ etc. are the elements of the matrix inverse to the matrix A which are given as follows :

$$
\begin{bmatrix} A_{11} \\ A_{22} \\ A_{33} \\ A_{23} \\ A_{31} \\ A_{12} \end{bmatrix}
=
\begin{bmatrix}
C_{11} & C_{66} & C_{55} & 2C_{56} & 2C_{15} & 2C_{16} \\
C_{66} & C_{22} & C_{44} & 2C_{24} & 2C_{46} & 2C_{26} \\
C_{55} & C_{44} & C_{33} & 2C_{34} & 2C_{35} & 2C_{45} \\
C_{56} & C_{24} & C_{34} & (C_{23}+C_{24}) & (C_{35}+C_{45}) & (C_{25}+C_{45}) \\
C_{15} & C_{46} & C_{35} & (C_{36}+C_{45}) & (C_{13}+C_{55}) & (C_{14}+C_{56}) \\
C_{16} & C_{26} & C_{46} & (C_{26}+C_{46}) & (C_{14}+C_{56}) & (C_{12}+C_{66})
\end{bmatrix}
\begin{bmatrix} f_1{}^2 \\ f_2{}^2 \\ f_3{}^2 \\ f_2 f_3 \\ f_3 f_1 \\ f_1 f_2 \end{bmatrix}
$$

For each projection the values of $K[f]_{hkl}$ have been evaluated along different directions of the wave vector defined by direction cosines, $f_1 f_2 f_3$. The values of K are then written in at the corresponding points on a stereogram with the rel vector at its centre, and finally contours of equal K-values are drawn over the whole stereogram. The elastic constants used in the computation are

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obtained from the study of thermal diffuse scattering of X-rays (Mukherjee & Sen, 1965), and they are given in units 10^{10} dynes/cm^2 as

$$C_{11} = 14{\cdot}00, \qquad\qquad C_{33} = 20{\cdot}40$$

$$C_{12} = -6{\cdot}30, \qquad\qquad C_{44} = 8{\cdot}40$$

$$C_{13} = 1{\cdot}60, \qquad\qquad C_{66} = 1{\cdot}00.$$

In terms of spherical polar coordinates the direction cosines may be expressed as :

$$f_1 = \sin\theta\cos\phi; \quad f_2 = \sin\theta\sin\phi \text{ and } f_3 = \cos\theta.$$

If θ varies from 0° to 180° and ϕ from −90° to +90° at an interval of 10°, practically 325 directions of wave vectors are obtained. K-values corresponding to different (θ, ϕ) values have been calculated by running a programme at the C.U. Computer Centre. Figure 1 represents the stereographic projection of K-surface of node $h00$ on (100). Evidently, the K-values have been calculated
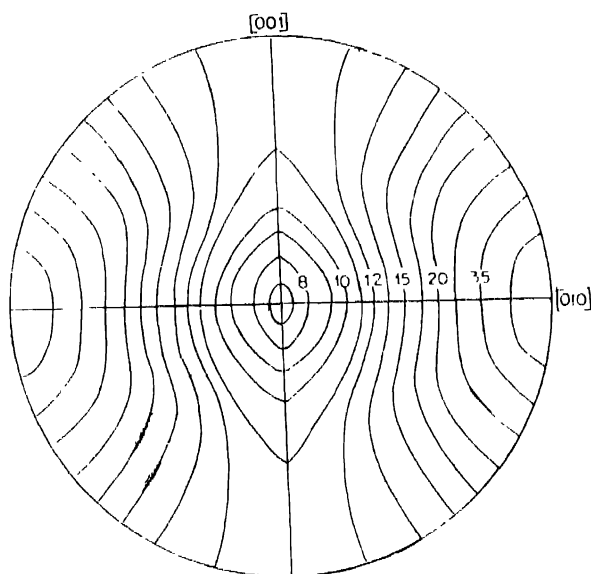

Figure 1. Stereographic projection of K-surface for 1,8-Dihydroxianthraquinone; node $h00$ projected on (100).

at all points lying on the interaction of (a) small circles round the [001] axis (const. θ value) separated by a 10° degree interval and of (b) great circles passing through the ends of the vertical diameter (const. ϕ value) also having a 10° degrees separation from one another. In special cases intermediate values are also calculated for facilitating contour drawing. Similarly the K-values have been

plotted for relps 00*l* and *hh*0 (figures 2 and 3) but in the latter case the computation runs from $\phi = -45°$ to $+135°$. The dimensions of K are cm^2 dynes^{-1}
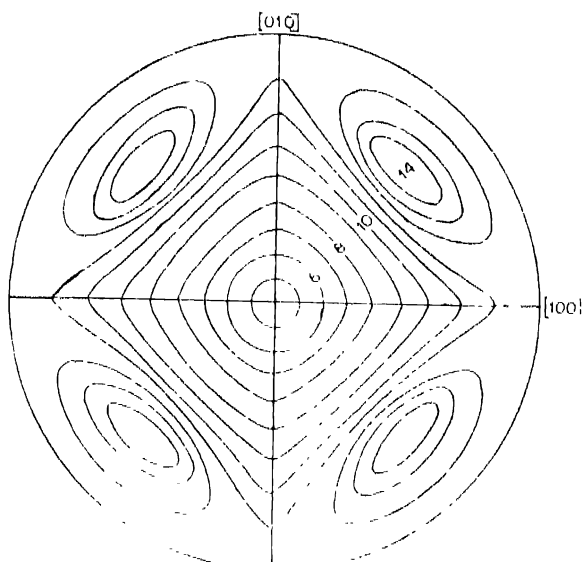

Figure 2. Stereographic projection of K-surface for 1,8-Dihydroxianthraquinone; node 00*l* projected on (001).
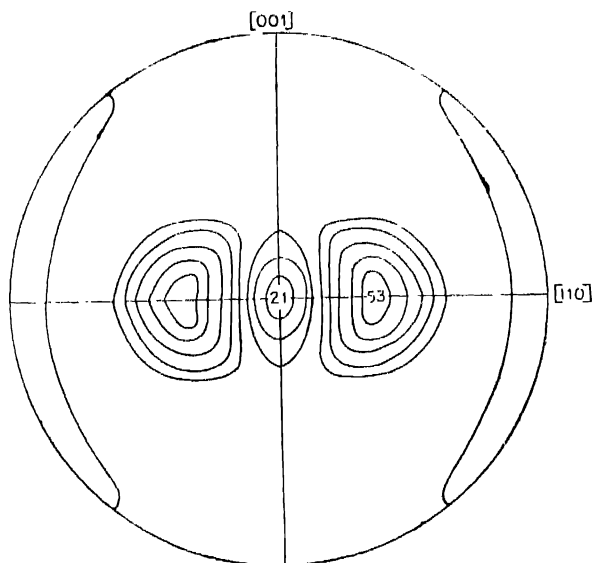

Figure 3. Stereographic projection of K-surface for 1,8-Dihydroxianthraquinone; node *hh*0 projected on (110).

and are the same as those of elastic moduli. The K-contours are, therefore, numbered in units of 10^{-13}.

The diagrams obtained are somewhat similar to those obtained by Wooster. Lack of spherical symmetry in the K-surface indicates considerable elastic anisotropy in 1,8-Dihydroxianthraquinone. The (100) projection shows that in directions nearly parallel to [111] [$\bar{1}\bar{1}$1] [1$\bar{1}$1] and [$\bar{1}$11] there are pronounced peaks. (110) surface also indicates the presence of two peaks parallel to the directions [100] and [010].

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Optical absorption spectra of Mn²⁺ in rhodonite

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The optical absorption spectra of rhodonite have been analysed by the earlier workers (Manning 1968, Lakshman and Reddy 1973) assuming a purely cubic crystal field around the chromophoric Mn^{2+} ion. Both the spectral data and structural data (Wyckoff 1968) indicate a distorted octahedral environment around the metal ion Therefore we think itw orthwhile to reexamine the spectra using a theoretical model which includes lower symmetric crystal field and also the spin-orbit interaction.

Rhodonite is a mineral with chemical composition $(Mn, Ca)SiO_3$. It has also been reported that this mineral contains some amount of Fe. (Deer *et al* 1962). The manganese ion is in divalent state in this crystal. So essentially the spectrum is characteristic of a d^5 ion in distorted octahedral environment. If we assume only a cubic field and ignore the spin-orbit interaction, the d^5 has a spin sextet ground state, 10 spin quartet excited states and 32 doublet excited states. All the electronic transitions are spin forbidden. But the spin-orbit interaction