APPENDICES

Appendix - 1

General Method of Calculations

Indexing patterns of orthorhombic system :

The Bragg's law is given below :

$$2d \sin\theta = n\lambda$$

λ = wavelength of X-rays

n = order of diffraction $\sim$ 1

d = Interplaner spacings

θ = diffraction angle

On the basis of reciprocal lattice concept, the relation for d and a lattice constant is given as for orthorhombic crystal structure.

$$\frac{1}{d^2} = \frac{h^2}{a^2} + \frac{k^2}{b^2} + \frac{1}{c^2}$$

where h,k,l are the muller indices

$$\text{Sin } 20 = Ah^2 + Bk^2 + Cl^2$$

where $A \quad \frac{\lambda^2}{4a^2} \quad B = \frac{\lambda^2}{4b^2} \quad C = \frac{\lambda^2}{4c^2}$

(where A, B, C are constant)

The indexing problem is considerably more difficult here in that three constants A,B and C have to be determined The general procedure which is too lengthy to illustrate here is to search for significant differences between various pairs of Sin 2θ values.

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For example consider any two lines having indices hko and hko with the hkl the same for each, such as 120, 121. The difference between the Sin 2 θ values of two lines such as 310 and 312 is 4C. In this way A, B, C sonstants can be evaluated.