

020228 Quiz 7 XRD

$$I(2\theta) = K |F|^2 p \left(\frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta} \right) e^{-\frac{(q^2 \sigma^2)}{2}}$$

is one equation for diffracted intensity for a certain type of radiation and for a certain type of camera.

- 1) The Debye-Waller Factor (last term) describes how “the intensity of diffraction is progressively more attenuated as the diffraction angle 2θ is increased”[1].
 - Explain this** in terms of thermal vibration of atoms and the relative effect on a lattice spacing as described by Bragg’s Law, $d = 2a/q$.
 - You will need to define** the term q in terms of d and the term σ qualitatively in terms of thermal vibrations.
 - Have you** observed this “progressive attenuation” in your diffraction measurements?
- 2) A Lorentz plot is a plot of Iq^2 versus q (used in the lab this week) and Lorentz corrected intensity is intensity multiplied by q^2 .
 - Is the Lorentz correction included** in the equation above?
 - Explain your answer.**
- 3)
 - Define** the term “ p ” in this equation.
 - What is** “ p ” for cubic (110) and (111) reflections?
 - Why** is “ p ” not included in the calculation of the degree of crystallinity for a semi-crystalline polymer?

[1] R. J. Roe p. 34 “Methods of X-Ray and Neutron Scattering in Polymer Science”, 2000 Oxford Press, NY.

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- 1) λ is the mean free path of a thermally vibrating atom about to the theoretically fixed lattice position. For smaller d , higher- q , the ratio of λ/d becomes much larger making the reduction in intensity greater at higher angle. This was observed for every diffraction pattern measured in lab, since it is a basic feature of diffraction. $q = 4(\lambda/d) \sin \theta$.
- 2) The Lorentz correction is included in the term $\sin^2 2\theta$. The intensity must be multiplied by $\sin^2 2\theta$ to obtain a function proportional to the number of atoms contributing to diffraction.
- 3) p is the multiplicity factor and it describes the number of planes of a given type in the unit cell. The normal to the (100) planes intersects the edge and there are 12 edges in the cubic unit cell so $p_{110} = 12$. The normal to the (111) plane intersects the corner of the unit cell and there are 8 corners in a cubic unit cell so $p_{111} = 8$.
 p is not included in the calculation of the degree of crystallinity since we are considering only the total number of atoms (or electrons) contributing to all crystallinity or all amorphous parts of the material. The term p is specific to comparisons of number of planes. The integral of Iq^2dq in the degree of crystallinity measurement for polymers yields what is termed the invariant, Q . The invariant is proportional to the total number of electrons contributing to diffraction/scattering.