

EFFECT OF THERMAL VIBRATIONS ON REFERENCE INTENSITY RATIO

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It is evident from the Debye-Waller equation that the intensity of Bragg reflections has a strong correlation with the thermal vibrations of the contributing atoms. This poster attempts to illustrate reliability of Reference Intensity Ratio (RIR) of a calculated pattern based on the thermal vibrations used in the calculation. The effect of thermal vibrations on the Reference Intensity Ratio is analyzed in terms of parameters including linear absorption coefficient, total number of electrons in the lattice and crystal density. Some case studies based on crystal structures having poorly refined temperature factors and their effect on the RIR are also discussed in the poster.