

this type of analysis are slightly in error because the assumed shape for the Maxwellian, $\alpha d^{-\gamma} e^{-\delta/d^2}$, with the 3 variable parameters α , γ , and δ , is not sufficient to exactly fit the background over the entire spectrum. For the least squares technique here described the ratio of χ^2 to the number of degrees of freedom which we shall designate the "goodness of fit" should lie between 0.8 and 1.2 for a perfect statistical fit.

Since the TOF diffraction method employs a continuous range of neutron wavelengths (λ), the measured intensities are modified by the thermal neutron spectrum and by a λ^4 multiplication.¹⁶

Relative structure factors were determined from the measured intensities ($I_{\vec{h}}^{\text{TOF}} = \alpha_{\vec{h}} S_i (\pi/4 \ln 2)^{\frac{1}{2}}$) according to the relation

$$m_{\vec{h}} |F_{\vec{h}}|^2 \propto \frac{I_{\vec{h}}^{\text{TOF}}}{\lambda^4 I_0(\lambda)} \quad (2)$$

where $m_{\vec{h}}$ is the multiplicity for the peak with label \vec{h} in the diffraction pattern, $F_{\vec{h}}$ is the structure amplitude including Debye-Waller factors, and $I_0(\lambda)$ characterizes the neutron flux from the reactor. In our case $I_0(\lambda)$ was determined from a measurement of the direct beam transmitted through the pressure cell containing the sample using a detector matched to those used in the 30 and 60° scattering angles, and so $I_0(\lambda)$ should implicitly contain absorption and multiple scattering corrections for both the sample and pressure cell as well as detector efficiency corrections. In fits to the diffraction pattern for well known cubic materials it was found that the measured $I_0(\lambda)$ predicted