

## MS43-05 | TEXTURE CORRECTION FOR TOTAL SCATTERING FUNCTIONS

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Preferred orientation (texture) is a complex effect that bridges powder diffraction to single crystal diffraction. Corrections for Bragg intensities are known [1-3]. However, within the Total Scattering approach, that prescind from periodicity and therefore avoids ragg formalism, the problem of evaluating the  $S(Q)$  and  $G(r)$  scattering functions in the presence of texture has never been quantitatively tackled. A complete treatment in the framework of spherical harmonics for the most common powder diffraction experimental geometries is presented. The  $S(Q)$  can be computed by an extended version of the commonly used Debye scattering equation (DSE) [4] comprising now sums over spherical Bessel functions of all (even) orders. Selection rules arising from sample and experimental symmetries are given. Concerning the  $G(r)$ , the effects of texture result in a fundamental indetermination that has important consequences. Example calculations for various interesting cases will be shown. As an aside, a second DSE-like formula for computing the antisymmetric intensity change in 3-D reciprocal space due to anomalous/resonant scattering is given. This is meant for single crystal or single particle studies. As with the DSE, this equation prescind from spatial periodicity and can be used for non-crystalline matter.

[1] *J. Appl. Phys.* **36** (1965) 2024

[2] H.J. Bunge, *Texture Analysis in Materials Science*. Butterworth:London (1982) ISBN:**0408104625**

[3] *J. Appl. Cryst.* **25** (1992) 611

[4] *Annalen der Physik* **46** (1915) 809