

Maximum likelihood applied to powder diffraction data

Bill David

ISIS Facility, Rutherford Appleton Laboratory, Chilton, OX11 0QX, UK

This talk will focus on the use of maximum likelihood (ML) techniques as applied to powder diffraction. Although ML techniques are widely used in macromolecular crystallography, their use in powder diffraction has been very limited. The reason for this lies in the mathematical complexity that results from the inevitable overlap in Bragg peaks resulting from the collapse of the three dimensions of diffraction data on to the one dimension of a powder diffraction. I will outline the mathematical issues associated with applying ML to powder diffraction data and illustrate the substantial improvement that can be obtained from using a full ML rather than a traditional least-squares analysis.