Versatile Rietveld – Applications to Real Materials

Steve Norval
Intertek MSG, Wilton Centre, Wilton, Redcar TS14 8PN

In principle, the Rietveld method is an extremely powerful means of extracting information from powder diffraction patterns. Crystal structure applications are well established and standardless quantitative phase analysis is becoming so. Other applications such as microstructure determination still seem a little esoteric to many. A basic and common limitation for many laboratories, especially in industry, is the reality of non-ideal materials. Real world materials often contain several phases, some of which can be non-stoichiometric or have uncertain composition. Microstructure often goes beyond simple crystallite size effects. Anisotropy, lattice distortion and stacking faults are common in nano-materials. Preferred orientation may arise during sample preparation, but it is often introduced during manufacturing processes.

The good news is that useful information can often be extracted from non-ideal samples using Rietveld techniques and the goodness-of-fit criteria considered necessary for establishing a crystal structure are often unnecessarily severe for other applications. Applications will be described that use Rietveld to extract information on preferred orientation, microstructure, bimodal lattice parameters and phase quantification. The examples relate to industries from biological to electronic.