THE EFFECT OF POINT DEFECTS ON X-RAY DIFFRACTION LINE INTENSITIES

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The presence of defects in crystals can cause severe problems for standard methods of extracting structure information from X-ray diffraction measurements. Concentrations of point defects of up to several per cent as observed in materials exposed to radiation environments such as wasteform ceramics or materials used in plasma fusion machines lead to lattice distortions and result in changes of the diffraction line intensities for which detailed models are hardly available. The Rietveld technique is based on crystallographic structure factors, and hence cannot a priori account for the effect of static distortions which break explicitly the periodicity of the lattice. When applied to irradiated materials, it will often either fail to converge or to provide reliable structure information. However, in analogy to the treatment of the effect of thermal vibrations, it may be possible in certain cases to parameterize the intensity changes caused by static lattice distortions in the form of a static Debye-Waller factor with a sufficiently smooth dependence on the scattering vector $\boldsymbol{K}$, and to include this correction factor into Rietveld refinement. The functional form of the $\boldsymbol{K}$-dependence should be obtained from model structures with a known defect configuration, containing a sufficiently large number of atoms to be representative of a macroscopic defective crystal.

In the present work the Molecular Dynamics (MD) simulation technique is used to generate defective crystal structures in the computer for which the $\boldsymbol{K}$-dependent X-ray scattering signal can be easily calculated. Static Debye-Waller factors are evaluated for different defect types and concentrations in an fcc metal, and it is discussed under what conditions the $\boldsymbol{K}$-dependence of the factor may be sufficiently simple for use in practical Rietveld refinement.