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*J. Appl. Cryst.* (1975). **8**, 183

# A Lattice-Statics Approach to the Calculation of Diffuse X-ray Scattering by Interstitials in Metals*

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(*Received* 29 *April* 1974)

The calculation of the intensity of diffuse X-ray scattering by interstitials involves the evaluation of a crystal structure factor which accounts for both the configuration of the interstitial atom and the distortion of the surrounding lattice. The lattice-distortion field surrounding an interstitial may be calculated using a Green's function lattice-statics approach described in earlier work [Benedek, R. & Ho, P. S. (1973). *J. Phys. F: Metal Phys.* **3**, 1285–1295]. In this approach, several atoms in the vicinity of the interstitial (the interstitial 'core') are treated formally on the same footing as the interstitial itself. Once the Green's function calculation of the lattice distortion field is performed the structure factor can be evaluated as follows. The contribution from the interstitial core is calculated explicitly using the core-atom displacements. The contribution from the remainder of the lattice is expressed in terms of 'Kanzaki forces' and certain 'virtual' displacements of core atoms, both of which are by-products of the Green's function calculation. Using this approach numerical calculations of diffuse scattering by self-interstitial atoms in tungsten were performed. Based on the results, typical features of the Huang scattering, small-angle scattering, and scattering far from reciprocal-lattice points are discussed. The sensitivity of the calculations to the interatomic potential are also discussed.

* This work was supported by the U.S. Atomic Energy Commission.
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*J. Appl. Cryst.* (1975). **8**, 183

# Investigation of the Strain Field of Bismuth in Lead by Diffuse Elastic Neutron Scattering

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(*Received* 29 *April* 1974)

The diffuse elastic neutron scattering due to distortion of the Pb host lattice around Bi substitutional atoms has been measured at the HFR in Grenoble. Two single crystals, with 2 and 4 at. % Bi and with 100 and 110 orientations respectively, were used. The diffuse elastic scattering intensity is equivalent to the scattering of 0·05 and 0·1 at.% of vacancies respectively. Using a wavelength of 4·3 Å and a time-of-flight technique, the measuring range in reciprocal space was extended to $\kappa = 2{\cdot}8$ Å$^{-1}$ compared with $\kappa = 1{\cdot}8$ Å$^{-1}$ of earlier measurements [Schumacher, H., Schmatz, W. & Seitz, E. (1973). *Phys. Stat. Sol.* (*a*), **20**, 109]. The scattering patterns agree within the common $\kappa$ range. The improved resolution, however, shows that the 110 peak at $\kappa = 1{\cdot}8$ Å$^{-1}$ observed earlier is more intense and has a smaller width than that described by the model calculations of Schumacher *et al.* These calculations assumed a distortion field around the Bi atoms caused by anisotropic forces acting on nearest neighbour Pb atoms. The new results require a more refined model.