Huang Diffuse Scattering by Mesoscopic Interstitial Defects in BCC Metals

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Microstructural evolution of materials in the extreme environment of a fusion or an advanced fission power plant is driven by migration of defects produced by irradiation. If the energy of collision cascades is low, only point defects (vacancies and single interstitial atoms) are generated. Agglomerating point defects form dislocation loops and voids. Huang diffuse scattering (HDS) is used for the determination of structure of single interstitial defects generated by irradiation.

We show that in addition to single interstitial atom defects, mesoscopic defect clusters containing two or more interstitial atoms give a strong contribution to the observed HDS patterns. The occurrence of clusters of interstitial atoms in e-irradiated bcc iron was proved in a recent study of resistivity recovery curves. The effect of interstitial atom clusters on HDS has not yet been investigated. The size of these clusters is comparable with the lattice constant making the infinitesimal dislocation loop approximation underlying the existing treatment of HDS not applicable. We show that the fact that the core of a mesoscopic interstitial cluster is fully three-dimensional has a strong effect on the long-range elastic strain field, and this masks the symmetry-related features of HDS associated with single interstitial atom defects. The new findings may help resolving the conflict between predictions of density functional calculations and the existing interpretation of experimental observations of HDS in bcc metals of the VIth group of the periodic table.

This work was funded by the UK EPSRC and by EURATOM.

Keywords: diffuse scattering, defect structures, defect clusters