

Electron Dynamical Diffraction Imaging and Diffuse Scattering by Small Dislocation Loops

Sergei L. Dudarev^a, Zhongfu Zhou^b, Adrian P. Sutton^c, Mike L. Jenkins^b, ^a*EURATOM/UKAEA Fusion Association, Culham Science Centre, Oxfordshire OX14 3DB,UK.* ^b*Department of Materials, University of Oxford, Oxford OX1 3PH,UK.* ^c*Department of Physics, Imperial College, Exhibition Road, London SW7 2AZ,UK.* E-mail: sergei.dudarev@ukaea.org.uk

Effects of dynamical scattering of high-energy electrons by elastic fields of interstitial or vacancy loops in a crystalline material provide a convenient means for diffraction contrast imaging. In this presentation we describe new developments in the methodology of simulation of diffraction images and *dynamical* diffuse scattering by small dislocation loops. To simulate diffraction images, a many-beam Howie-Basinski equation approach has been developed where strong dynamical effects as well as the non-parallel propagation of diffracted beams in the crystal are treated using a combination of the adaptive spatial mesh and wave field interpolation techniques. The significance of dynamical diffraction as well as practical applications of the new approach are illustrated by the comparison of simulated and experimentally observed images. The treatment of diffuse scattering includes effects of Kikuchi diffraction on Huang diffuse scattering patterns that we simulate using the atomic displacement fields evaluated using anisotropic elasticity solutions and atomistic modelling.

Keywords: electron microscopy and diffraction, quantitative electron diffraction, dynamical diffraction