Microsc. Microanal. 8 (Suppl. 2), 2002
DOI 10.1017.S1431927602101218



# Characterization of Dislocation Structures in Hexagonal Close-Packed Metals by X-ray Line-Broadening Analysis

M. Griffiths*, D. Sage* and D. Galindo**

* Atomic Energy of Canada, Chalk River Laboratories, Chalk River, Ontario, K0J 1P0.
** McGill University, Department of Mathematics, Montreal, Quebec.

In deformed hcp metals such as Zr, X-ray diffraction line profiles are determined by the convolution of a number of different broadening factors: (i) instrumental; (ii) intergranular strain distributions; (iii) coherent diffracting domain size; and (iv) lattice microstrains (strain distribution around a dislocation), [1]. Dislocation structures can be characterized by Fourier analysis methods, [2], provided that the only contributions to the line profile arise from the latter two factors, (iii) and (iv). The instrumental broadening effect, (i), can be extracted from the line profile using conventional deconvolution methods with an appropriate standard, [2,3]; the line-broadening is then compared relative to the standard (normally an annealed single crystal). The intergranular strain distributions, (ii), introduce an error into the determination of dislocation densities unless they too can be deconvoluted. Unfortunately, as the intergranular strains are dependent on the extent of deformation, there are no practical means by which a standard can be generated that is independent of the dislocation structure, that is also dependent on the extent of deformation. In principle, the intergranular strain distributions and lattice microstrains from dislocations are both dependent on the order of diffraction. This provides a means of separating them from the coherent domain size effect, which is independent of the order of diffraction, using the Fourier method of Warren and Averbach [2]. The residual peak profile will be comprised of a convolution of the two components, (ii) and (iv), and can only be separated if the functional form of each component can be defined or measured.

The aim of this work is to determine the functional form of dislocation microstrains and intergranular strain distributions. Experimental data for both types exist. For microstrains, the diffraction peaks from an irradiated single crystal containing dislocation loops are analysed. The single crystal peaks are, in principle, unaffected by intergranular strain distributions and can be processed using the method of Warren and Averbach [2] to obtain type (iv) profiles. For intergranular strain distributions, the diffraction peaks from a deformed sample are analysed. Those peaks corresponding with planes that are relatively undistorted by dislocations and are, in principle type (ii). Both peak shapes are compared with the calculated shape of the diffraction peak resulting from the strain field around a dislocation in order to verify the premise that the two effects originate from different sources and are separable. The dislocation loops are shown in Figure 1(a) and the corresponding prism plane line profile, with superimposed Gaussian and Lorentsian fits, for neutron irradiated single crystal Zr are shown in Figure 1(b). The line profile calculated from first principles, with superimposed Gaussian and Lorentsian approximations, is shown in Figure 2. These preliminary results indicate that the diffraction line profile for the strain around a dislocation is primarily Lorentsian in nature. Similar fits for intergranular strain distributions indicate that a Gaussian distribution is the better fit.

References

[1] M. Griffiths et al., *Trans. AIME, in press.*
[2] B.E. Warren and B.L. Averbach, *J. Appl. Phys.*, 21 (1950) 59
[3] S. Ergun, *J. Appl. Cryst.*, 1 (1968) 19.

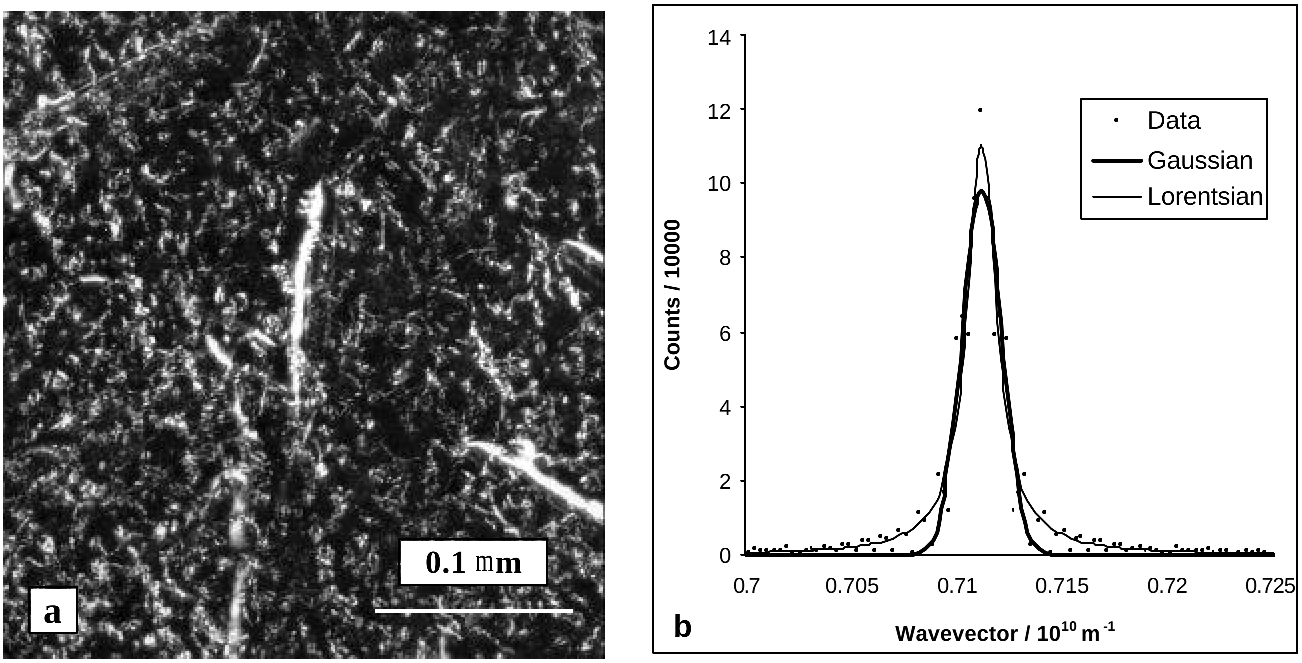


FIG. 1. (a) Micrograph showing dislocation loops in neutron irradiated single-crystal Zr; and (b) corresponding deconvoluted prism plane diffraction line profile.

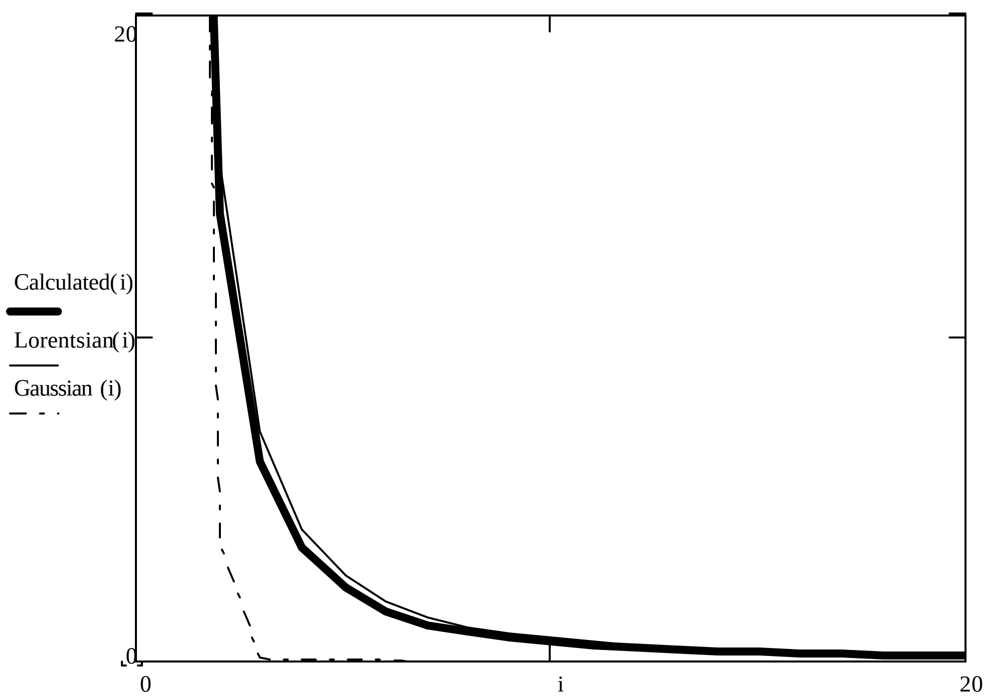


FIG. 2. Calculated diffraction line profile, based on the theoretical strain field around a single edge dislocation, compared with Gaussian and Lorentsian approximations.

https://doi.org/10.1017/S1431927602101218 Published online by Cambridge University Press