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**DIRECT RETRIEVAL OF CRYSTAL STRUCTURES BY MAXIMUM
ENTROPY ANALYSIS OF INCOHERENT Z-CONTRAST IMAGES**

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DIRECT RETRIEVAL OF CRYSTAL STRUCTURES BY MAXIMUM ENTROPY ANALYSIS OF INCOHERENT Z-CONTRAST IMAGES

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Z-contrast imaging¹ of crystalline specimens in a scanning transmission electron microscope (STEM) can provide directly interpretable images of crystal structures at atomic resolution with strong compositional sensitivity. The key feature of the technique is that, by recording images using high-angle thermally diffuse scattered electrons, the resultant image is incoherent, and can be interpreted as a convolution between the incident electron probe and the projected crystal structure of the specimen. Consequently, the technique is ideally suited to the application of deconvolution routines which enable the retrieval of the original crystal lattice by means of an incident electron probe approximation, and with no prior assumption of the nature of the crystal itself. Here, we show that by applying the image processing technique of maximum entropy, such a retrieval can be achieved with high accuracy, enhancing spatial resolution whilst preserving Z-sensitivity.

Maximum entropy² is an image processing routine based on Bayesian probability which produces a 'most likely' reconstruction of the original image given a particular point spread function, or in this case, electron probe current density distribution. The results described here were obtained using a VG Microscopes MaxEnt software routine on an IBM 486 PC with special accelerator card. Experimentally acquired images were taken on a 300kV STEM at 1.3Å spatial resolution. As a measure of the capabilities of maximum entropy in the analysis of Z-contrast images, the technique was applied to the study of simulated 300kV images of a graded SiGe structure in the <110> orientation (Fig.1). Shown in figures 1(a) and (b) respectively is the original simulated image using the theoretical optimum probe and the full maximum entropy processed image obtained using a gaussian probe approximation. It can be seen that even with a simple probe approximation, the original crystal structure on which the simulation is based is retrieved in terms of an array of delta functions with coordinates that match those of the initial column positions to within 1%. In addition, variations in signal intensity corresponding to columnar scattering power are preserved. The robust nature of the maximum entropy approach is demonstrated by processing simulations with increasing levels of noise (Figs 1c and e) and retrieving the original structure (Figs 1d and f). These figures show that unless nearly all image information is lost, column positions can be retrieved to within an accuracy of <10%.

As-acquired 300kV Z-contrast images of Si and GaAs in the <110> orientation are shown in figures 2(a) and 3(a) respectively. Qualitatively, it can be seen that contained in these images alone is information on both column positions and composition at a resolution better than the nearest neighbor spacing. However, more accurate analyses can be obtained by applying maximum entropy to each image (figs 2b, 2c, 3b and 3c). The power of this approach is clearly demonstrated, showing that not only can coordinates be assigned to each column position, but also, in the case of GaAs, that column intensity information enables the assignation of elemental species to specific column sites in the sublattice. In addition to the materials discussed here, maximum entropy has also been applied to the study of grain boundaries in SrTiO₃³.

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4. This research was sponsored by the Division of Materials Sciences, US Department of Energy contract DE-AC05-84OR21400 with Martin Marietta Energy systems Inc, and by the Oak Ridge National Laboratory Postdoctoral Research Program administered by the Oak Ridge Institute for Science and Education.

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FIG. 1. Simulated Z-contrast images of a graded SiGe structure with increasing levels of noise (a, c and e) and their corresponding maximum entropy images (b, d and f)

FIG. 2. (a) As-acquired, (b) partial and (c) full maximum entropy images and (d) schematic diagram of Si in the $\langle 110 \rangle$ orientation.

FIG. 3. (a) As-acquired, (b) partial and (c) full maximum entropy images and (d) schematic diagram of GaAs in the $\langle 110 \rangle$ orientation.

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