**Z-CONTRAST IMAGING: QUANTITATIVE ASPECTS OF THE DYNAMICAL OBJECT FUNCTION.**

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In this paper, we use a Bloch wave approach to show that the elastically scattered electrons from neighbouring atomic columns in a zone-axis oriented crystal contribute incoherently to a Z-contrast image regardless of the fact that we have coherent dynamical scattering from a stationary lattice with no absorption. This incoherent nature of the elastic scattering means that through the filtering of the 1s-type Bloch states by the detector geometry[1] we approach the Rutherford $Z^2$ dependence of the column intensity for sufficiently large inner detector angle. Thus, annular dark-field (ADF) imaging provides us with a direct incoherent structure image of the atomic-column positions in a zone-axis oriented crystal.

Bloch wave simulations were carried out at 300 kV for the $\langle \quad \rangle$ orientation of InAs (a = 6.06Å) with full, half and empty columns of In atoms. Calculations including 411-beams were carried out for each of the above structural configurations for a single incident partial plane wave vector parallel to the optic axis. Residual object functions (ROF's) were constructed from just the In and As 1s-type states and from all 411 Bloch states for comparison. Figure 1a and 1b show the profiles across the classic "dumbbell" structure of the residual object functions for inner detector angles of 26 and 60 mrad respectively. It can be clearly seen that the intensity of the peaks in the ROF's comes predominantly from the 1s-type Bloch states; the other 409 Bloch states contributing only to the tail regions of the column positions. Since the 1s Bloch waves do not vary strongly over the small range of incident wave vectors defined by a typical objective aperture, similar behaviour is obtained for other incident wave vectors, and the ADF image intensity can therefore be described as a convolution between the probe intensity and an object function. The most important feature of these plots is the invariance of the As peak intensity to changes in the physical structure of its neighbouring In column. The maximum deviation in the intensity of the As column peak intensity is ~ 8% and ~1% for the 26 and 60 mrad inner detector angles respectively as the In column is completely removed.

The variation of the intensity of the In column changing from full to half In columns varies for the two inner detector angles; the In peak intensity falls by a factor of 0.38 and 0.22(~_) for the 26 and 60 mrad inner detector angle respectively showing that for the larger inner angle we begin to approach the classical $Z^2$ dependence of Rutherford. Further calculations were performed for eleven atoms with a range of Z values (Z = 6 – Z = 79). The unit cell of InAs was used with the atoms placed on the In positions only (the As positions being left empty). The calculations were also expanded to include 781 Bloch beams, each with 781 plane wave components, to ensure convergence and adequate sampling of reciprocal space at high angles. The parameter $C_{jj}$ describes the strength of the intensity contribution of the $j^{th}$ Bloch state on the ADF detector and in the high-angle-limit is reported to have a $Z^2$ dependence; and the excitation of the $j^{th}$ Bloch state have a $Z^{-1}$ dependence[1]. Figure 2a shows a plot of these parameters for the 1s-type states as a function of Z for a 60 mrad inner detector angle. Figure 2b shows the column peak intensity values of the corresponding ROF's for just the 1s-type states and all 781 Bloch states. It is assumed that these parameters have a power law dependence ($A_Z^n$), which has been fitted to the data points (see curves in Figure 2 and Table 1). Both the $C_{jj}$ and the excitation parameters have a stronger Z-dependence than expected but overall the high-angle limit of the ROF intensity approaches the Rutherford $Z^2$ dependence, with a value of n = 1.770±0.046 and n = 1.880±0.031 for the 1s-type states and all states respectively.

In conclusion, we have shown that the intensity contributions from neighbouring columns in a crystal structure contribute incoherently to the ADF image intensity. The detailed structure of one column does not affect its neighbours since the intensity contributions are dominated so strongly by the highly localised 1s-type Bloch states.

References:

1. P D Nellist, S J Pennycook, Ultramicroscopy 78 (1999) 111
2. Supported by Lockheed Martin Energy Research Corp. under DOE Contract No. DE-AC05-96OR22464, and by appointments to the ORNL Postdoctoral Research Associates program administered jointly by ORNL and ORISE.

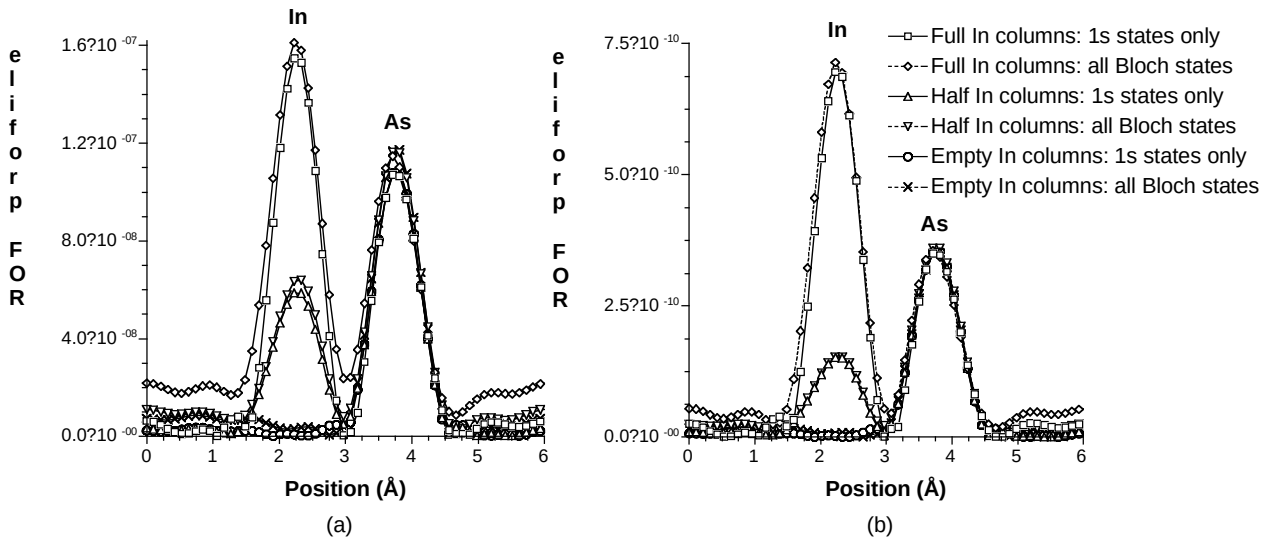


**Figure 1: ROF profiles across the InAs "dumbbell" structure with full, half and empty In columns for (a) 26 mrad and (b) 60 mrad inner detector angles.**

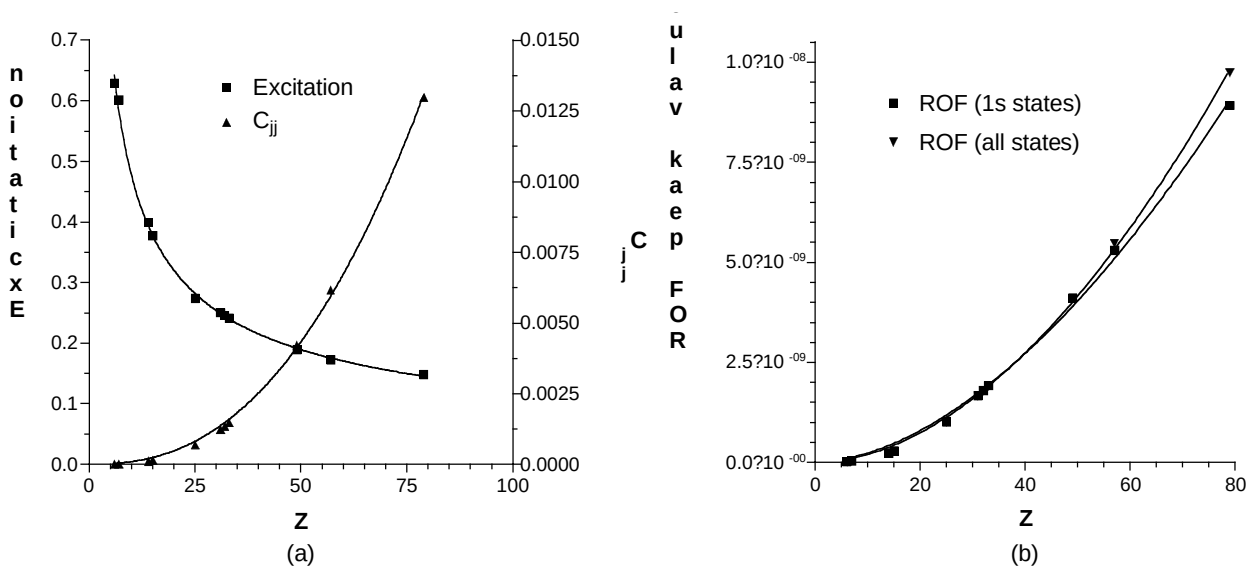


**Figure 2: Plot of (a) the excitation co-efficient and $C_{jj}$ parameter for the 1s-type states and (b) the peak intensity of the ROF for 1s-type states and all states as a function of Z. The curves are the fitted power-law dependencies to the data points.**

| | Excitation | $C_{jj}$ | ROF (1s state) | ROF (all states) |
|---|---|---|---|---|
| **n** | -0.5762 | 2.419 | 1.770 | 1.880 |
| **σ** | 0.008406 | 0.03694 | 0.04579 | 0.03147 |
| **95% confidence interval** | -0.5952, -0.5572 | 2.336, 2.503 | 1.667, 1.874 | 1.809, 1.951 |
| **$R^2$** | 0.9983 | 0.9991 | 0.9970 | 0.9988 |

**Table 1: A summary of the results of the power-law fitting to the data points in figure 2.**