Characterisation of the composition and structure of ultrathin Si layers in GaAs using bright and dark field Fresnel contrast

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Here we assess the degree to which dark field (DF) and bright field (BF) Fresnel contrast data can be applied together to provide both structural and compositional information about two thin Si layers, which are grown 50nm apart on [001] GaAs with Si concentrations (nominally 100at% and 200at% Si) that are intended to differ by a factor of two. The Fresnel data can be interpreted solely in terms of changes in tetragonality and electron scattering factor, as contributions to the potential from electrical activity are known to be negligible at the high Si concentrations that are present. The experimental images examined below were obtained at 200kV on a JEOL 2000FX, digitised and scaled to proportionality in electron dose. The specimen thickness was determined using several sets of weak beam thickness fringes, and atomistic multislice calculations incorporating neutral atom scattering factors were performed to model the data, with the strain at the Si layers included using conventional elasticity theory.

Fig. 1 shows one image from a BF through-focal series taken at a systematic row orientation approximately 7° from [100], with beam convergence and objective aperture semi-angles of 0.45 and 3.5 mrads respectively. The sense of the contrast (the bright central fringe underfocus) indicates that both of the layers have a lower scattering potential than GaAs. The width of each layer is known to be sensitive to the spacing of the Fresnel fringes, and a comparison of the experimental and simulated data in fig.3 indicates that the Si has spread over approximately 2 GaAs unit cells in both layers. The magnitude of the experimental contrast, which has been extrapolated to a specimen thickness of 5nm for each defocus in figs. 4 and 5 to account for contrast reductions due to inelastic scattering at higher thicknesses, exhibits both the expected ratio of two between the layers and clear asymmetry with defocus which is reproduced in the simulations. However, the most surprising observation is that the experimental contrast is much *higher* than that of simulations for the intended Si concentrations, whether Si is predicted to substitute for Ga or for both Ga and As. A Si concentration of more than 600at% is required to match the contrast at each layer whichever model for the site occupancy of the Si is used. Although this value would be reduced if the lattice contraction at each layer were smaller than that predicted using conventional elasticity theory or if the effects of bonding were included in the simulations, it would still be substantially higher than the intended values.

DF Fresnel contrast data were obtained at a g=002 diffracting condition with a positive deviation parameter, again using a 3.5 mrad objective aperture, with the aim of obtaining strain information to complement the BF data. One image from the series is shown in fig.2, and line profiles taken across each of the layers at a specimen thickness of 40nm are shown in figs. 6a and 6b. Interestingly, the dark contrast which is seen on both sides of focus in the experimental data is only reproduced in the simulated contrast shown in figs. 6c-6f when Si substitutes for both Ga and As, and this conclusion is independent of the strain included in the models. Thus, while the original aim of the DF approach was to determine strain, the sensitivity of the contrast to the site occupancy of the Si shows that the Si in the layers examined here *cannot* be confined to one type of site on the GaAs lattice, and the full explanation of the intriguing BF data still requires strain information to be obtained using a technique such as regressional analysis applied to a high resolution image or convergent beam electron diffraction.

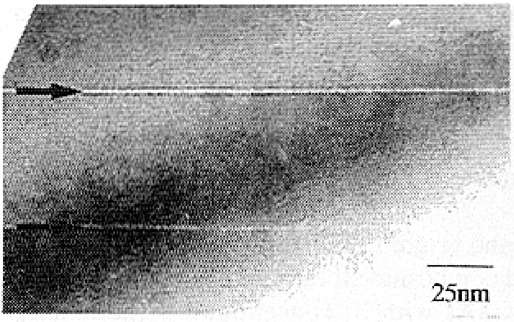

Fig.1 BF image, taken approximately 600nm underfocus, showing the higher (top) and lower (bottom) concentration Si layers.

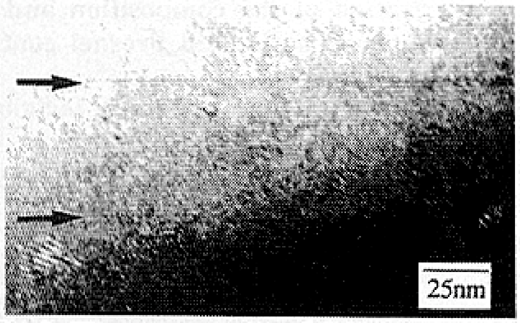

Fig.2 The corresponding DF image, taken at g=002 with a positive deviation parameter, approximately 600nm underfocus.

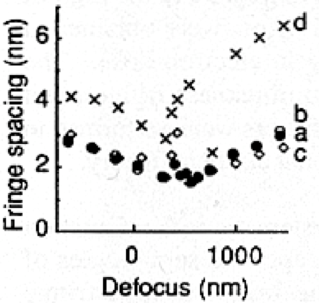

Fig.3 BF fringe spacing for a) higher and b) lower concn Si layer, and simulations for 100 at% Si spread over c) 2 and d) 4 unit cells on Ga & As sites.

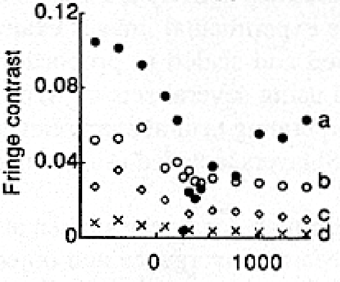

Fig.4 BF fringe contrast for a) higher and b) lower concn Si layer, and simulations for c) 400 and d) 100at% Si spread over 2 unit cells on Ga sites.

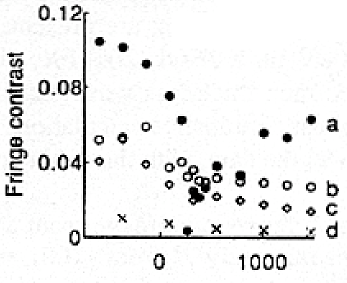

Fig.5 BF fringe contrast for a) higher and b) lower concn Si layer, and simulations for c) 400 and d) 100at% Si spread over 2 cells on Ga & As sites.

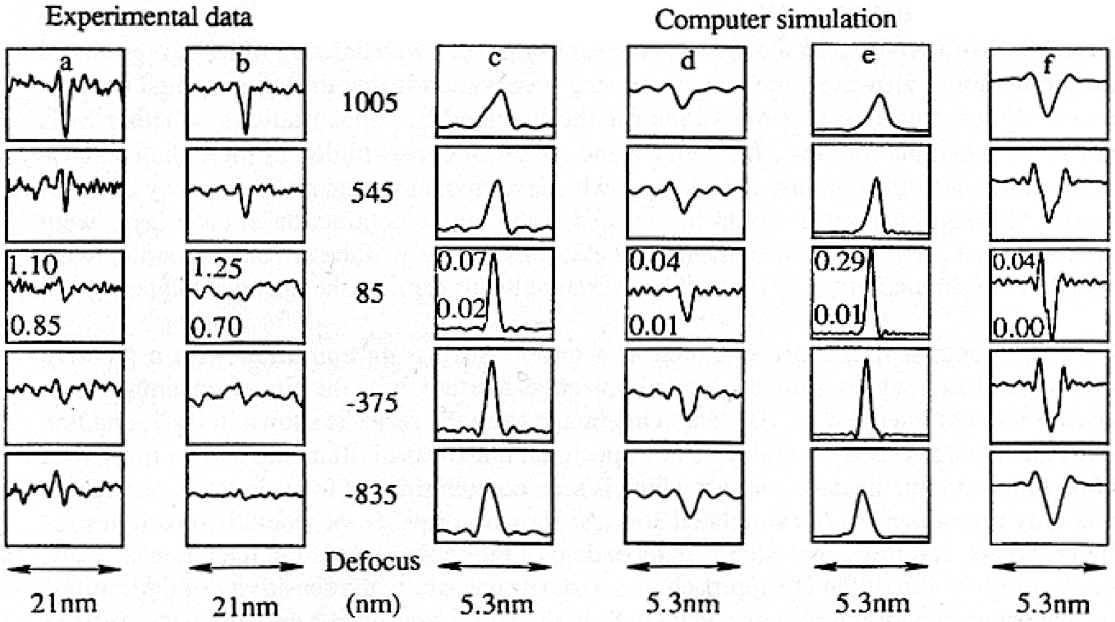

Fig.8 DF Fresnel data at specimen thickness of 40nm for a) lower and b) higher concn Si layer, and simulations for 100at% Si spread over 2 unit cells on c) Ga and d) Ga & As sites, and for 400at% Si spread over 2 unit cells on e) Ga and f) Ga & As sites, at the defoci indicated (nm).