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Modelling the intensity distribution of the Fresnel contrast of sub-unit cell Si layers in Ge

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ABSTRACT: The Fresnel Method has been used to determine the interfacial abruptness of a Si/Ge multilayer comprising 2 monolayers of Si and 22 of Ge within one period of the structure using details of the form of the contrast change with defocus. There are, however, inconsistencies between both the magnitudes and some of the contrast features for the experimental and theoretical profiles. Here we discuss the probable origins of these differences between the predicted and observed behaviours.

1. INTRODUCTION

The compositional abruptness of interfaces in a semiconductor heterostructure often needs to be determined to monolayer accuracy if a unique test is to be made of models for properties in fields such as the optoelectronic. We have successfully applied the Fresnel Method to the determination of heterostructure composition profiles for both coarse and fine layers of AlAs in GaAs (Ross and Stobbs 1991a) and to multilayers in the much more compositionally abrupt Si/Ge system (Shih and Stobbs 1991). In the latter case the monolayer accuracy required was achieved through the effects on the Fresnel contrast associated with the layering being periodic and of low spacing. We recently reported data obtained for 2 monolayer Si layers at a greater Ge separation (22 monolayers) (Dunin-Borkowski et al 1991) grown under the same conditions as the former system. We were able to infer that the Fresnel contrast exhibited was not inconsistent with the less than monolayer diffuseness of the interfaces as measured for the former system. However a more positive characterisation was not possible for the more isolated layers in the latter system because we were not able to model some features of the contrast behaviour using conventional approaches that have previously proved to be successfully applicable (e.g. Ross and Stobbs 1991a). Our concern is thus that there might be some characteristic of the fundamental modelling of the Fresnel behaviour of isolated abrupt interfaces which precludes their accurate characterisation. Accordingly we assess here the potential importance of contributions to the Fresnel contrast of this class of system both from inelastic/elastic scattering and as a function of the various ways in which the beam convergence can be affected. The experimental methods used and the general techniques required for the atomistic (in this case) modelling of fringe contrast are described elsewhere (e.g. Ross and Stobbs 1991b). The specific experimental Fresnel data discussed here have been previously reported (Dunin-Borkowski et al 1991 (Paper 1)).

2. RESULTS OF FRESNEL METHOD APPRAISAL OF Si/Ge INTERFACES

The Si/Ge multilayer examined had a wavelength (λ) of 3.36nm, nominally comprising 2 monolayers of Si and 22 of Ge. The long wavelength of this specimen allowed the examination of the relatively low contrast individual Fresnel effects for each Si layer, as are seen before overlap effects contribute (non monotonically) for defoci of more than about 250nm. The Fresnel contrast profiles, as digitised, are shown in Fig. 5 of Paper 1 and it was the double-peaked feature of the contrast seen between the Si layers, which proved to be

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sensitive to the form of the interface composition profile. A tendency for a strong "half-spacing" peak, even at low defoci, can also be seen in these profiles and results from the "lattice imaging" effect of the periodic multilayer. This effect, which must be sensitive to the partial spatial coherence, can amplify the Fresnel overlaps leading to changes with defocus in the form of the interlayer contrast which can typically have triple, double or single peaked character between the fringes centred on the marked Si layers.

Figs. 1a-1b show conventionally simulated profiles (at the experimental foil thickness of 80nm) for the interesting defocus values and for interfaces which are atomically abrupt and graded over one monolayer. The main feature which we should be able to use easily to assess the experimental profiles (since it changes rapidly with the degree of grading) is the contrast of the central double peaks relative to that of the Si peak. The contrast features are defined in Fig. 2. The behaviour of $(I_c-I_f)/I_o$ and $(I_c-I_s)/I_o$ as a function of defocus can be compared for simulated and experimental profiles. We can see immediately from Fig. 1 that an abrupt interface should show a change of sign of $(I_c-I_s)/I_o$ and this was not seen experimentally. Data from the experimental profiles in fig. 5 of Paper 1 are shown graphically as $(I_c-I_f)/I_o$ and $(I_c-I_s)/I_o$ in Fig. 3, while graphs of $(I_c-I_f)/I_o$ (modelled using experimental parameters) for an abrupt and monolayer diffuse model are compared with the experimental data in Fig. 4.

Interestingly, a comparison of the fringe contrast with defocus for experimental profiles and simulations shows clear features indicating both abruptness and diffuseness. The ranges of defocus over which the profiles exhibit triple, double and single intermediate peaks experimentally are marked as 3,2 and 1 respectively in Fig. 3. For "2" we see an interesting dip in the values of both contrast measures which can be associated with the effects of "overlap" even for the low defoci used. A Fourier approach suggests that this behaviour would indicate a fair degree of squareness of the Si potential profile and yet we have the clear contradictory evidence of the negative values of $(I_c-I_s)/I_o$ for the square model which are not found experimentally. On the other hand the defocus values for the dips (fig.4) referred to above relate to those at which this feature is seen for the abrupt but not for the more diffuse models though again the contrast values do not relate well. The experimental contrast is low, and its changes with defocus are less than predicted. This suggests the effects of multiple inelastic/elastic scattering. Further spreading the potential does <u>not</u> yield better fits with the data. The point of the original exercise was to examine the Fresnel effects for "isolated" layers but the multilayer spacing is still small and the abrupt nature of the interfaces strengthens the multilayer effects. At the same time irregularities in the spacings of the layering were noted which would weaken the "half spacing" lattice fringe effect predicted from the modelling. Clear comparisons with the modelled data are thus more difficult than had been hoped and the strength of the contrast is lower than we would expect. Even so, remembering that changes in the form of the contrast with defocus are more reliably interpreted than are their absolute values the data, particularly for the higher defoci giving multilayer effects, indicate that the layering is less than a monolayer diffuse. Furthermore the horizontal plane irregularities indicate comparable 'waviness' through the thickness of the specimen leading to a greater projected diffuseness than is present locally. Again however such an effect could not explain the contrast anomalies in question.

This is of some concern in relation to the confidence we can have in the use of the Fresnel Method for the atomic level profiling of interfaces, particularly if they are abrupt. Accordingly we are investigating the relative importance of a variety of effects which might change the Fresnel contrast under such circumstances and it is our findings in this area which we are primarily interested in here. Beam convergence uncertainties, hollow cones of coherently scattered electrons due to amorphous contamination and inelastic scattering are the primary candidates as the potential causes for the disagreement between the experimental and modelled profiles and each effect was investigated for a crystal thickness of 80nm. Figs. 1c-1d show the profiles of Figs. 1a-1b now with a larger value of beam convergence, and the fringe contrast is compared in Fig. 5 for abrupt interfaces. Although the nature of the fringe pattern has not changed, the fit of first fringe contrast has improved dramatically with the increase in convergence. In fact, using a 2000FX with an objective lens of C_s=2.3mm we are more likely

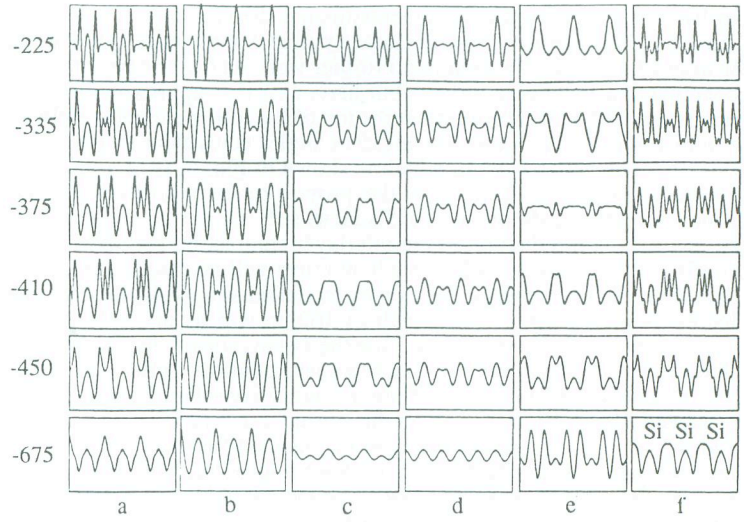

Fig. 1 Simulations for the defoci shown (nm) and at a thickness of 80nm
a) Abrupt well, 0.42 mrad conv.
b) 1 monolayer spread, 0.42 mrad conv.
c) Abrupt well, 1.0 mrad conv.
d) 1 monolayer spread, 1.0 mrad conv.
e) 1D hollow cone images
f) Abrupt well, 0.42 mr conv. plus plasmon losses (coherent limit).

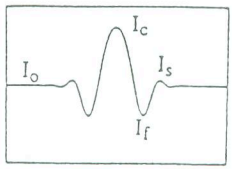

Fig. 2 Definitions of I_c, I_f, I_s and I_o.

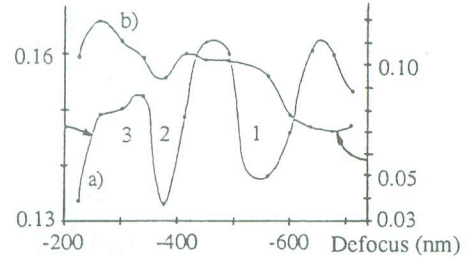

Fig. 3 Experiment : a) $(I_c-I_f)/I_o$ b) $(I_c-I_s)/I_o$

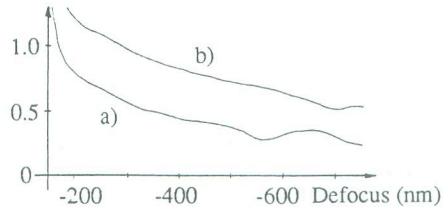

Fig. 4 A comparison of simulated first fringe contrast $(I_c-I_f)/I_o$ for a) abrupt and b) 1 monolayer spread at 0.42 mrad convergence.

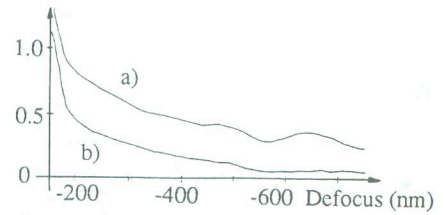

Fig. 5 A comparison of simulated first fringe contrast $(I_c-I_f)/I_o$ for abrupt interfaces at a) 0.42 mrad and b) 1.0 mrad convergence.

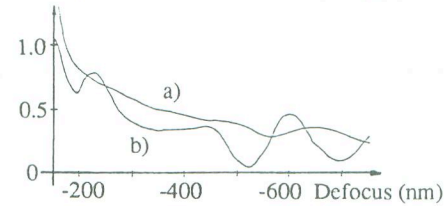

Fig. 6 The effect of hollow cone simulations ; $(I_c-I_f)/I_o$ for abrupt interfaces at 0.42 mrad convergence with a) 0% and b) 30% Ge hollow cone simulations added incoherently.

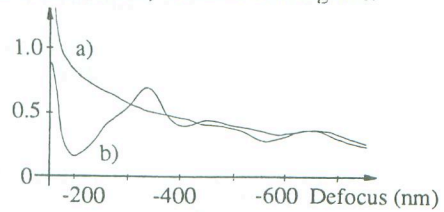

Fig. 7 The effect of inelastic scattering ; $(I_c-I_f)/I_o$ for abrupt interfaces at 0.42 mrad convergence a) no inelastic scattering and b) plasmon-loss images coherently added to a).

to have overestimated than underestimated the convergence onto the specimen. However scattering in contamination will cause a partial convergence increase, though coherently rather than incoherently. We need to do further work on differences in the contrast caused by such coherent and incoherent effects but here, as a first approximation for the effects caused by relatively high angle scattering at the top of the foil, we incoherently added the Fresnel fringe contrast profiles calculated for incident angles equivalent to a 1D Ge amorphous halo (see Fig. 1e). The general trend, which is shown in Fig. 6, is of a gradual shift of the prominent contrast features overfocus as the proportion of amorphous halo images added to the simulations for an abrupt interface is increased. For a coherent addition there will undoubtedly be more general reduction in the interlayer contrast but, while further work is being done to confirm this, the magnitude of such an effect will be insufficient to explain the experimental data. The effect of energy losses was modelled simplistically considering only the plasmon losses. A plasmon mean free path of 162nm was assumed for Ge, and both coherent and incoherent limits were analysed for the behaviour of the electrons which had lost energy (Howie 1963). Fascinatingly, and in sharp contrast to the way these two limits have very different effects on the high resolution contrast contributions of such electrons, the two models produced very similar effects on the Fresnel contrast (Fig. 1f and Fig. 7). Significantly, the addition of the appropriate fraction of plasmon-loss electrons to the images for an abrupt interface has produced features in the contrast profiles, which agree very well in form (if not in magnitude) with experiment. We can conclude that for a near abrupt model an appropriate combination of the effects of a coherent hollow cone (due to contamination) and of loss electron contributions would allow an accurate match both of the contrast levels and of their form with the contrast behaviour seen experimentally. The effective convergence change reduces the contrast level and energy loss effects yield the changes in contrast with defocus.

3. CONCLUSIONS

Since we can now qualitatively explain the general reduction in contrast level as well as the changes in detail of these levels with defocus we can return with more confidence to the use of changes in the detailed form of the Fresnel contrast with defocus for the characterisation of a composition profile. However it should be noted that for the current test case our confidence that the layers exhibit less than a monolayer's diffuseness derives again from features in the Fresnel profiles due to overlap effects. If we could energy filter and maintain a lower contamination level then the lower defocus contrast forms could be used less equivocally.

We are unsurprised that we have been able to confirm that the contrast effects that were causing problems in the interpretation of the Fresnel data can be explained sufficiently well for our retained confidence in the use of the approach for measurements of composition changes to the atomic level. The Method has a proven track record. Our more interesting conclusion is that, whether loss electrons contribute detail in the coherent or the incoherent limit is of minimal importance for the (still strong) effects such electrons have on Fresnel contrast for moderately thick foils at necessarily conventionally high defoci. In contrast it is uncertainty in the relevant ratio which makes filtering essential for quantitative high resolution imaging. For Fresnel profile analysis our preliminary result is that it is merely desirable.

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