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MODIFIED DISLOCATION STRUCTURES IN Ge_xSi_{1-x} DOUBLE EPILAYERS ON (001)Si

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ABSTRACT

Double epilayers of different compositions of Ge_xSi_{1-x} on (001)Si are observed to have dislocation contents which differ markedly from similar single epilayers. An initial epilayer, grown below its critical thickness, underwent substantial misfit dislocation introduction, while a second epilayer, grown at a composition where edge-type misfit dislocations are normally observed to dominate the morphology, contained mostly 60° type dislocations. It is suggested that dislocation entry into the upper, high mismatch epilayer allows many dislocations to enter the buried, low mismatch epilayer, and that this in turn affects the dislocation morphology in the upper layer through strain relief.

INTRODUCTION

The stability against misfit introduction of single epilayers was predicted by Matthews, et alia [1,2], and in essence has been confirmed by many experiments. One of these, a combined X-ray topography and TEM experiment [3], has established that misfit dislocations gradually extend from their source points; in this case, the beginning of extension was found to be at Ge content $x = 0.20$ for a thickness of 200nm. It has also been shown that, as misfit strain increases, the character of misfit dislocations changes from predominantly 60° (at $x \leq 0.38$) to predominantly edge type (at $x \geq 0.45$) [4,5].

In this experiment, a double epilayer was grown, the first grown below the single-epilayer critical thickness, h_c, the second well above and into the edge-dominated strain region. Both epilayers were grown by MBE at 350°C onto a (001) Si substrate, and alloy growth was preceded by Si buffer layer growth. The epilayer compositions were determined by RBS to be $x = 0.18$ and $x = 0.48$, and each epilayer was 150nm thick. Materials were examined by TEM in both plan and cross sectional views. Preparation was done by mechanical thinning followed by Ar ion milling. Both conventional and weak beam dark field techniques were employed, and accelerating voltages from 100 to 1500 keV were employed.

RESULTS

The double epilayer material was observed to have substantial dislocation introduction of 60° type dislocations at both heterointerfaces (epi-Si and epi-epi). In Figure 1 is shown an edge-on cross-sectional view of this material. Numerous epithreading dislocations can be seen within each layer; in tilted images, a number of interfacial misfit dislocations could also be discerned at each interface.

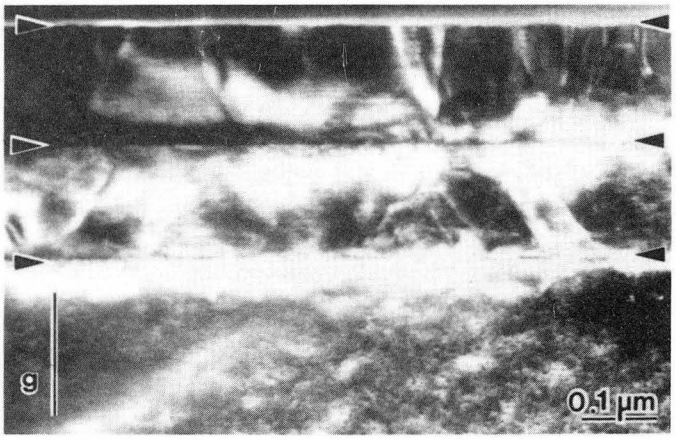

Figure 1.
Cross section view of double epilayer. Arrows indicate interfaces (from top:growth surface, epi-epi interface, epi-Si interface). Substantial dislocation line structure can be seen running in inclined directions within each epilayer.

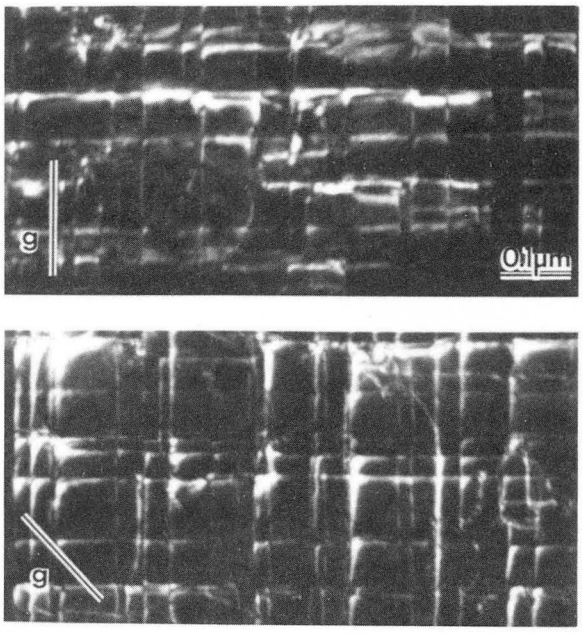

Figure 2.
Plan view of upper epilayer and epi-epi interface. Weak beam images illustrate 60° character of orthogonal sets of interfacial misfit dislocations, (a) in equal contrast in each direction using a 400 reflection, and (b) in unequal contrast (but not extinct) using a 220 type reflection.

A plan view of the upper (high mismatch) layer and upper (epi-epi) interface can be seen in Figure 2. Here the Si wafer and most of the lower (low mismatch) epilayer have been removed to allow observation of the misfit dislocations at the epi-epi interface. If the misfit dislocations were of the edge type typically observed for epilayers of this composition, those parallel to g in Fig. 2(b) would be out of contrast. It is seen that this is not the case, and that nearly all dislocations are in contrast for both **g** = (220) and (400). (N.B. Misfit dislocations of non-screw character are all in contrast for **g** = (400) due to the $\mathbf{g} \cdot (\mathbf{b} \wedge \mathbf{u})$ contrast.) The misfit dislocations at this interface are, therefore, predominantly of 60° type. It should be noted that the epithreading dislocation density measured at the growth interface was $\sim 2 \times 10^{10} cm^{-2}$.

As a test, a single epilayer of the same composition was similarly grown and imaged. This material did indeed show almost complete dominance of misfit dislocation morphology by edge dislocations.

DISCUSSION

As mentioned, TEM and x-ray topography of a thicker, similar mismatch epilayer (grown at higher temperature) have shown that the first, low mismatch epilayer here was very probably deposited below its critical thickness. However, deposition of the upper, high mismatch epilayer has clearly altered the 'system' in such a way as to allow copious misfit dislocation introduction. The method by which this could occur can be explicated by using either of the two models developed initially by Matthews, et alia, namely (i) bending over of existing threading dislocations [1], or (ii) surface nucleation of dislocation half-loops [2]. In each case, we first assume (for simplicity and clarity) that misfit dislocations have begun to relax the mismatch strain in the upper epilayer, leaving a glissile misfit dislocation at the epi-epi interface.

In the former case, illustrated schematically in Figure 3(a), it can be seen that as the epithreading segment moves from position I to II, no new dislocation line length need be created, and the dislocation self-stress is invariant. Since dislocation line tension is by far the most energetic aspect in the Matthews model, the dislocation may move under misfit stress encumbered essentially only by the Peierls stress. The only remaining back-stress is the image force, but this is small: for a dislocation moving downward from a 10nm-buried interface (the predicted critical thickness of the upper epilayer), this force would be counterbalanced by a strain of just 0.001 (corresponding to $x = 0.025$).

Threading dislocations have been seen to make relatively little contribution to the total misfit dislocation density at high mismatch, however, and it has been suggested that the large number of misfit dislocations seen for $x \geq 0.40$ is due to surface nucleation [6]. This situation, illustrated in Figure 3(b), is not so intuitive, but still straightforward to understand. In this figure a half-loop has begun to extend along the epi-epi interface, and the movement from this

position (A-B) to one inside the lower epilayer (A'-B') is the critical step. To move from A-B to A'-B', two new lengths of dislocation must be created, A-A' and B-B'. Computationally, this is similar to the case of a buried epilayer (e.g. in a SLS), and to the threading case previously discussed, where the thickness is doubled by mirroring the epilayer onto itself perpendicular to the growth surface. The system is thus most easily viewed by bisecting it along A-B, and imagining the movement of a single threading segment (from the epi-epi interface to some position within the low mismatch epilayer), leaving dislocation line length along B-B'.

In such a case, the critical thickness corresponds closely to one-half the distance A-B. We will refer to the A-B distance as l_c, the critical length to move into the lower epilayer. For the lower epilayer, x = 0.18, so $h_c \sim 300$nm, meaning that the distance l_c need only be 600nm, well within the range of misfit dislocation lengths observed in materials at the composition of the upper epilayer near h_c. It should also be noted that the diagram (and above approximation of l_c) assume the most difficult case of absolutely rigid Peierls valleys; if the dislocation is allowed to bow out along an arc, the energy barrier (and l_c) would be correspondingly lower.

The morphology of the misfit dislocations at the epi-epi interface (60° rather than edge) is understandable in terms of the relative mismatch of the epilayers only if the low mismatch epilayer has undergone some relaxation (i.e. misfit dislocation introduction). If no strain relaxation has taken place, then the lower layer would remain tetragonally strained to match the Si substrate, and the in-plane lattice parameters presented to the upper layer would be those of Si. This would result in the strain in the upper layer corresponding to that layer's bulk mismatch to Si, and dislocation introduction and reaction should take place accordingly. However, if some relaxation of the lower layer is allowed, the in-plane lattice parameters would expand, leaving a lower than bulk-to-Si misfit strain in the upper epilayer. (The point being made is that the net upper epilayer strain, not composition or strain change at the epi-epi interface, is the parameter of interest.)

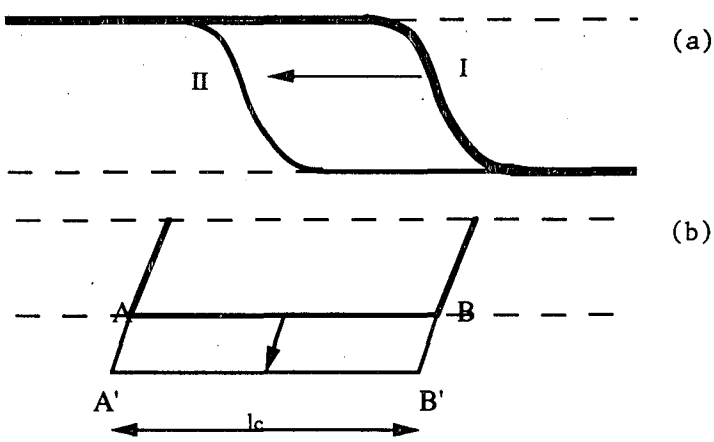

Figure 3.
The two possible mechanisms for dislocation glide from upper to lower epilayer: (a) internal source and (b) surface source for misfit dislocation introduction.

The 60° character of the epi-epi heterointerfacial dislocations indicates not just that the relaxation of the lower mismatch layer has taken place (a fact already presented), but also that the relaxation has taken place prior to edge dislocation formation.The composite structure certainly reached h_c (the point where total intergrated misfit strain force could overcome the restoring line tension and image forces) prior to the point where the high mismatch epilayer would, by itself, have reached h_c. The critical question is whether (a) the relaxation at this stage was sufficient to drop below the edge dislocation formation point, or (b) edge dislocation formation occurs by a multistep process, and the latter step(s) was (were) delayed or shunted until their completion was no longer favourable.

It has recently been argued [5,6] that the inception of surface nucleation occurs somewhere near a misfit strain of 0.015, and that edge dislocation formation occurs at a slightly higher strain (~0.019). The proposed mechanism for edge dislocation formation is a

two-step process: initial surface nucleation of a glissile 60° half-loop, followed by nucleation of a second 60° dislocation (either at the surface or upon the initial dislocation), which combines with the initial dislocation to form an edge type misfit dislocation.

In this experiment, it seems very likely that surface half-loop introduction of dislocations was a dominant mechanism, in light of the very high epithreading density. This density is related to the number of individual misfit dislocations, which in turn is related to the number of sources (since dislocation multiplication has been shown to be a low-probability event [6]). Since a high density of growth defects was not observed, the source for most dislocations was very probably the surface.

As has been shown, surface-nucleated half-loops could easily be swept from the epi-epi interface into the low mismatch layer. Such an operation would remove the precursor stage to edge dislocation formation (the initial 60° misfit dislocation [5]) soon after its creation. Although the removal of dislocations from the epi-epi interface requires that the dislocations be longer than many of those observed in, e.g., x = 0.50, 10nm thick epilayers, it should be recalled that the lengths in such epilayers are artificially short. For single epilayer materials, it has been observed that dislocation pinning takes place due to the repulsive force exerted on a gliding dislocation by other dislocations lying across its path [7], thus preventing further extension along the interface. In the case of this experiment, the dislocations would not be so permanently pinned, since the obstructing dislocation could easily glide into the low mismatch epilayer, and thus be removed as an obstacle (or, glide downward before it can become an effective obstacle). Thus the average epi-epi interfacial dislocation length is likely to have been far greater, and the time spent to reach 'critical length' before being swept into the low mismatch layer quite low, leaving very little incubation time for an edge-forming event.

Any relaxation process need only continue until the lower mismatch epilayer is sufficiently relaxed for edge dislocation formation to no longer be favoured. In this case, the upper layer was not far above this critical strain level, so not much dislocation introduction would have been necessary. The evidence for surface introduction, however, indicates that the upper epilayer was at least near this regime for some time, since surface nucleation is so closely followed by edge formation.

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REFERENCES

1. J.W. Matthews, **Phil. Mag.**, 13, 1207 (1966)

2. J.W. Matthews, S. Mader, and T.B. Light, **J. Appl. Phys.**, 41, 3800 (1970)

3. D.J. Eaglesham, E.P. Kvam, D.M. Maher, C.J. Humphreys, and J.C. Bean, **Appl. Phys. Lett.**, 53(21), 2803 (1989)

4. E.P. Kvam, D.J. Eaglesham, D.M. Maher, C.J. Humphreys, J.C. Bean, G.S. Green, and B.K. Tanner, in Defects in Electronic Materials, edited by M. Stavola, S.J. Pearton, and G. Davies (Mater. Res. Soc. Proc. 104, Pittsburgh, PA 1988) p. 623

5. E.P. Kvam, D.M. Maher, and C.J. Humphreys, this volume

6. R. Hull and J.C. Bean, **J. Vac. Sci. Tech.**, A7(4), 2580 (1989)

7. R. Hull and J.C. Bean, **Appl. Phys. Lett.**, 54(10), 925 (1989)

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