A TEM study of Ge-on-(111)Si structures for potential use in high performance PMOS device technology

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Abstract. We have performed a transmission electron microscopical study of samples where pure Ge has been grown on differently oriented Si wafers by reduced pressure chemical vapour deposition. In the present study we examine pure Ge layers grown on (111)Si wafers by annular dark-field (ADF) scanning transmission electron microscopy (STEM) and by high-resolution electron microscopy (HREM). There is evidence of immediate strain relaxation taking place by dislocations and twinning. A novel configuration of micro-twins has been observed at the interface between the pure Ge and the underlying (111)Si wafer. Growth mechanisms and models to explain the interfacial configurations of this type of wafer are suggested.

1. Introduction

In recent years, there has been an increased interest in using Ge as a higher charge carrier mobility alternative to Si, for advanced complementary metal-oxide-semiconductor (CMOS) device applications, based on hole transport [1].

One consideration is the choice, type and orientation of the substrate used. In recent years, Ge, or an alloy of SiGe, has been grown commonly on (001)Si wafer orientation; however, enhancements in hole mobility have been theoretically found if alternative orientations of the surface normal of the Si wafers are utilised; namely growth on (101)Si or (111)Si wafers [2-4]. However, growth upon these latter two orientations can impose difficulties in terms of the final microstructure observed. Growth on these latter types of wafers is very challenging because it is the way in which the layer relaxes by the nucleation of dislocations into the final microstructure that can have an impact on the electrical properties [5]. Ideally we would like to grow layers onto virtual substrates; however, the microstructure of the virtual substrate is non-ideal with significant defects and non-planar uniformity of the surface of the substrate. Micro-twins and extended stacking faults are prevalent in structures grown on non standard orientated wafers [5]. The main consideration is the orientations of the various (111) slip planes in Si or Ge grown on top of the wafers. In (001)Si there is a symmetry in the orientation of the various (111) planes which can balance the effects of misfit relief and also the tilt components in the final microstructure. One compromise would be to grow pure Ge, or alloy SiGe,
layers directly onto the differently oriented wafers which circumvents the need to fabricate potentially defective virtual substrates.

In the present work, we focus on growth of pure Ge on (111)Si wafers through transmission electron microscopy studies. We will show that relaxation of the pure Ge layer is evident and also an unusual twinning effect appears at the boundary between the pure Ge layer and the underlying Si.

2. Experimental Details
The Ge layers investigated in this study were grown by reduced pressure chemical vapour deposition (RP-CVD) using an ASM Epsilon 2000 reactor on (111) orientated p-Si substrates. The Si substrates were cleaned using a high temperature in-situ H bake immediately prior to epitaxial growth to remove any native oxide. The Ge layers were all grown at 400°C using a GeH₄ precursor gas. The growth time was 15 mins. The control of precursors, carrier gas flows and chamber pressure resulted in a GeH₄ partial pressure of around 10mTorr.

[110] cross-sectional specimens, for TEM, were prepared in the usual manner with 3mm disks thinned mechanically to ~30-40µm followed by Ar⁺ ion thinning to electron transparency. Finished specimens were then analysed using a JEOL 2010F field-emission gun instrument, operating at 197kV) and a JEOL Z3100 R005 (300kV) aberration corrected cold-FEG scanning (S)TEM, both equipped with Gatan Imaging Filters as well as bright-field (BF) and annular dark-field (ADF) detectors.

3. Results and Discussion
As an overview of the morphology of Ge layers grown onto (111)Si wafers, a low magnification annular dark-field image is provided in figure 1. The average thickness of the Ge layer on (111)Si of 8 nm corresponds to an average growth rate of 0.5nm/min. It is clear that the surface of this ‘pseudo’-continuous layer is rough with an amplitude of roughness of ~5nm.

![Figure 1. ADF image of Ge layer on Si(111)](image)

If the thinnest region of the TEM specimen is now focused upon, where the material is suitable for high resolution phase contrast imaging, we observe discrete islands such as the one shown in figure 2. This image is obtained using the JEOL 2010F analytical TEM and shows clearly the atomic columns close to the island/wafer interface. There appear to be small regions on this boundary that are amorphous-like in appearance. If a Burgers circuit is drawn around these amorphous regions, as in the two regions of figure 2, we find that the centres of these amorphous regions contain dislocation cores.

One interesting feature of the present (111)Si grown wafer is the occurrence of twinning. Since the basal plane is {111} type, there is a possibility that the (001) direction of deposited material can be oriented in one of two ways. Either the (001) direction can follow the (001) direction of the substrate wafer. Or, alternatively, a twinned configuration can be established whereby the (001) of the deposited material is mirrored about the interface plane. An example of this can be seen in figure 3. Here, we see a grain (indexed B) which is a mirror twin of the underlying substrate, and also the surrounding material (grains A and C).
Figure 2. Lattice images of boundary between Ge island (top) and underlying (111)Si. Burgers circuits show non-closure.

Figure 3. HREM image showing twinned (B) and untwinned (A+C) grains.

In addition, edge dislocations are observed in those grains grown epitaxially without the occurrence of twinning; whereas no dislocations are observed at the grain-substrate interface for the twinned configuration. This would indicate that twinning or, more precisely, the introduction of twin boundaries, may be regarded as an alternative to the introduction of misfit dislocations; however, the situation is more complicated. If the microscope point resolution is sufficient to resolve individual atomic columns of the diamond structure along the <110> zone axis (so-called dumb-bells), i.e. better than 0.14 nm, we can determine at the atomic level the orientation of these dumb-bells, which are aligned along the (001) orientation of the local crystal lattice.

Figure 4. High Resolution ADF image showing twinned configuration at island substrate interface.

In the ADF image shown in figure 4, taken using the JEOL Z3100 R005, the Ge atomic columns appear much brighter than the Si columns, in agreement with the contrast expected for pure Ge/Si [6]. It can be clearly seen that there is a switching of orientation of the Ge dumb-bells at various regions of the interface (these areas are marked transparent yellow in figure 4). Upon further growth of the island the orientation of the (004)Ge lattice planes reverts back to the correct alignment where they are parallel to those dumb-bells of the underlying Si wafer. These micro-twins observed at the boundary between the deposited island and the underlying wafer are very narrow and found to be always exactly 2 monolayers (=½ unit cell), 4 monolayers (=1 unit cell) or 6 monolayers (=1½ unit cell) in thickness. Their origin is still unclear, although it is likely due to the energy of formation of the twinned orientation being very similar to the untwinned because growth on a (111)Si wafer has the option of adopting a non-mirror or a mirrored orientation.
In the case of growth upon the (111)Si surface, we observed what seems to be an array of dislocations at the island/substrate interface. A Burgers circuit around the amorphous like regions showed non-closure; however, the closing vector does not seem to represent the full Burgers vector. It appears that this closure is simply the edge component of the Burgers vector observed in projection.

Upon analysis, we find that this dislocation is not a pure edge dislocation such that the total Burger’s vector is perpendicular to the beam direction. If this were the case then the Burgers vector would not be a normal translation vector. Instead, the Burgers vector is inclined to the beam direction to give a conventional $a/2\langle 110 \rangle$ vector. So, what is observed in the image (figure 2) is a projection of the Burgers’ vector along the beam direction. Moreover, these dislocations are very efficient at relieving interfacial misfit because the edge component of the Burgers vector is actually in the interface plane and not inclined to it as would be seen in growth in the other two systems ((001) and (101)).

If there is a (111) glide plane parallel to the sample surface then it is possible to introduce dislocations quite efficiently at the edges of this plane. This is reminiscent of dislocations introduced in materials which grow via the Volmer-Weber growth mode where growth proceeds immediately in a 3D islanding mode and relieves misfit strain energy quite efficiently by introducing dislocations at the edges of islands as the island size increases. What is clear is that misfit relief in the (111)Si system proceeds by introducing dislocations in a glide plane parallel to the island/wafer interface. In any case, this may have important implications in that it may be difficult to produce pseudomorphically strained layers on such (111)Si wafers.

The interfacial twinning observed in growth of Ge on (111)Si is interesting in that this behaviour would not have been observed without the use of an aberration corrected instrument with the necessary resolution to resolve the (004)Ge ‘dumb-bells’. What is clear is that the (111) surface acts as a mirror plane and allows growth in one of two configurations where (004)Ge is aligned with that of the substrate or grows in a mirror related twin configuration. Both alternatives seem energetically equally favourable and are perhaps evidence of a misfit relieving mechanism in this system. Moreover, it appears that with further growth the required (001)Si//(001)Ge epitaxial relationship is obtained as the micro-twins achieve a lateral length of only 6-7 nm and so cover only a small fraction of the substrate. These twin structures appear to be confined to the film-substrate interface and do not have components which extend up to the final free surface.

4. Conclusions

On (111) surfaces it has been shown through high resolution images that an array of misfit relieving dislocations are present at the island/substrate interface indicating that the islands are not fully strained. This has been explained in terms of the presence of a slip/glide plane parallel to the film substrate interface along which misfit dislocations can be introduced. These dislocations are mixed type and have the usual $a/2<110>$ Burgers vector. A novel configuration of micro-twins has also been observed at a portion of the Ge/Si(111) interface where the twins appear to be confined to the interface and do not extend up to the surface.

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