Inhomogeneous Strain Distribution in Epitaxial SiGe/Si Multilayers Visualized by Dark-field Inline Electron Holography

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Elastic strain arising from the epitaxial growth of thin film on a lattice-mismatched substrate can be utilized to enhance the material's properties and functionalities. Detailed nature of the epitaxial strain varies sensitively with the geometry of thin film system. In the case of an alloy thin film system, the strain state may vary in strong correlation with the distribution of alloy element within the film and vice versa. In this aspect, elastic strain engineering of a SiGe/Si system relies primarily on accurate measurement and thereby precise control of the lattice strain and Ge distribution. Here we show the detailed strain state of the 10 nm-thick $Si_{0.85}Ge_{0.15}$ epitaxial layers grown in multilayer with Si with various thickness ratios by using dark-field inline electron holography strain mapping [1-3] and atom probe tomography (APT) for the correlation of Ge distribution to the stain results.

The cross-sectional TEM specimens were prepared by mechanical wedge polishing. The wedge-polished samples were ion-milled first by using Ar^+ ion beam at a few kV, followed by low energy ion milling. The electron holography experiments were performed using a JEOL-2100F, equipped with a 200 kV field emission gun. All TEM images were recorded using the Gatan's GIF Tridiem imaging filter to remove inelastically scattered electrons. For the in-plane and the out-of-plane strain mapping, the (0-22) and (004) diffracted beam were selected, respectively.

The in-plane strain maps demonstrate that the lattice matching between the SiGe and Si in the multilayer is accomplished by (compressive) strain of SiGe layers to fit onto Si substrate. This is quite understandable in the classical thin film mechanics. The out-of-plane strain maps clearly show that the strain within each SiGe layer is non-uniform with exhibiting local maxima at the interfaces (**Fig.1**). Interestingly, the APT results reveal that the spatial distribution of Ge in each SiGe layer is closely linked to the strain (**Fig.2**); the Ge content is higher at the regions of higher strain. More interestingly, we found unexpected strain distribution in the out-of-plane strain maps; the compression of Si interlayers, which increases with decreasing its film thickness. Previously, we have also found a similar compressive strain in the GaN layer of InGaN/GaN multiple quantum well structures [2]. This compressive strain, however, is hardly accounted for by any of the existing models developed for the epitaxial strain in thin film structure [4]. To understand this phenomenon, we propose a stress-compensation model in which the total out-of-plane stress is zero ($\sum \sigma_{33}^{SiGe} = 0$) but the local out-of-plane stress is non-zero ($\sigma_{33}^{SiGe} \neq 0$). The implementation of the stress-compensation model using finite element modelling (FEM) reproduces the fundamentally the same strain distribution (the inset in **Fig.1**). Further elaborate analysis based on molecular dynamic simulation and phase field modelling will be discussed .

Reference

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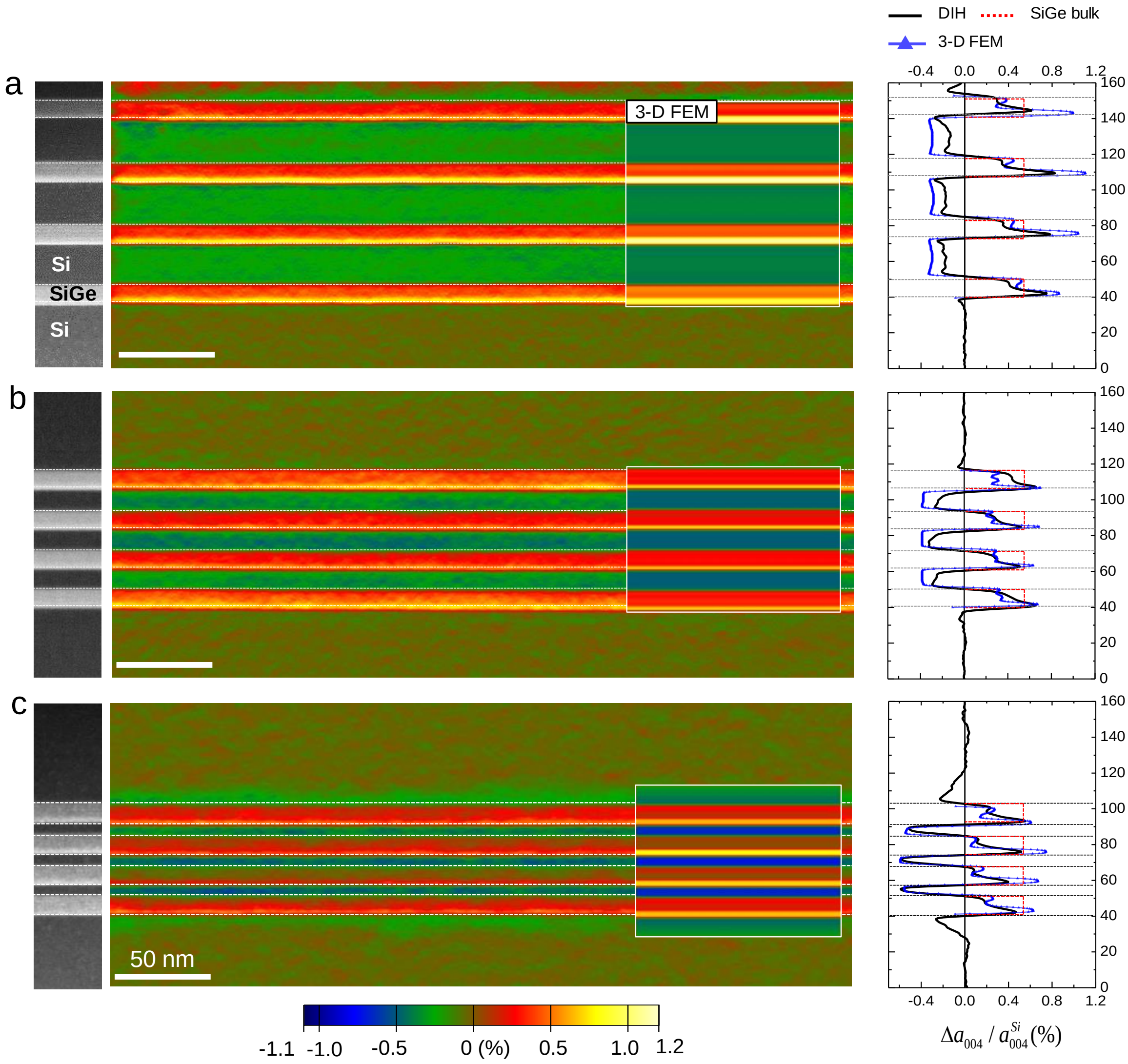

Figure 1. Out-of-plane lattice parameter ($\Delta a_{004} / a_{004}^{Si}$) maps and corresponding FEM simulation results. (a) Thickness ratio of Si/SiGe$_{0.15}$ = 2.0; (b) 1.0; and (c) 0.5. The out-of-plane strain maps show that not only SiGe but also Si layers are strained in opposite sign, to amounts which depend on the relative Si/SiGe thickness ratio.

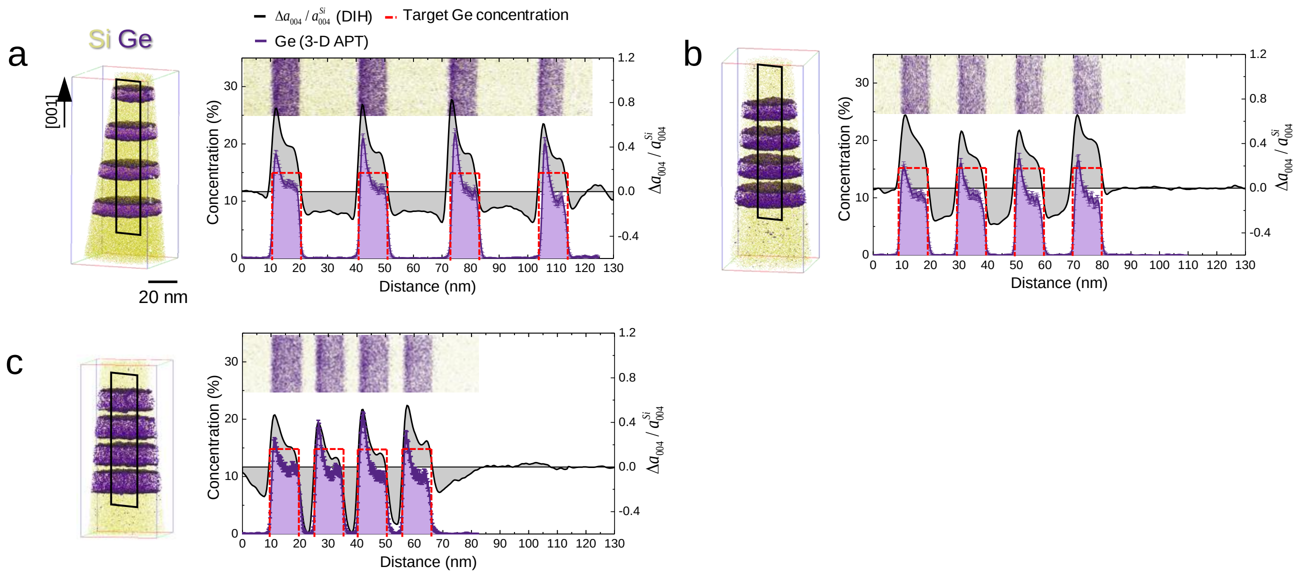

Figure 2. Ge concentration analysis by 3-D APT. (a) Thickness ratio of Si/SiGe$_{0.15}$ = 2.0; (b) 1.0; and (c) 0.5. Inhomogeneous Ge concentration distributions were observed in within the Si/SiGe$_{0.15}$ layers with local maximum at the lower interface.