Combining SIMS with GPA of aberration corrected HAADF STEM images for measurement of misfit strain in epitaxial SiGe layers

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Nanoscale mapping of strain in Si and SiGe alloys is of critical interest to the microelectronics industry since strains less than 1 % will be engineered into next generation device structures to continue along the performance-scaling roadmap.[1] In this study, Geometric Phase Analysis (GPA) of aberration corrected high-angle annular-dark field STEM images is used to measure lattice strain in Si and epitaxial SiGe multilayers to assess sensitivity to strain at nanometer length scale. GPA of phase-contrast TEM has been widely used to map the 2D strain in a range of systems and recent applications of STEM have been reported[2]. A key benefit of HAADF STEM is that contrast does not reverse with focus and is monotonic with sample thickness. Since acquisition takes 30s or more, the scan instability can exceed a 1% standard deviation which poses the biggest challenge. An assessment of the scan of was made using polished Si. Corrections made to the intermediate phase image allow strain measurement with 0.1% accuracy.

Fig. 1 shows the HAADF image and strain maps of a biaxial compressively strained epitaxial $Si_{1-x}Ge_x$ multilayer structure grown on (001) Si . The in-plane e_{xx} map shows that the layers are pseudomorphically strained and the out-of-plane e_{zz} misfit oscillates. The average x through the SiGe multilayer stack measured by SIMS is 0.44 with modulation between minimum (~32.5at%) and maximum [Ge] ~60.3at%, fig 2. Fig 3 shows line profiles of the strain along through a box drawn perpendicular through the stack. Misfit out of plane rises to 4%. Since the $Si_{1-x}Ge_x$ lattice spacing varies as $d_{SiGe}=0.5431+0.0199\,x$, the misfit for a relaxed $Si_{0.56}Ge_{0.44}$ alloy would only be 2%. Since the epilayers are compressively constrained in-plane, this observation confirms an out-of-plane tetragonal distortion of up to 2%. The strain may be estimated from the composition assuming an isotropic strain model. The HAADF intensity profile averaged over a width of 0.5A is calibrated using the SIMS composition assuming linear-proportionality to x. Applying the Poisson's ratio, $\nu = 0.278$, the out-of-plane misfit with respect to Si is derived assuming the in-plane lattice is fully stained. There is good agreement between the strain calculated and the GPA measurement, fig. 4. Strain measurement with 0.1 % sensitivity and sub-nanometer resolution will be applied to map strain in CMOS device structures.

This Work was performed by Alliance Teams at various IBM Research and Development facilities

[1] Haensch et al IBM Journal of Research and Development, **50**, (2006) 339

[2] Vajargah et al App Phys Letts **98**, (2011) 082113;

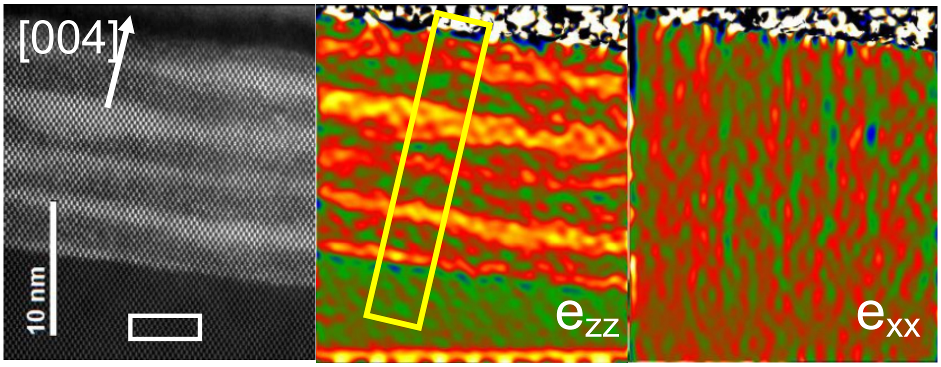

Figure 1 HAADF STEM of SiGe multilayer structure on Si, recorded on FEI Titan STEM with 1A resolution. e_{zz} axis is along Si [004] shows out-of-plane strain modulations Null contrast in e_{xx} confirms in-plane pseudomorphic epitaxy.

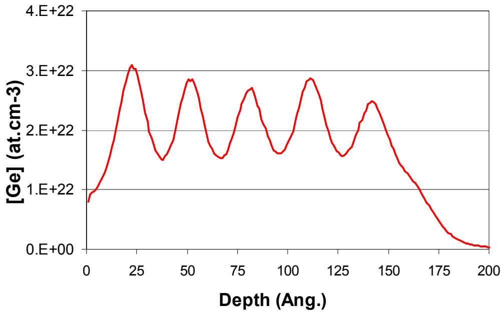

Figure 2. SIMS depth profiles showing composition modulations of $Si_{1-x}Ge_x$

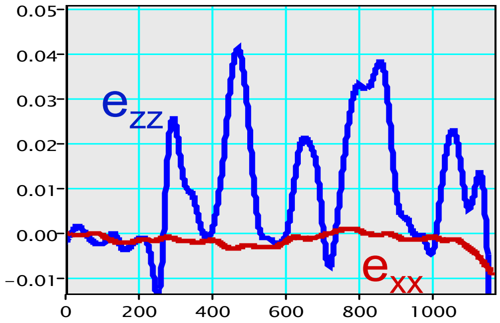

Figure 3. Average misfit profiles from box shown of $Si_{1-x}Ge_x$ misfit through multilayer (x-axis units is pixels)

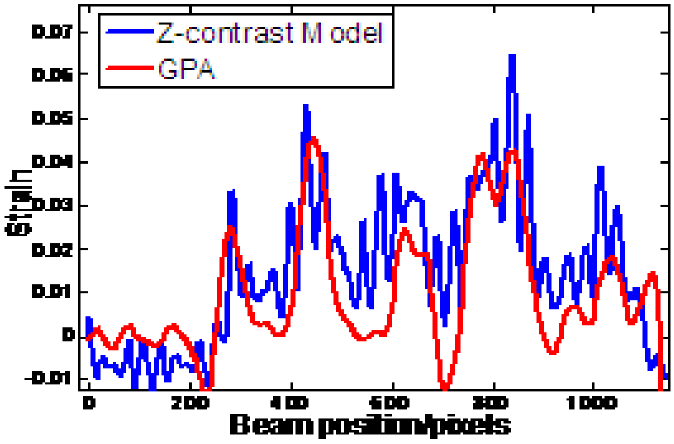

Figure 4. Misfit measured by GPA compared to misfit calculated from isotropic elastically strained model of $Si_{1-x}Ge_x$, where x is determined from the "SIMS-calibrated" HAADF intensity line profile. The difference is attributed to strain relief associated with the thin TEM lamella.