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EBSD Strain Analysis of Epitaxial Si_{1-x} Ge_x on Si

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High resolution electron backscattered diffraction (HR-EBSD) is a rapidly evolving technique for measuring lattice strains and rotations [1], with the potential for broad application, for example in the areas of MEMS, NEMS, and the analysis of CMOS and developmental semiconductor metamaterials such as quantum dots and multiple quantum wells. In this technique, cross-correlation methods are applied to high resolution EBSD patterns obtained from unstrained and strained points on the same planar sample in such a way that the crystal lattices at the two points can be accurately compared to determine lattice strain and rotation [2,3]. This study is part of a project to create a reference artifact consisting of a die of silicon partially covered with a coherent epitaxial film of $Si_{1-x}Ge_x$ of known composition (x), thickness and interplanar spacing. Thin films of Si_{1-x} Ge_x were deposited on six inch Si wafers; the films had nominal Ge contents of 17% and 28%, and thicknesses up to 200 nm. Test structures were created, including lines of various widths, and large blanket areas surrounded by bare Si.

The equilibrium lattice constants for these Si-Ge alloys were calculated using relationships from the literature; for x = 0.17 and 0.28, the calculated lattice constants were 0.642 % and 1.07 % larger than the Si lattice constant, respectively [4]. EBSD measurements of the strain tensor relating the SiGe film to the Si substrate indicated tetragonal expansion normal to the substrate caused by the epitaxial misfit; the magnitude of the distortion can be related to the film composition and the degree to which epitaxy is relaxed by misfit dislocations, which typically occurs with thicker films and higher values of x. X-ray diffraction (XRD) was used on the blanket film samples to measure the d-spacing of the film parallel to the substrate. Where perfect epitaxy could be justifiably assumed, the XRD measurements allowed the composition of the film to be determined; the validity of this approach will be discussed. Energy dispersive x-ray spectroscopy (EDS) measurements were also made to determine film composition. Contact resonance atomic force microscopy (CRAFM) was applied to quantitatively observe the difference in the elastic response of adjacent SiGe and Si regions. From CRAFM point measurements as well as mapping, the indentation moduli of SiGe of various compositions were determined relative to the indentation modulus of the Si substrate. Fig. 1 shows a line scan of the strain of the SiGe film relative to the adjacent substrate measured using HR-EBSD, allowing both the film-to-substrate strain and the details of the strain variation at the edge of the film to be elucidated. Relaxation of the epitaxial strains was observed over a length scale about five times the film thickness. A critical comparison between the film-to-substrate strain determined by HR-EBSD and XRD will be presented.

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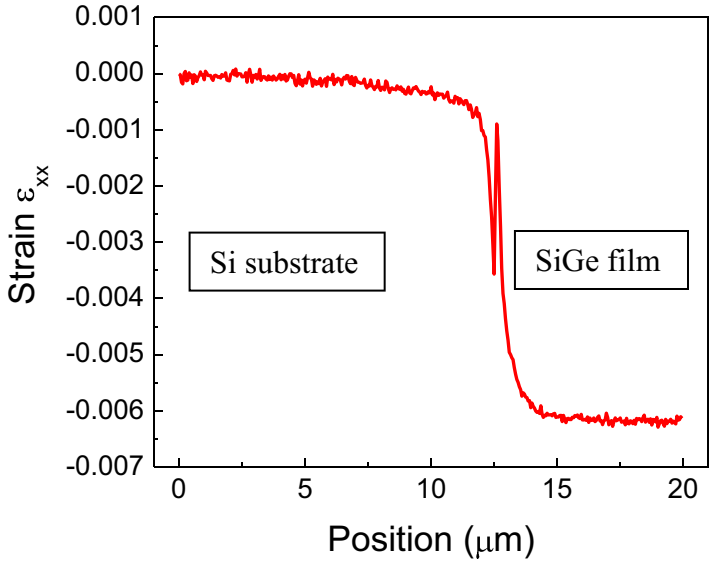
FIG. 1. Strain (ε_{xx}) vs. position measured across edge of 100 nm $Si_{0.83}Ge_{0.17}$ blanket film on Si determined using HR-EBSD



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