doi:10.1017/S1431927613005448
Microsc. Microanal. 19 (Suppl 2), 2013
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Excellent Agreement Between High Resolution EBSD and XRD Strain Measurements on $Si_{1-x}Ge_x$ films on Si

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High resolution electron backscattered diffraction (HR-EBSD) is a rapidly evolving technique for measuring lattice strains and rotations with the potential for broad application in a number of areas, for example in microelectronics and microelectromechanical systems. The method measures strain differences between positions on a sample in a scanning electron microscope by cross correlating several equivalent regions in EBSD patterns obtained at those positions; the method has been described by Wilkinson et al. [1], and implemented in commercial software. This work describes ongoing efforts at NIST to establish an experimental basis for the accuracy of measured strains, and the spatial and strain resolutions of the technique. One primary goal of the work is to produce a Reference Material (RM) that contains strained and unstrained crystalline material in adjacent, coplanar regions of the artifact. To be useful, the regions must be at similar orientations (≈ 1°) and the strain must be known to an accuracy of 10^{-4}. The artifacts chosen to fulfill these requirements consisted of $Si_{1-x}Ge_x$ films on Si, with film thicknesses (t) selected so that the films were epitaxial and electron diffraction occurred entirely in the film, and composition (x) in the range 0.2 to 0.4 to produce coherency strains in the 1 % to 2 % range. The tetragonal strain, ε_{tet}, in the film was defined:

$$\varepsilon_{tet} = \varepsilon_{33} - \frac{\varepsilon_{11} + \varepsilon_{22}}{2} , \tag{1}$$

where the 1- and 2-axes are in the plane of the film and the 3-axis is normal to it.

Wafers of (001) Si with $Si_{1-x}Ge_x$ films of specific x and t values deposited on them were obtained from commercial semiconductor companies. Prototype devices were fabricated at NIST on 25 mm square dies with a number of features for various experiments, including stripes of $Si_{1-x}Ge_x$ with various widths and pitches for HR-EBSD measurements of strain, and a 20 mm × 12.5 mm pad for x-ray diffraction (XRD) measurements. XRD scans across the Si 004 and $Si_{1-x}Ge_x$ 004 peaks were taken, using equipment with a Johansson optic to suppress the x-ray beam $K\alpha_2$ component, from which the d-spacings of the (004) planes of the film and substrate (d_{Si004} and $d_{SiGe004}$) were determined. The scan in Figure 1 from a film with nominal $x = 0.3$ and $t = 35$ nm shows the Si and $Si_{0.7}Ge_{0.3}$ 004 peaks and also residual $K\alpha_2$ component on the right side of Si 004. The $Si_{1-x}Ge_x$ 004 peak has a number of oscillations on each side due to the perfection of the $Si_{0.7}Ge_{0.3}$ film and these oscillations were modeled to determine film thickness; this work is not presented here. Under the assumption that the film was epitaxial with the substrate so that the in-plane ((400) and (040)) d-spacings of $Si_{0.7}Ge_{0.3}$ and Si were the same, ε_{xrd} can be calculated as

$$\varepsilon_{xrd} = d_{SiGe004} / d_{Si004} - 1 \tag{2}$$

On the same sample, EBSD scans were made across several 50 µm stripes of $Si_{0.7}Ge_{0.3}$, and Figure 2 shows the normal strains (ε_{11}, ε_{22}, ε_{33}) generated from two 50 µm stripes (marked A and B) using commercial software [2] to calculate the strains, followed by the use of eq. 1. The shaded regions indicate the data that were averaged to give the strains in the substrate (nominally zero) and film. These

https://doi.org/10.1017/S1431927613005448 Published online by Cambridge University Press

strains were subtracted to give the measurements in Table 1, which also contains the strain calculated from the XRD plot in Figure 1 using eq. 2. The agreement between the two EBSD measurements is good and their average agrees with the XRD result to within 3×10^{-4}. XRD is the more mature and tested technique and can easily yield results of high accuracy; $\pm10^{-4}$ can be achieved on a routine basis. These results suggest that a RM of this type can be fabricated to validate the accuracy of EBSD strain measurements at the $\pm3\times10^{-4}$ level, and potentially better.

References:

[1] A. Wilkinson, G. Meaden, D. Dingley, Ultramicroscopy **106** (2006), 307-313

[2] A. Wilkinson, G. Meaden, D. Dingley, Materials Science and Technology **22** (2006), 1271-1278

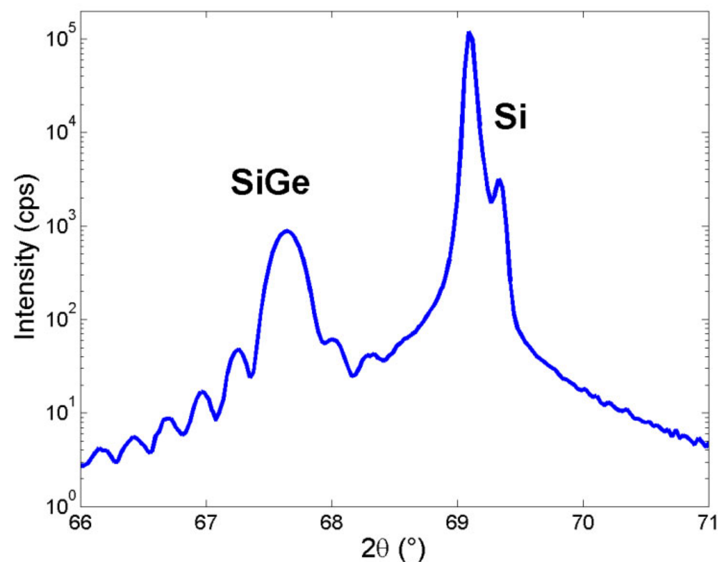

Figure 1. X-ray diffraction scan from 35 nm $Si_{0.7}Ge_{0.3}$ on Si

Measurement	Strain
XRD	0.0189
EBSD A	0.0187
EBSD B	0.0185

Table 1. EBSD and XRD results

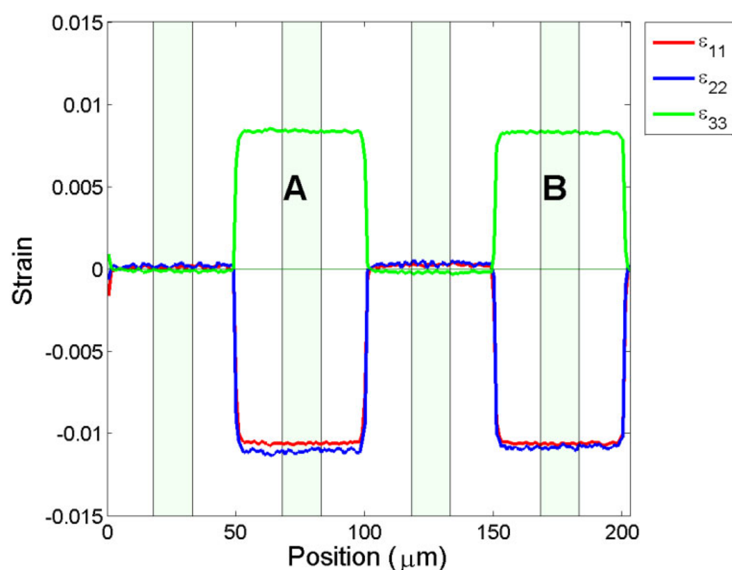

Figure 2. EBSD data from 35 nm $Si_{0.7}Ge_{0.3}$ on Si

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