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Strain Measurement of 3D Structured Nanodevices by EBSD

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Abstract

We present a new methodology to accurately measure strain magnitudes from 3D nanodevices using Electron Backscatter Diffraction (EBSD). Because the dimensions of features on these devices are smaller than the interaction volume for backscattered electrons, EBSD patterns from 3D nanodevices will frequently be the superposition of patterns from multiple material regions simultaneously. The effect of this superposition on EBSD strain measurement is demonstrated, along with an approach to separate EBSD patterns from these devices via subtraction. The subtraction procedure is applied to 33 nm wide SiGe lines, and it provides accurate strain magnitudes where the traditional EBSD strain analysis method undervalues the strain magnitude by an order of magnitude. The approach provides a strain measurement technique for nanoscale 3D structures that is high spatial resolution, nondestructive, and accurate.

Keywords

EBSD; strain; strain measurement; cross-correlation; Electron Backscatter Diffraction; nanoscale; SiGe; silicon

Introduction

Stress and strain effect fundamental material properties and govern the performance, both mechanical and otherwise, of things both large and small. Strain measurement of large-scale parts (e.g. steel beams) allows engineers to understand performance and failure behavior of the material, and the same insight is also useful in nanoscale devices like transistors and micro-electro-mechanical systems (MEMS). Although some traditional non-destructive strain measurement techniques like confocal Raman microscopy can be applied to small-scale devices, nearly all existing approaches fail when spatial resolution below 100 nm is required. Transmission electron microscopy (TEM) is capable of measuring strain[1] at very high resolution, but sample preparation is slow, expensive, destructive, and alters the mechanical boundary conditions for most structures generating a strain state that is not representative of the in-service state. Due to the impact strain has on both semiconductor and MEMS devices during fabrication and operation, the ability to accurately measure strain in sub-100 nm devices is essential. To address this need, we present an extension to strain measurement using electron backscatter diffraction (EBSD) that improves spatial resolution,

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preserves the original strain state, is non-destructive, and is accurate compared with traditional EBSD methods.

EBSD is routinely used to measure crystal orientation and strain using a scanned electron probe—typically a Scanning Electron Microscope (SEM)[2]. In an idealized description, the SEM probe provides a sub-surface point source of monochromatic electrons that propagate radially outward through the sample. Some of these electrons will meet the diffraction criteria for the crystal and will form Kikuchi bands that are centered about the intersection of the EBSD detector plane and the diffracting lattice planes. This pattern of Kikuchi bands, or Electron Backscatter Pattern (EBSP), can be analyzed to provide the orientation of the diffracting crystal relative to the detector[3]. Furthermore, as strain is the distortion of a crystal structure, and the distortion of the crystal lattice generates a predictable distortion in the EBSP, EBSPs can be analyzed to measure strain, as described by Wilkinson et al.[4] and others[5–10].

In reality, the idealized sub-surface monochromatic point source is much more complicated. High energy electrons (>10 keV) from the SEM scatter both elastically and inelastically within the sample and travel large distances, typically 100s of nm, before losing a large fraction of their initial energy. Many of these electrons will scatter along a trajectory that causes them to leave the sample again while still maintaining a large fraction of their initial energy. These electrons (termed backscattered) form EBSPs, but do so with energies distributed below the initial energy and from a position that may be many 100s of nm[11,12] away from the incident location.

Neither the energy nor spatial distribution of the source disrupt strain measurement for many applications. However, in microelectronics applications where feature sizes are well below 100 nm, the spatial distribution of the source can strongly affect strain measurements and requires that the fundamental physics that generate EBSPs be considered. Here we describe an entirely new analytical approach that applies electron trajectory models to analyzing EBSD strain measurements from sub 200 nm structures, and demonstrate that this advanced analysis is essential to accurately measuring strains in nanoscale 3D devices.

EBSD Strain Measurements of Nanoscale SiGe Lines

To adequately illustrate the strain magnitude problem with nanoscale features, SEM imaging and EBSD line scans were performed across SiGe lines of several widths. The strain measurements are presented in Figure 1 and include the surface strains predicted by finite element analysis (FEA) for the structures.

The FEA-predicted values for ϵ_{22} are constant regardless of line width (as expected), and the values for ϵ_{11} and ϵ_{33} show only a small change in average magnitude as nanoscale line width decreases. This elastic state is confirmed by independent Raman and microspot x-ray diffraction experiments that indicate a uniaxial stress state along the line that does not vary in magnitude with decreasing line width, particularly ϵ_{22} which should be invariant. In contrast, the magnitude of the EBSD-measured strain decreases dramatically with decreasing line width. Although Raman and microspot x-ray diffraction experiments

measure ensembles of lines simultaneously, the EBSD-measured strain magnitude vs. line width trend is determined to be incorrect.

The discrepancy of the EBSD measured strains with Raman and microspot x-ray diffraction is larger at smaller line widths. This trend, along with the knowledge that backscattered electrons emanate from a volume that is likely larger than the width of an individual line, leads to a testable hypothesis: electrons striking the line scatter through the 3D structure and produce backscattered electrons from both the strained SiGe and the unstrained silicon regions simultaneously[13,14], causing the EBSD measured strains to be incorrect for both regions.

By mixing an EBSP from equibiaxially strained SiGe and an EBSP from unstrained silicon in a linear fashion, superimposed EBSPs can be generated with known weights and known strains, expressed as

$$Obs = SiGe \cdot w + Silicon \cdot (1-w) \quad \text{Eqn 1}$$

where *SiGe* and *Silicon* are pure EBSPs, *Obs* is an observed EBSP, and *w* is a weight factor. The SiGe and Silicon EBSPs were taken in the center of un-patterned 50 μm square regions. A 150 μm stage translation in the 1 direction was required to shift between these two regions, and care was taken to prevent pattern center motion between the two collection points (see SI). Figure 2 shows the result of performing EBSD strain analysis on the linear mixture of two such EBSPs with *w* ranging from 0 to 1.

Although the strains determined from analyzing mixed patterns with increasing *w* values are not perfectly linear with *w*, Figure 2 shows that analyzing an observed EBSP that is formed from both strained SiGe and unstrained silicon regions will result in a strain magnitude that does not represent either region. For strain measurements on samples where superposition of EBSPs is unavoidable, this effect must be accounted for to obtain an accurate strain magnitude for either region.

Experimentally, we collect the observed EBSP and frequently the silicon EBSP as well (used as the reference pattern for the cross-correlation analysis technique[4]), but without *w*, the desired SiGe EBSP is unknown. If the strain magnitude of the SiGe is known, then *w* could be inferred by performing strain analysis on an array of mixed EBSPs. Although possible, that approach limits the usefulness of the strain measurement technique. An independent method of calculating *w* is needed.

Modeling of EBSD Screen Illumination

Modeling of EBSPs is a complicated topic that is well described, including its limitations[15,16]; however, the *w* weight factor that is required to subtract (or un-mix) a SiGe pattern from the observed EBSP does not require modeling of the diffraction. Instead, *w* is determined by the quantity and energy of electrons arriving at the EBSD detector and the region from which they originate. By applying a Monte Carlo simulation procedure like

those commonly used for x-ray microanalysis, it is possible to simulate w for structures with known geometry and material composition. This procedure does not include diffraction scattering physics, but instead simulates electron trajectories in solids and allows the non-ideal nature of the “monochromatic sub-surface point source” to be addressed. Therefore, this is not a simulation of an EBSP, but rather a simulation of illumination of the EBSD detector.

Screen illumination simulations were performed using a newly developed extension to JMONSEL[17], an open source simulation packaged developed at NIST. Within the simulation environment, the geometry of both the sample and the SEM chamber are recreated, and the material properties needed to inform the electron scattering physics are entered. Once this simulation environment is established, electrons can be “fired” from the gun and their complete trajectories tracked. Using this process, the location and energy of the electron is known at every scattering event, and for each electron a terminal status can be classified: (a) absorbed in the solid, (b) scattered out of the solid on a trajectory that intersects the EBSD detector, and (c) scattered out of the solid on a trajectory that misses the EBSD detector. For this work, an electron is considered absorbed once its energy is below 5 kV (accounting for 95% of total intensity, see SI), which is consistent with experimental work.[11] Only electrons from case (b) contribute to screen illumination, and for these electrons additional pieces of information are accumulated: (1) the position of the electron where the last scattering event occurs, (2) the position where the electron leaves the solid bound for the EBSD detector, (3) the location on the EBSD detector that the electron trajectory intersects, and (4) the energy of the electron at the detector. With this information accumulated, a binning operation is performed to sum all the energy each pseudo-pixel receives. Figure 3 shows the results of this procedure for a flat amorphous silicon (a-Si) sample.

The visual agreement between the experimentally collected pattern in 3(a) and the simulated illumination inside the dashed rectangle of 3(b) is excellent. Validating the EBSD detector illumination simulation on a-Si is useful because it does not produce a crystalline diffraction pattern—which is the physical aspect that the simulation method neglects—but is otherwise similar to the silicon 3D nanostructures of interest.

To transfer the usefulness of monte-carlo illumination simulation between a-Si and crystalline Si with epitaxial SiGe structures requires some assumptions. The largest is that the observed local contrast of an EBSP (namely the Kikuchi lines), is simply a modulation of the backscattered intensity in that direction.[18] Given that unprocessed EBSPs from crystalline Si are dominated by the background contrast, and Gaussian blurring of a Si EBSP yields an image very similar to the screen illumination from amorphous Si (see SI, Fig S4), this assumption seems appropriate for this application.

Using simulations of SiGe lines on Si, the screen illumination of a 40 nm wide $\text{Si}_{0.7}\text{Ge}_{0.3}$ line is shown in Figure 4(a):

Because the simulation provides the exact location where the electron exits the solid, it is easy to select the illumination as a function of the material from which the electron exited

the solid. For the simulation in Figure 4, electrons were incident into the center of a 40 nm wide and 50 nm tall SiGe line, and electrons exiting from the SiGe (light grey of Fig 1(b)) and Silicon (dark grey of Fig 1(b)) are accumulated separately in Fig 4(b) and 4(c) respectively. The summed EBSD detector illumination in Fig 4(a) contains no diffraction information, but otherwise qualitatively matches the raw detector illumination created by EBSD experiments on SiGe lines.

In addition to identifying the last material an electron scattered through, the simulation data provides the location where the electron exits the material. For this work, the strain gradients within a material region are small compared to the difference between the two regions (Si and SiGe); however, the exit location information appear to provide some insight in to the information volume of the technique. Although exit locations provide one essential input to assessing information volume, an information volume estimation likely requires convolving the lateral exit positions with a “skin” thickness and an energy dependent parameter.[16] Because this simulation approach offers no insight into these additional parameters, and the lateral extent is strongly influenced by the beam landing position being on top of a tall and narrow line, attempts to construct an information volume provide little value.

Subtraction of EBSPs by Illumination

As shown in Figure 4a–c, simulating the EBSD screen illumination allows for the contribution of different material regions to the total screen illumination to be separated. These simulations are performed on the specific 3D geometry (e.g. line width, line height, SiGe composition, beam position, etc.) for the SiGe on Silicon line, and thus the intensities shown in Figures 4b and 4c are the weights that the Si and SiGe materials contribute to the observed EBSP—in other terms, w from Eqn 1. However, unlike Eqn 1, w is not a scalar chosen arbitrarily and applied to a pair of known EBSPs. In contrast, the simulation provides $w_{i,j}$, which is a 2-dimensional weight map that is the ratio

$$w_{i,j} = \frac{SiGe_{i,j}}{Silicon_{i,j} + SiGe_{i,j}} \quad \text{Eqn 2}$$

where i,j denotes the pseudo pixel from the spatially binned simulation results. It is technically possible to choose the pseudo pixel size to match the actual pixels of the EBSD detector, but to reduce the number of simulated electron trajectories required to achieve a statistically reasonable weight map, we bin actual pixels to produce 1 mm square pseudo pixels. To prevent introduction of high contrast artifacts between pseudo pixels, the simulated weight maps ($w_{i,j}$) are Gaussian smoothed and then interpolated by cubic spline from 32×24 pseudo pixels to the EBSP resolution of 1344×1024 (see SI). In both cases, the meaning of $w_{i,j}$ is unchanged: it is the ratio of desired signal from the SiGe to total observed signal, and it is spatially distributed over the EBSP. By continuing to assume the linear mixing of EBSPs from both SiGe and silicon region, Eqn 1 can be adapted to accommodate the 2-dimensional nature of the weights

$$Obs_{i,j} = SiGe_{i,j} \cdot w_{i,j} + Silicon_{i,j} \cdot (1 - w_{i,j}) \quad \text{Eqn 3}$$

where $SiGe_{i,j}$ and $Silicon_{i,j}$ are the EBSPs from the two material regions that mix to form the observed EBSP, $Obs_{i,j}$.

Although the $w_{i,j}$ maps have significant character which has complicated implications for the cross-correlation strain measurement technique, the average value of w for the 40 nm SiGe line (0.57), combined with the results of the linear mixing shown in Fig 2, provide a clear explanation of why EBSD underestimates the magnitude of the strains from small 3D structures like the SiGe lines measured here. Effectively, the desired signal ($SiGe_{i,j}$) is superimposed with an almost equal part of undesired signal ($Silicon_{i,j}$). However, for this and many other technologically significant cases, these two signals can be separated by subtraction.

The SiGe lines for this work are relatively narrow with a large pitch; thus essentially all of the silicon is unstrained. As a result, all of the illumination from the silicon region can be assumed to be coming from unstrained silicon. Because unstrained silicon is the reference pattern of choice for this cross-correlation strain measurement, the $Silicon_{i,j}$ pattern is recorded with the SEM beam positioned away from the SiGe line. Thus, every component of Eqn 3 is known— $Silicon_{i,j}$ and $Obs_{i,j}$ experimentally, and $w_{i,j}$ from simulation—and the desired $SiGe_{i,j}$ EBSP can be calculated. Figure 5a–c show $Obs_{i,j}$, $w_{i,j}$, and $SiGe_{i,j}$ respectively.

As expected from a signal subtraction technique, the noise level in the $SiGe_{i,j}$ EBSP (Fig. 5(c)) is somewhat larger than in the observed EBSP, but the edges of the Kikuchi bands in the subtracted $SiGe_{i,j}$ pattern are sharper than the $Obs_{i,j}$ pattern and the additional high frequency noise does not obfuscate the EBSP (See SI for animation).

It is important to note that the weight map $w_{i,j}$ is a function of both the sample geometry and the SEM beam location. Thus, to perform a line scan, $w_{i,j}$ must be calculated for the specific structure of interest and for each beam position. Although computationally intensive, the simulation process parallelizes readily and libraries of weight maps can be produced in a semi-automated fashion.

Results and Discussion

EBSD line scans were performed for SiGe lines of several widths, and cross-correlation-based strain measurement was performed[19] on both the observed and subtracted SiGe EBSPs. The results of both approaches are shown in Figure 6.

When strain measurement was performed on the observed EBSPs from 63 nm and 33 nm line widths, where values of w are small (more unstrained silicon present in the observed EBSP), the measured strain magnitude decreased significantly. In contrast, performing the same strain analysis technique on the subtracted SiGe EBSPs resulted in ϵ_{22} magnitudes that were invariant with decreasing line width and normal strains that agree very well with the

FEA-predicted results. This result demonstrates the necessity of considering electron scattering through multiple material regions when performing EBSD on nanoscale 3D structures.

As with any measurement technique that requires simulation to interpret results, the interplay between the two—specifically what adjustable parameters are available in the simulation—must be discussed. Although full details of the simulation are provided in the supplemental information, the important aspect for this approach is that there is no feedback between the simulation that yields w_{ij} and the strain measurement. w_{ij} is determined entirely by sample composition and geometry (both sample and microscope). Because these parameters are determined by independent methods, the strain results from the subtracted SiGe EBSPs are stable. In fact, w_{ij} varies sufficiently smoothly with line width, SiGe thickness, over-etch depth, SiGe composition, and SEM beam position that a library of these free parameters can be interpolated to find weight maps for points within the parameter set of the library.

The technique described here has tremendous practical application. Both the microelectronics and MEMS industries incorporate strain in devices with physical dimensions smaller than 100 nm and must be able to measure these strains to control device yield and performance. The analytical approach described here enables strain measurement on features 33 nm and smaller on a bulk substrate and in an SEM—avoiding the cost, sample preparation complexity, and destructive nature of TEM based nanoscale strain measurements.

Although the experimental limit of this approach has yet to be determined, it is not without limitation. First, the linear combination of EBSPs from discrete regions to form the observed EBSP requires that one of the EBSPs from one of the two regions be known experimentally. In practice, this is only slightly limiting because there are many measurement applications where the substrate is both the reference pattern and the source of the unwanted signal. Second, the signal to unwanted signal ratio needs to be moderately large because EBSD is a relatively noisy technique. For small values of w_{ij} (< 0.2), the subtraction of the unwanted Si pattern yields an EBSP with a noise level that disrupts the cross-correlation strain measurement technique in unpredictable ways. SEM operating voltage can be reduced and acceptable signal to noise can be achieved on features smaller than 40 nm made from low atomic number materials.

Conclusions

We have presented a method for subtracting EBSPs collected from very small (< 40 nm) features and demonstrated the necessity of this method to accurately interpret EBSD strain measurements from nanoscale 3D structures. Without simulation-based subtraction, strain magnitudes measured by traditional EBSD analysis from features below 200 nm are subject to large errors due to the superposition of the EBSPs from both the interrogated position and other regions from which backscattered electrons are generated. Although the simulation component of the measurement is not trivial, it is also independent from the strain measurement with no feedback between the strain measurement and simulation. Ultimately,

this analytical approach allows accurate strain magnitudes to be measured from bulk devices in an SEM with a spatial resolution that would previously have required TEM-based techniques.

Supplementary Material

Refer to Web version on PubMed Central for supplementary material.

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Figure 1.

(a) Plan view SEM of 33 nm SiGe lines, with the 3D structure and orientation convention shown in (b). Applying cross-correlation strain measurement to EBSPs observed from these structures yields approximately the predicted strain magnitudes for a large 5 μm wide line, but for decreasing nanoscale line widths an increasing deviation in strain magnitude from the simulated value is shown (c).

Figure 2.
Strains measured by mixing EBSPs from Si and Si_{0.76}Ge_{0.24} at increasing values of w .

Figure 3.

An experimentally observed EBSP from a-Si (a) and a simulation of the screen illumination from accumulated electron energy (b). The orange dashes in (b) denote the bounds of the experimental EBSD detector. As the position of the sample is an experimental variable, the geometric extent of the simulated EBSD screen exceeds the experimental screen (See SI). Two profiles in both horizontal (c) and vertical (d) directions are provided to allow quantitative evaluation of the agreement between experimentally and simulated screen illuminations. The simulated intensities in (c) and (d) were scaled by 2.025×10^{-9} such that the mean intensity (in a.u.) of both images was the same.

Figure 4.

The simulated illumination of the EBSD screen from a beam centered on a 40 nm wide $\text{Si}_{0.7}\text{Ge}_{0.3}$ line: (a) is the sum of illumination from SiGe (b) and Si (c) regions.

Figure 5.

An observed EBSP from the center of a 63 nm SiGe line (a) and the simulated weight map (without Gaussian smoothing or interpolation) for the structure (b) yield a SiGe EBSP after subtraction (c).

Figure 6. Strain measurements for 63 nm (a–c) and 33 nm (d–f) SiGe lines. By applying the deconvolution scheme (selected w_{ij} in (c) and (f)) and processing SiGe EBSPs, the measured strain magnitude ((b) and (e)) is consistent with FEA, Raman, and microspot XRD measurements. The incorrect strain magnitudes measured from Observed EBSPs are shown in (a) and (d).