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Meeting-report

Towards Atomic Scale Tomography Using Correlative 4-D STEM, Strain Mapping, and Atom Probe Tomography

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In quantum information applications, accurate spatial measurement of isotopes within quantum wells, point defects at superconductor interfaces, and single extrinsic dopant atoms are necessary to characterize structure-property relationships. Atomic Scale Analytical Tomography (ASAT) with subatomic precision and high efficiency is well suited to provide insight into these measurement challenges. One possible path towards ASAT involves correlative diffraction and spatial information from the scanning transmission electron microscope (STEM) and single isotope information from atom probe tomography (APT), referred to as STEM-centric ASAT [1]. In this method, TEM diffraction information is used to generate a crystal lattice the size and shape of the specimen volume evaporated during APT [2]. In this work, we extend that approach by using 4D-STEM data to determine the local crystal structure, orientation, and strain within smaller volumes of the APT specimen and take an automated approach to integrating the datasets to improve reproducibility. The 4D-STEM data are used to create a specimen function of the lattice points contained by the volume evaporated during the APT experiment with atom position resolution approaching 5 pm. Isotopic information about each lattice position is then applied using the mass spectral information collected during APT.

In this work, 4-D STEM + APT is applied to Ge quantum wells grown via molecular beam epitaxy on a (100) Si substrate with SiGe buffer layers accommodating the lattice mismatch. The evaporated material matches neither the Si nor Ge lattice parameters and any average parameters or ion volume applied to the specimen will not be locally accurate in all areas. STEM micrographs and 4D STEM datasets were collected from the atom probe specimen before analysis, and post-mortem micrographs were collected after analysis. Pre- and post-analysis STEM micrographs are combined using the computer vision tool OpenCV to determine the 2-dimensional extent of the evaporated area [3]. The un-evaporated bottom of the specimen is template-matched between the two micrographs (Figure 1a) and spatially registered to each other. Subsequently, edge features are found and connected (Figure 1b), and the outline of the evaporated volume (Figure 1c) is converted to dimensioned coordinates. The 4D-STEM dataset yields crystallographic information at each 2-D pixel. Local strain due to the lattice mismatch between Si_xGe_{1-x} and pure Ge can be observed using exit-wave power cepstrum (EWPC) analyses at each pixel to determine the local lattice parameters and orientation in that volume (Figure 1d) [4].

The 2D outline is then rotated in 3D about its central axis to realize the evaporated volume (Figure 2a). Lattice positions within the evaporated volume are identified using the crystal structure information and constrained by the STEM micrographs. This lattice is then populated by the ions collected during the atom probe experiment, accounting for detector inefficiency, following the method developed by Ceguerra, et al [2]. The resulting reconstruction will account for both bulk shape effects and local apparent density differences caused by uneven evaporation fields in the specimen during the experiment that would otherwise be created by evaporation-centric reconstruction algorithms. Although this Ge specimen is nominally epitaxial and analysis is relatively straightforward, this analysis is also suitable for determining local phase and orientation in more complicated microstructures.

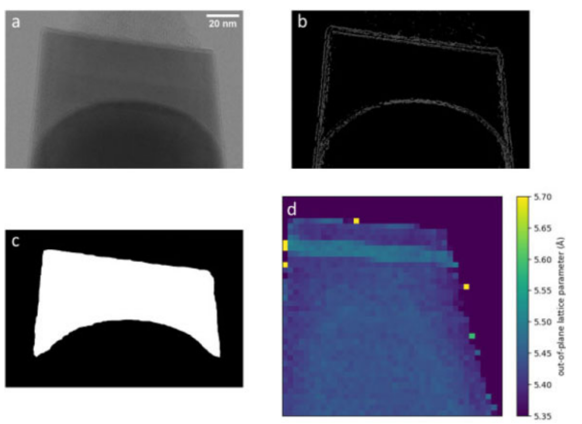

Fig. 1. a) Overlaid TEM images of Ge quantum well in SiGe pre- and post-APT experiment, showing extent of evaporated material in one specific atom probe experiment. B) Automatic edge detection result on image from (a), showing identification of the extent of the evaporated material. C) Map of evaporated material generated from (b) after dilation and etching. D) Strain map of the atom probe tip shown in (a), showing increase of the out-of-plane lattice parameter in the Ge quantum well and unstrained SiGe throughout the rest of the visible material.

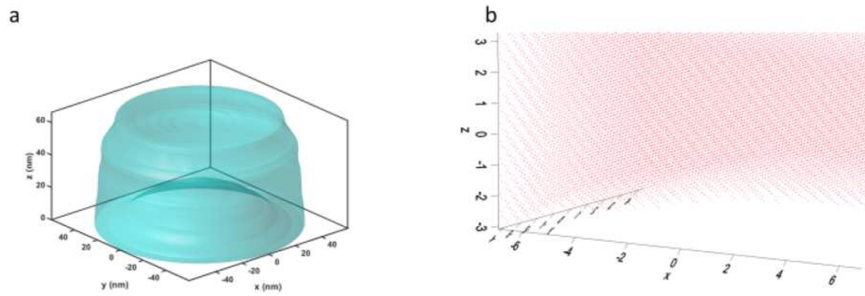

Fig. 2. a) Evaporated volume from a Ge quantum well specimen determined using pre- and post-mortem STEM micrographs. B) A small portion of the reconstructed lattice from the bottom of the evaporated volume showing the curve of the volume bottom. Note moiré fringes due to the underlying lattice.

References

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