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Measuring the Roughness of Buried Interfaces in Nanostructures by Local Electrode Atom Probe (LEAP®) Analysis

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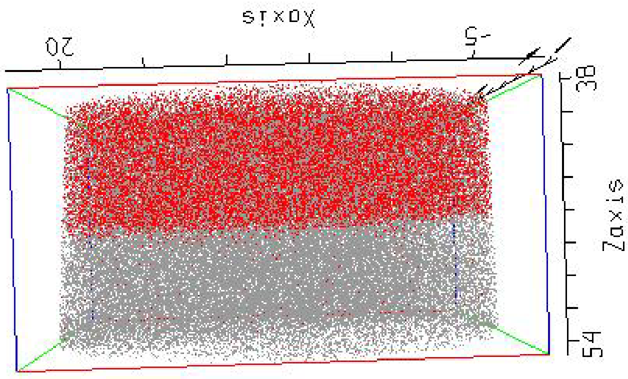
As the size of nanostructure devices continues to decrease, the inherent quality of deposited thin films continues to be a primary force for determining device performance feasibility. The surface roughness of these films plays an important role in understanding the operation and optimal manufacturing of such devices. To date, there have been a small number of diagnostic tools available for determining the roughness of target interfaces. Atomic force microscopy has been used extensively to measure surface roughness [1], but to do so an interface must be exposed at the specimen surface and only a topographical morphology and/or composition may be determined. X-ray reflectivity is another approach currently used, with which a number of buried interfaces may be collectively measured for roughness [2]; however this somewhat method is limited by the electron density of the area to be measured. The LEAP® offers a novel approach to measuring the roughness of buried interfaces. Using time-of-flight 3-D tomography, the LEAP® affords the ability to measure surface roughness of buried interfaces on the near-atomic scale.

The sample chosen for this study was a Si/SiGe/Si structure [3] analyzed in the LEAP®. The lower SiGe/Si interface was chosen for surface roughness measurements (Fig.1). The first step in measuring the buried interface roughness was to establish an isoconcentration surface [4] between the Ge-containing and non-Ge-containing layers (Fig. 2). Once the interface has been established, utilizing the Imago Visualization and Analytical Software (IVAS™), it is possible to select a ~5nm long by ~2nm radius analysis cross-section of the region of interest (gray cylinder shown in Fig. 2). The resulting 1D composition profile illustrates the transition from the SiGe region (at a concentration of Si-20at.%Ge) into the intrinsic Si substrate (Fig. 3). In order to define the buried interface for the roughness measurement, it is necessary to select analysis voxel (grid spacing) and delocalization sizes for the isoconcentration surface calculation. The delocalization defines a Gaussian-weighted moving average where the value of delocalization is set equal to 6σ of the distribution (Fig. 4). Once these have been established it is possible to measure the roughness of the desired region by fitting a plane to the interface and measuring the spatial deviation at each point in the interface from the plane.

The roughness of the SiGe/Si interface was measured using a number of voxel and delocalization values in order to ensure the precision of the measurement and to optimize for computational time. As the delocalization value increases (more spatial averaging), there is an inverse effect on the root mean square (RMS) roughness value. The delocalization will eventually reach a value however where it has a minimal effect on the RMS value (~3 nm as shown in Fig. 5). The selection of different voxel sizes also has an effect on the RMS measurement, but to a much lesser degree. As the voxel size increases, there is minimal effect on the roughness measurement (Fig. 6). This work suggests that a voxel size equal to 0.5 nm with a 3.0 nm delocalization value produces a precise value of 0.22 nm for the RMS roughness and maintains reasonable computational time**.**

[1] S.W. Crowder et. al., Appl. Phys. Lett. 65(13) (1994) 1698.
[2] T. Roch and G. Dehlinger et. al., J. of Appl. Phys. 91(11) (2002) 8974.
[3] K. Thompson et al., Solid State Technology, In Press.
[4] M. K. Miller et al., Atom Probe Field Ion Microscopy, Oxford University Press, 1996.

1



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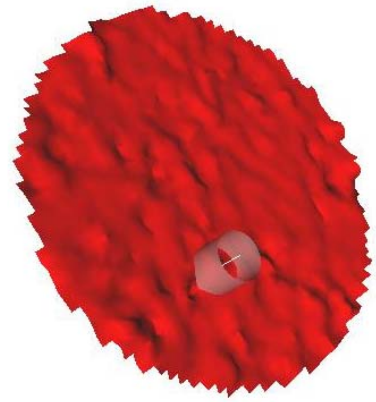

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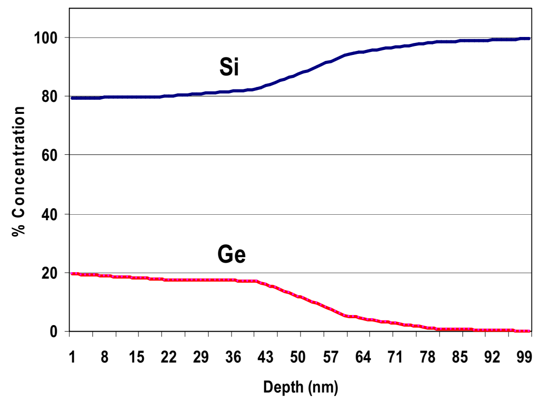

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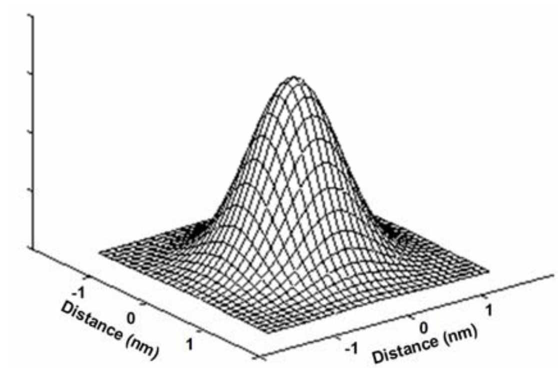

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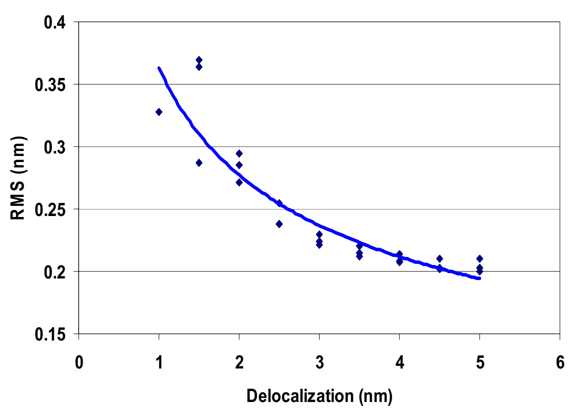

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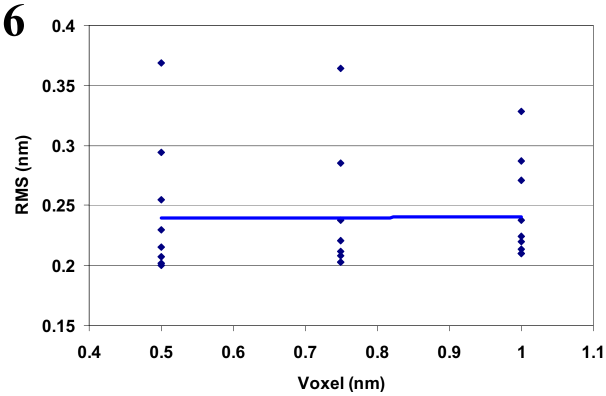

Fig. 1. 3D reconconstruction (25nm x 25nm x 16nm) of a Si(gray)Ge(red)/Si buried interface.
Fig. 2. SiGe/Si interface isosurface with cross-section analysis cylinder of 5nm x 2nm.
Fig. 3. Composition profile of SiGe/Si interface within 5nm x 2nm analysis cylinder.
Fig. 4. Interface calculation parameters with 0.5 nm grid spacing and delocalization value of 3 nm.
Fig. 5. RMS roughness of SiGe/Si interface as a function of delocalization value.
Fig. 6. RMS roughness of SiGe/Si buried interface as a function of analysis voxel size.

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