

A scheme to correct for inaccuracies in the compositional analysis of $\text{Si}_x\text{Ge}_{1-x}$ by Atom Probe Tomography

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Atom probe tomography, thanks to the advent of laser-assistance (LA-APT), is becoming a promising tool for confined volume materials characterization in the semiconductor industry. A prime example is APT's potential for dopant profiling, or more general compositional analysis, in confined three dimensional nanostructures and nanodevices [Van17]. Nevertheless, the standard APT analysis of heterogenous systems still encounters several artefacts, due to for instance the non-stoichiometric evaporation and detection of different atomic species, non-ideal reconstruction algorithms for 3D volumes and differential laser light adsorption. Therefore more (fundamental) studies are required to bring APT up to the required accuracy and precision. In this work we specifically address the challenge of quantification accuracy and compositional profiling of $\text{Si}_x\text{Ge}_{1-x}$ compounds in thin films and the more complicated 3D devices (such as the gate-all-around (GAA) field-effect transistor, Fig A.), which are of high interest for future semiconductor applications (see e.g. [Mer17]).

The choice of the experimental conditions has a significant impact on the elemental composition quantification of $\text{Si}_x\text{Ge}_{1-x}$, a reoccurring issue in the APT community when characterizing semiconductor alloys and compounds [Mar19,Cud20]. The charge state ratio (CSR) not only offers a measure for the apex electric field, but has been identified as a parameter to link and compare the APT elemental quantification between different experimental conditions [Man14]. The origins of the field dependence of the apparent $\text{Si}_x\text{Ge}_{1-x}$ composition are still topic of debate [Est15, Mar19]. Our analysis demonstrates a good empirical agreement to what is reported by [Mar19] in view of the trend of the measured $\text{Si}_x\text{Ge}_{1-x}$ composition as function of CSR. Furthermore, we can pinpoint an optimum measurement condition, i.e. the CSR value at which the elemental composition quantified by APT matches the one determined by complementary Rutherford Backscattering Spectrometry (RBS) on blanket reference layers (Fig. B).

Moreover, the correlation between apparent elemental composition and the CSR holds also for local variations within a single APT dataset, which originate from field variations across or along the tip, for instance due to crystallographic features [Mor19] or those typically arising at interfaces between two materials. We demonstrate this here in detail for LA-APT with different laser wavelengths and field conditions for $\text{Si}_x\text{Ge}_{1-x}$ ($x \sim 0.2 - 0.8$). These repeatable observations, tip-to-tip and across each position within a tip volume, put forward an interesting possibility for more accurate 3D elemental mapping in APT: the elemental composition as function of CSR can be used as a calibration curve. In detail, the actual CSR during APT measurement can be employed to calibrate, i.e. rectify any deviation from the CSR optimal for the quantification of this compound. This correction can be applied on the individual voxels of a sub-divided dataset, provided that the quantification error is larger than any additional uncertainty due to reduced counting statistics (related to the voxel size).

For the APT analysis of contemporary 3D semiconductor architectures, it is often very difficult, if not impossible, to perform the measurement at the optimal (or same) experimental conditions (i.e. CSR) for the (local) region of interest in the device. This can be due to the different components that make up these systems which have very different field evaporation properties e.g. the dielectric gate material and (doped) semiconducting channel region. The proposed correction scheme provides a solution for such a complex situation, which we demonstrate by correcting the apparent $\text{Si}_x\text{Ge}_{1-x}$ profile in the APT analysis of a state-of-the-art Gate-All-Around nanosheet field effect transistor (Fig. C).

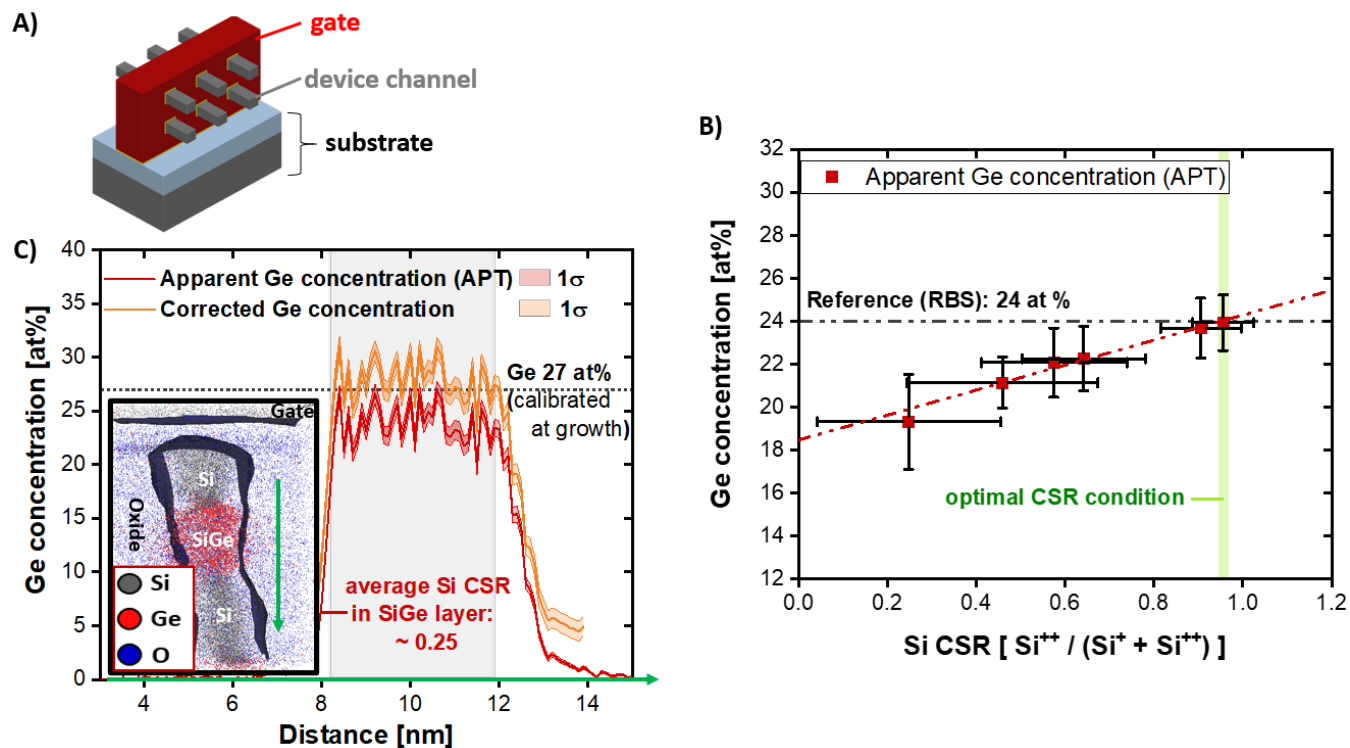


Figure 1. Fig. A) Sketch of the Gate-All-Around field-effect transistor. Fig. B) Apparent Ge concentration from APT analysis of a SixGe1-x film ($x \sim 0.76$ as measured by RBS) as function of the Si CSR. The optimal CSR value for which the apparent concentration matches the reference value is indicated in green. Fig. C) Apparent Ge concentration profile from a GAA device as obtained by APT analysis (red). Using the calibration curve of Si_{0.76}Ge_{0.24} (Fig. A) and according to the (local) Si CSR within the region of interest, the Ge profile was corrected (orange). Inset shows the reconstructed device volume.

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