BAPVC Annual Project Report

Project Title: Design principles and defect tolerances of silicon / III-V multijunction interfaces

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Summary:

Atom Probe Tomography(APT) is a novel, high-resolution three-dimensional spatiochemical mapping technique capable of observing single atomic impurities at interfaces and in the bulk. Applying it to photovoltaic absorbers and devices allows the performance-limiting impurities and compositional inhomogeneities to be directly characterized. However, the technique is still in its adolescence, and truly quantitative measurement of semiconductors requires considerable care and material-specific technique development before reliable information can be acquired in wild-type specimens; to this end, custom specimens of Si and III/V materials have been fabricated and characterized, to measure interface compositions, bulk impurities, and compositional inhomogeneities and compare them to correlative measurements to ensure accuracy and precision of the Atom Probe technique.

Key Accomplishments:

Three separate avenues of investigation have been brought either to publication or to submission of the manuscript. The first has focused on using Atom Probe Tomography to investigate a series of carefully-prepared transition-metal contaminated Si specimens, with correlative SIMS, TEM, SEM, and diffraction measurements to establish the accuracy of the technique; see Fig 1 for an example. At the same time, this research has also investigated the dynamics of rapid solidification in supersaturated solutions of Si and a transition metal, in this case Co. The resulting manuscript has been published in Advanced Functional Materials, and can be found here: http://dx.doi.org/10.1002/adfm.201501450 . The main result of this work, in addition to establishing the accuracy of APT for measurement of some transition metals in Si, has been to greatly extend our knowledge of rapid solidification of alloys, cellular breakdown dynamics, filament formation and pinch-off in far-from-equilibrium systems, and impurity diffusion during solidification from the melt.

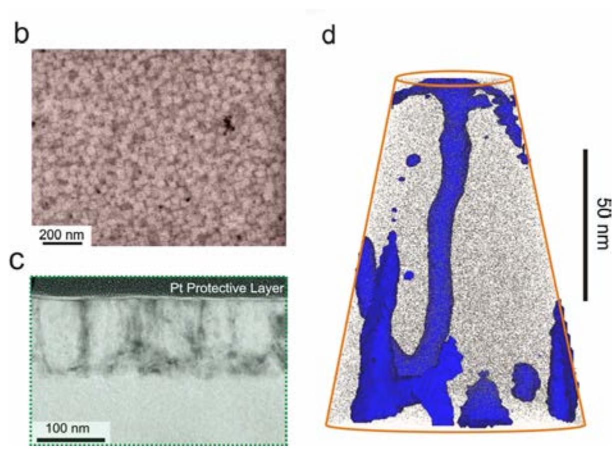

Fig 1. Taken from the linked AFM article. SEM (b), TEM (c), and APT (d) data showing the segregation of Co atoms into filamentary structures embedded within a Si matrix.

A second major direction has been the characterization of III/V-IV interface. Although Si-III/V interface specimens were not available, a series of Ge-InAlAs specimens have been acquired and characterized. These have been found to consist of impure Ge nanowires, ranging from 75 to 95 % atomic Ge with the balance As, embedded in an InAlAs matrix, seen in Fig 2. The interfaces between these materials are seen to be somewhat graded, with evidence of As segregation at the interface in addition to the As incorporation within the nanowires. The mechanism of formation has been modeled using a similar adatom-diffusion and phase separation model to the one mentioned above, and this work is currently being prepared for submission.

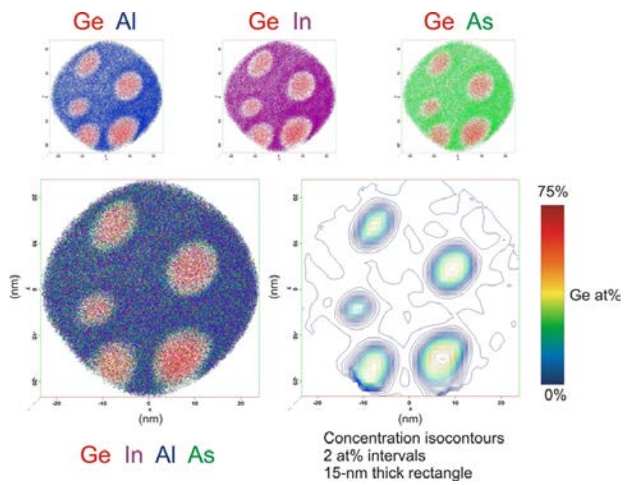

Fig 2. Cross-sectional views of APT dataset from InAlAs-Ge material, showing the distribution of the component atoms within the matrix and the embedded Ge nanostructures. A Ge concentration plot is also provided.

Finally, the third avenue of investigation has been characterization of the interface between Si and a transparent conductive oxide used as a contact material in some photovoltaic devices, in this case Aluminum-doped Zinc Oxide. This interface is known to exhibit Fermi-level pinning, with the mechanism of this pinning not being ully understood. Two separate types of AZO, one grown by pulsed-laser deposition and the other by sputtering, have been deposited on Si, and the interface composition has been investigated by APT. We have observed a layer of Al segregated within the AZO at the interface (seen in Fig 3), raising the local Al concentration to approximately the solubility limit in AZO, possibly leading to the formation of a degenerately-doped layer at the interface and leading to classic metal-on-semiconductor Fermi level pinning. This work is currently in preparation for submission as two manuscripts, one covering the mechanism of Al segregation, and the other the electronic effects of this Al-enriched layer.

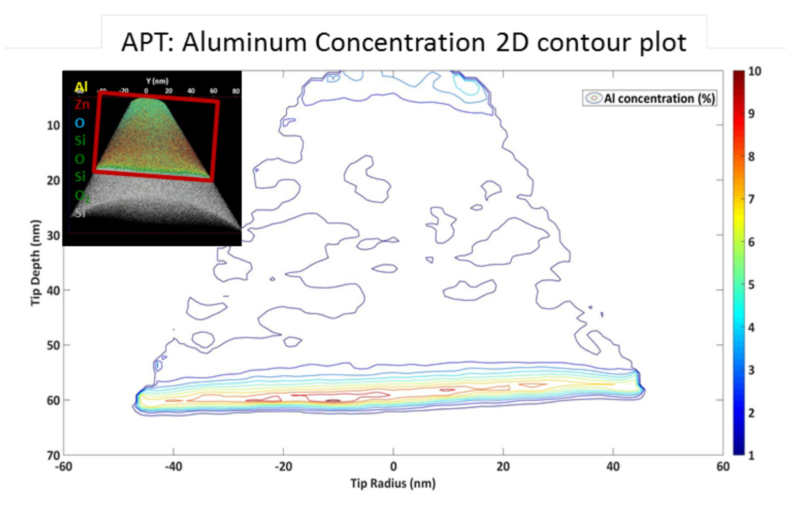

Fig 3. Al Composition profile of AZO on Si, showing Al enrichment at the AZO-Si interface (bottom of profile). Inset, a view of the full APT dataset, showing AZO on top of Si, with red box indicating the view window for the composition profile.

Future Work:

In addition to completing the above-mentioned work and submitting for publication, further efforts on III-V materials continue, as do efforts to verify APT's suitability for measurement of bulk impurities in Si. This last has proven surprisingly variable, as different impurity elements have wildly varying behavior during the APT measurement. Fe and Cu, in particular, have demonstrated behaviors that necessitate in-depth investigation before APT measurements of these elements can be treated as trustworthy; work in this direction is underway. Several other impurities, including Au and Pd, have been found to be, at present, undetectable in Si by APT, even when the impurity atoms are present in tremendous excess of the solubility limit. This is believed to be the result of the difference in ionization energies between the impurities and the matrix atoms, so theoretical investigation of the local electronic environment around these atoms during APT measurement has begun. Lastly, we will commence measurement of III-V / Si interfaces.