**BAPVC Annual Project Report**

# Project Title: Design Principles and Defect Tolerances of Silicon/ III-V Multijunction Interfaces

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**Summary:**
Promising multijunction solar cell devices, composed of III-V compound semiconductors on silicon, have high theoretical maximum efficiencies. However, efficiencies to date achieve a fraction this maximum. For a single two-absorber device, the theoretical optimal bandgaps for top and bottom cells match closely those of GaAs and Si. However, the optimization of the III-V/Si interface presents many challenges, primarily from the 4% lattice mismatch that can result in impurity segregation, formation of dislocations, interface dipoles, and interlayer diffusion, all of which may affect negatively the device performance. Exploring these interfaces with Atom Probe Tomography (APT) enables a fundamental understanding of the device performance, by elucidating chemical and structural behavior with atomic resolution.

**Key Accomplishments:**

ATP is used in our group to characterize solar cell materials down to the atomic scale. Transition metal impurities in silicon were chosen as a first target, acting as both an important avenue of scientific investigation, and as useful control samples for determining the correct operating conditions for detection of embedded impurities in semiconductor matrices, a non-trivial and largely unstudied problem. This having been achieved, the interface between GaAsP and SiGe is now the next goal on the list, as an example of the kind of III-V/Si interfaces that are the goal of the larger study.

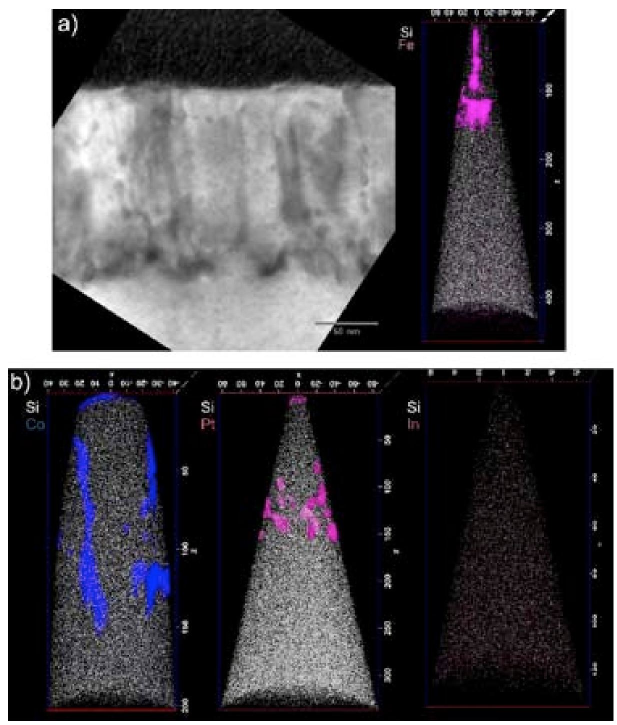


Figure 1. (a) Left, Cross-sectional TEM of Silicon with $Fe^{56}$ impurities visible as dark regions. Right, APT of same specimen, with Fe shown as pink dots and 0.1% of Si shown as white dots, for visual clarity. (b) Three different morphologies of impurity segregation in Si found by APT. From left: one-dimensional structures in Co-contaminated Si; small roughly spherical impurities clouds in Pt-contaminated Si; homogeneously-distributed In in In-contaminated Si. All axes are in units of nm.

Initial investigations of two transition-metal impurities in silicon have been promising. A variety of transition metals have been ion-implanted into silicon, then the silicon recrystallized and the impurities induced to redistribute and precipitate by a single pulse from an Nd:YAG laser. Atom probe samples have been fabricated using the Focused Ion Beam (FIB) assisted liftout method, and analyzed using a Cameca LEAP 4000HR 3DAPT instrument at Harvard University's Center for Nanoscale Systems. Analysis was carried out in laser-assisted mode, using laser pulse energies of between 10 and 40 pJ/pulse, with the sample background temperature held at 20–40 K to minimize surface migration of atoms during analysis and prevent diffusion of the impurities.

Results: while both gold and iron can be identified in the samples, the charge states observed for the impurity atoms differs significantly from that predicted in past literature. Differential ionization effects cause the detected concentration of gold observed from APT to be approximately one order of magnitude lower than that measured by secondary-ion mass spectroscopy (SIMS) in the same sample (peak concentration observed from APT for Au is ~0.1% atomic, compared to ~1.2% atomic observed in SIMS). Further investigation of this effect is ongoing, and understanding the nature of the ionization of these elements in the presence of the silicon matrix should be improved by analysis of a full range of elements. At present, samples which have been fabricated include Pt, W, Co, Cu, Zn, Pd, Cr, and Ag in silicon, which should provide enough variety for larger trends to become evident.

Regardless, the observed distribution of impurities in the APT data matches well to TEM performed on the same samples. Iron precipitates are observed in the analyzed volume, with a shape which differs from that postulated from TEM examination in past literature. Iron detection has been found to be highly dependent on local fields internal to the specimen, and theory has been developed to predict spatially varying iron detection limits in silicon. Here, the three-dimensional nature of APT has made it possible to fully visualize the shape and local composition of these impurities in a way that has never before been possible. Further data on Co, Pt, and In in silicon have recently been acquired and are in the process of being analyzed.

Initial measurements have been carried out on a candidate III-V/Si interface material, in this case, GaAsP/SiGe/Si with the SiGe layer acting as a strain-relieving layer (Fig 1). The samples were provided by the Fitzgerald group at MIT, cross-sectioned by Argon-ion polishing, and then prepared for APT. Initial measurements reveal a variety of complex issues with this material system, including local field enhancement (presumably caused by small compositional variations created during differential evaporation of some of the five component atoms), clustering visible in the time-of-flight and mass spectra, resulting in degradation of lateral resolution, and possibly diffusion of various species either in the bulk or at the surface during APT analysis. As expected, this type of material system represents the cutting edge of APT technique, and more development will be necessary to properly and repeatably analyze these interfaces.

**Future Work:**

TEM/APT compatible holders have been fabricated following the designs found in the literature and are now in use to allow correlative measurement of precipitates, interfaces, and defects in samples. This should greatly enhance the reliability of generated reconstructions. We are also pursuing a novel form of sample characterization, based on the collection of field-emitted electrons from the sample tip at various points during an APT measurement. Briefly, the APT samples are ideal field-emission sources for electron emission, and the geometry of the instrument is well suited to the generation of electrons by classic Fowler-Nordheim field emission. By performing voltage sweeps and measuring the resulting electron current, it should be possible (based on recent and ongoing advances in theory) to derive sample geometry parameters from this data, allowing a simple in-situ characterization of the sample shape during an ongoing APT measurement. This would help to solve some of the largest problems in the technique's reliability, related to the sometimes-arbitrary choice of reconstruction parameters necessary to generate the three-dimensional projected dataset.

Significant additional effort will be needed to realize reliable, repeatable measurements of compound semiconductor interfaces. The observed clustering and diffusion issues will require in-depth investigation, already begun in our lab. These problems are well known in the literature[14], and their solution will benefit both the efforts outlined in the BAPVC grant and the APT community generally. Control samples of GaAs interfaces with a variety of other materials are being fabricated to test the evaporation, ionization, and diffusion conditions present during analysis. Additional data analysis capabilities, including correlation of different ion detection events both temporally and spatially, and crystallographic identification and analysis techniques, are being developed.