Invited Paper

Enriching and purifying silicon epilayers for quantum information

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High quality, enriched silicon contains an exceptionally low density of defects and unpaired electron and nuclear spins that allow candidate qubits (single donors or quantum dots) to exhibit very long dephasing times compared to silicon with a natural abundance of isotopes[1]. Unfortunately, high quality enriched silicon is not a readily available resource. Only a few niche supplies exist and the advancement of silicon based quantum information is limited by access to these. As quantum information has made progress, efforts to increase supply have been made, but these are also hampered by sparse evidence for determining what level of enrichment is sufficient for eliminating the effects of nuclear spin dephasing.

In this talk, I will describe very highly enriched silicon films that are grown epitaxially on Si(100) substrates. We have been refining the quality of these films with the aim of experimentally determining the relationship between important metrics, like coherence time, and the physical mechanisms limiting them, like nuclear spin density or chemical impurity density. At present, we have suppressed the minor isotope fraction in these films to $\approx 10^{-7}$, grown the films epitaxially with high crystalline quality and are successively reducing contaminant densities (mostly light gas components.) As the quality of the films has improved, we have begun making electronic test devices from this silicon, in particular, diodes, capacitors and transistors on the way to realizing single and multiple quantum dot devices.

The extreme suppression of the minor isotopes is accomplished through the use of ionized mass separation in a high vacuum environment. An ionized beam of essentially monoisotopic ^{28}Si is generated by 1) introducing natural abundance silane gas into an ionization cell, 2) producing a plasma of ionized silicon and silane fragments, 3) extracting and collimating an ion beam from the cell, 4) passing the ion beam through a mass analyzer composed of a magnetic field and a small aperture, 5) refocusing and transporting the monoisotopic beam into the ultra-high vacuum (UHV) growth chamber and 6) decelerating the ions onto the sample for gentle, epitaxial growth[2]. Once the sample is removed from UHV we can perform a wide range of analyses, including secondary ion mass spectroscopy (SIMS) to evaluate the distribution of isotopes in the sample. An example of a SIMS depth profile for one of our samples is shown in Figure 1. During SIMS, the sample is successively sputter eroded from left to right (surface to substrate) while progressively measuring the number of secondary ions for the three silicon isotopes. After an initial surface transient, the measured isotope fractions become stable at values of $\approx 1.27 \times 10^{-7}$ for ^{29}Si and $\approx 5.2 \times 10^{-8}$ for ^{30}Si[3]. Once the sputter depth reaches the sample substrate the isotope fractions are observed to return to the natural abundance values. In analyzing the possible contamination sources limiting the enrichment, we find that the minor isotope contamination is not a consequence of the mass selectivity, but due to silane diffusion. Through further analysis of the pressure and temperature dependence, we have developed a predictive model for the enrichment as a function of these parameters that we expect to use targeting specific levels of enrichment from natural abundance down to the levels shown in Figure 1, i.e., $\approx 10^{-7}$.

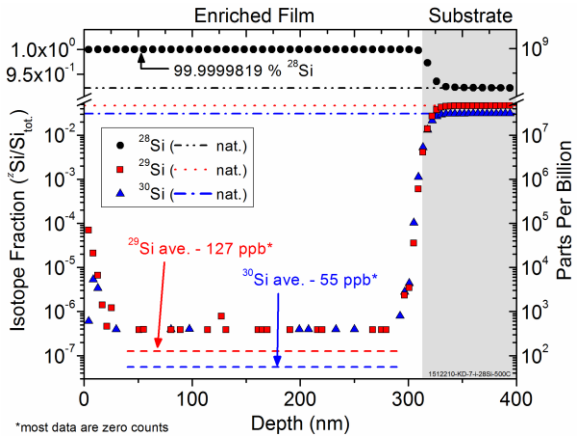

Figure 1- Secondary Ion Mass Spectroscopy (SIMS) depth profile showing nearly complete suppression of the minor isotopes of silicon in this highly enriched film.

In order to achieve the goals of very long coherence times, a high level of enrichment alone is not sufficient, but must also be accompanied by

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excellent crystalline quality and very low densities of chemical impurities. In order to assess these properties, we have conducted a number of additional analyses, including *in situ* scanning tunneling microscopy of every substrate and film. Shown in Figure 2 is a transmission electron microscopy (TEM) image taken on an enriched silicon sample with less than 10^{-6} contribution from the minor isotopes. The image is from the interface region between the substrate at the lower left and the enriched film toward the upper right. The enriched film seems to show a more "mottled" overall contrast, but exhibits a crystalline orientation identical to the substrate. We perform rigorous assessments of the chemical composition by using SIMS and selecting a suite of likely targets, e.g., targets known to the semiconductor industry to be deleterious. Results from SIMS analysis of this type is shown in Figure 3 for silicon and 22 other elements, including heavy metals, transition metals, alkalis and light gasses. Of these, only light gasses and aluminum was detected. We attribute the aluminum to auto-doping that has since been eliminated and note that the light gasses have since been reduced by almost a factor of 100 with further improvements in progress expected to improve more than 100 times more.

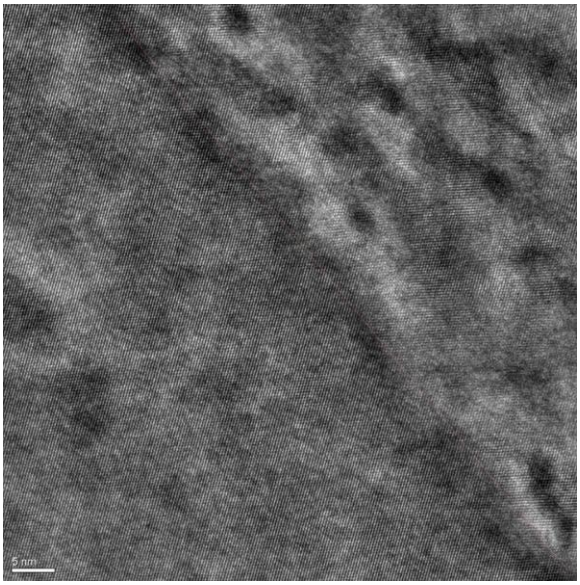

Figure 2- Transmission Electron Microscope (TEM) image of a highly enriched silicon film (upper right) grown on a natural abundance Si(100) substrate (lower left).

As we move forward with this project, we are fabricating and measuring electrical test devices while also developing the techniques to produce arbitrary targeted levels of enrichment. The fabrication of test devices has met with challenges in growing high quality oxide isolation layers, which we attribute to a self-limited growth arising from the excess nitrogen. None-the-less, we have plans to mitigate these difficulties even while we seek to substantially reduce the nitrogen. Additionally, we are pursuing collaborations to conduct electron spin resonance (ESR) studies of small numbers of donors in our highly enriched silicon to directly correlate the coherence properties with the materials and electrical properties independently measured.

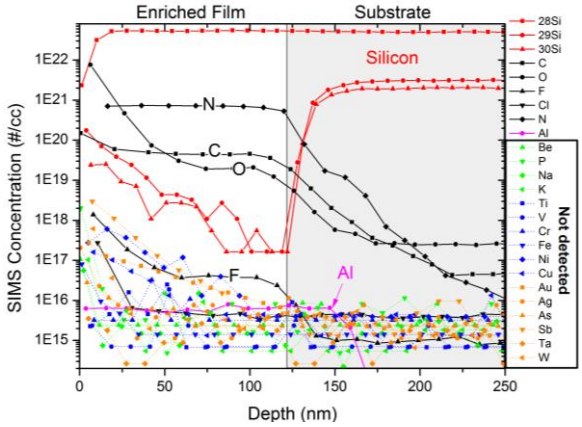

Figure 3- SIMS measurements for a wide range of target contaminants. The dominant elements found are from incorporated light gasses.

References

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