Final Progress report

1. DOE Award Number: DE-FG02-05ER46208, University of Houston, Houston, TX 77204.
2. Title: Nano Vacancy Clusters and Trap Limited Diffusion of Si Interstitials in Silicon
3. Principal Investigator: Wei-Kan Chu
   TEL: 713-743-8252 (O); FAX: 713-743-8201, E-mail: wkchu@uh.edu
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5. Personnel:

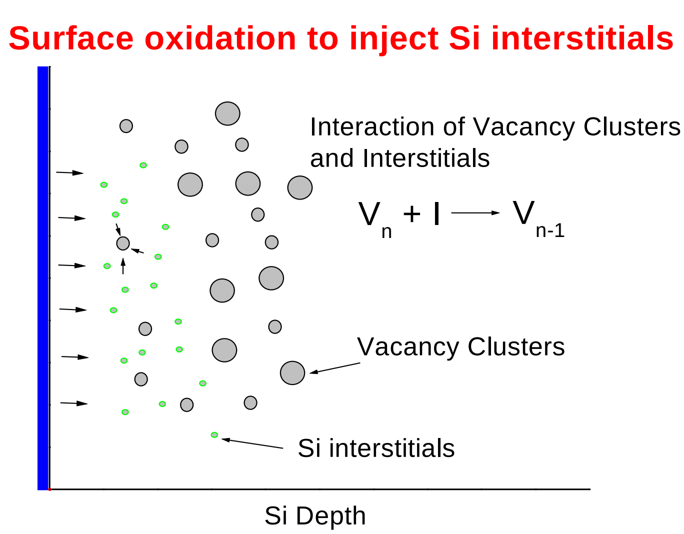
Dr. Wei-Kan Chu, Dr. Quark Y. Chen, Dr. Ki Bui Ma
Doctoral students: Dharshana Wijesundra, Omar Lozano Garcia, Priya Chinta, Paritosh Wadekar .

6. Unexpended Fund: (None)

7. Recent Progress:

Three students obtained their Ph.D degree from the Physics Department at the University of Houston during the year of 2010. They are Omar Lozano Garcia, Priya Chinta, Paritosh Wadekar. 18 publications are generated during the 4 year period.

The objective of this project is to develop a method to characterize nano vacancy clusters and the dynamics of their formation in ion-irradiated silicon. It will impact (1) semiconductor device processing involving ion implantation, and (2) device design concerning irradiation hardness in harsh environments. It also aims to enhance minority participation in research and curricula on emerging materials and ion beam science. Vacancy defects are of scientific and technological importance since they are ubiquitous when the host materials are exposed to particle irradiation. Studies on vacancy clustering in the past decades were mainly theoretical and the approach heavily relied on the total-energy calculation methods. The lack of experimental data is mainly due to the formidable task in measuring the cluster size and density using modern metrological techniques, including transmission electron microscopy and positron annihilation spectroscopy. To surmount these challenges, we proposed a novel approach to tackle the metrological problems on the nano vacancy clusters, especially in determining densities and sizes of the nano vacancies based on the premise that the vacancy-clusters act as diffusion-trapping centers. For a silicon substrate containing vacancy-clusters, the diffusion of interstitials (from the surface) can be classified into three phases: (1) an ultrafast phase-I in which the trapping centers



have little effect on the diffusion of interstitials; (2) a prolonged phase-II in which the loss rate of interstitials by trapping balances the influx of interstitials from the surface; and (3) a phase-III diffusion in which surface influx of interstitials depletes the trapping centers and interstitials consequently propagate deeper into the bulk. By measuring diffusion profiles of Si interstitials as a function of diffusion time, void sizes and void densities can be obtained through fitting.

Experimentally, our approach to characterize voids is realized through three consecutive steps. (a) First, high energy self ion irradiation is used to create a wide vacancy-rich region, and to form voids by post implantation annealing. (b) In an additional annealing step in oxygen ambient, Si interstitials are injected in by surface oxidation. (c) Analyzing trap-limited diffusion of Si interstitials, which is experimentally detectable by studying the diffusion of multiple boron superlattices grown in Si, and enables us to characterize the nano voids, e.g. their sizes and densities.

Fig. 1. A schematic show of void-limited penetration of Si interstitials from the surface. Modeling of interstitial diffusion is able to extract void sizes and densities.

Binding energies of vacancy clusters:

We have experimentally derived the binding energy of vacancy clusters as a function of sizes. Comparison with theoretical prediction has been conducted. (a) We used Sb-doped Si superlattice markers to detect the free vacancy concentration at the annealing stages when void growth and decay have reached the equilibrium. Under such a quasi static state, the free vacancy concentration is determined by the binding energy of voids. Therefore, we derived the binding energy of voids as a function of mean void size. (b) We have conducted large scale molecular dynamic simulations based on the potential derived from modified embedded atom methods. The binding energies of vacancy in voids as a function of void size have been obtained and compared with the experimental data.

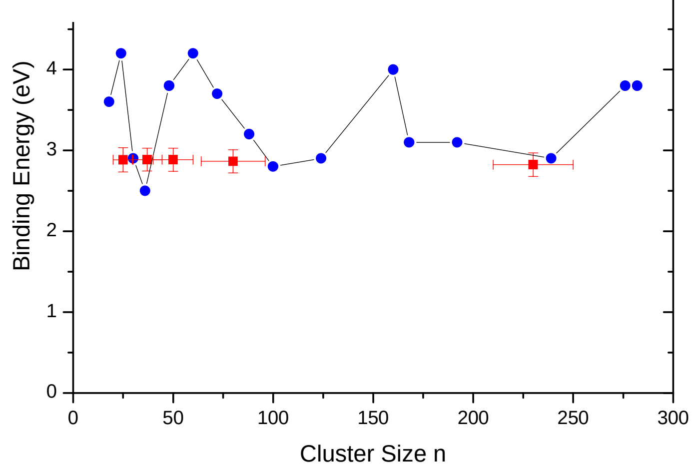


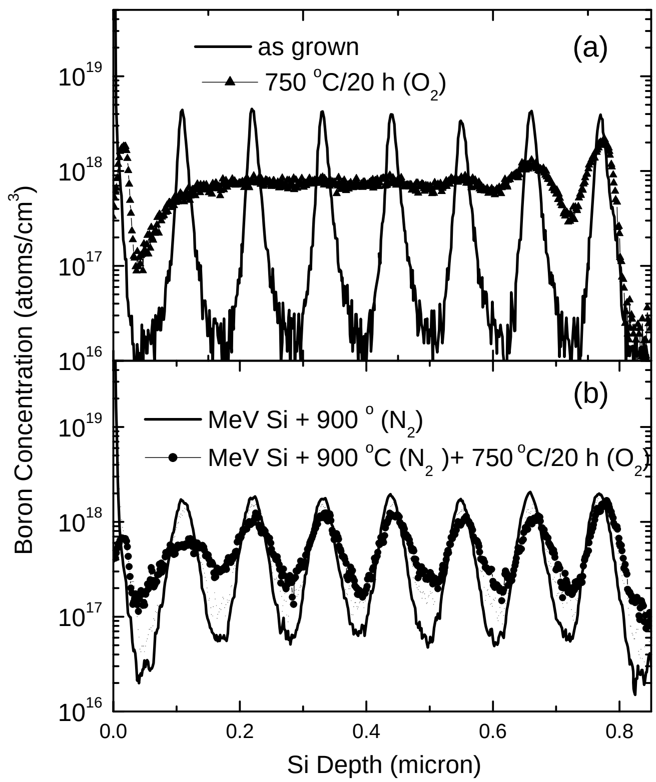
Fig. 2. The binding energy of vacancy clusters as a function of cluster size. The values are extracted from the diffusion experiments, and in a comparison with the values calculated from MD simulations.

High thermal stability of voids formed in Si

We found considerable amount of vacancy defects introduced by MeV Si self ion implantation were able to sustain a high temperate annealing, i.e. 900 ^{o}C for 5 minuets. By analyzing the trap-limited Si interstitial diffusion, we have characterized these vacancy clusters. Furthermore, we showed that the remnant vacancies are sufficient to reduce B diffusion, which suggests that MeV ion implantation can be inserted before gate formation (involving high temperature annealing) to avoid irradiation damage on gate structures. The finding is significant since it suggests a promising approach for ultra shallow junction formation in metal-oxide-semiconductor device fabrication.

FIG. 3. B diffusion profiles before and after oxidation at 750 °C for 3 h for (a) the as-grown sample and (b) the sample with MeV Si ion implantation + 900 °C /5 min anneal (N_2), respectively.

Surface oxidation results in Si interstitial injection. The deep penetration of Si interstitials is obvious in (a), which shows significant spreading of B markers. However, the interstitial penetration is significant retarded in (b). The suppressed diffusion is due to the presence of vacancy types defects in Si. Our study suggests a high thermal stability of voids formed in MeV Si ion implanted Si (voids did not disappear after 900 °C /5 min anneal.



Atomic scale diffusion of dopants in vacancy excessive region

It has been known for quite some time that the diffusion of dopants in Si is strongly influenced by the presence of defects. In particular, the diffusion of Sb is enhanced by vacancies and suppressed by interstitials. Later on, Cowern et al proposed a quantitative basis for the description of this phenomenon in terms of highly mobile defect-dopant complexes as crucial intermediaries, and demonstrated this concept in an application to the B-Si system. In this model, the diffusion coefficient is no longer the only materials parameter governing the process of diffusion. At least one other parameter, chosen here to be the mean 'free' path of the mobile complex in a single hop of the diffusing dopant, is involved and has to be considered. This mean free path is referred to as the migration length. Using this model, we have extracted the migration length for the diffusion of Sb in Si through a thorough analysis of the concentration profiles of Sb in Sb-delta-doped Si after diffusion of the Sb dopants was allowed to proceed for various time intervals and temperatures in the presence of excess vacancies previously created within the sample by high energy implantation of Si itself.

Development of a low temperature characterization method to detect vacancies

Characterization of voids by studying trap limited Si interstitial diffusion requires an oxidation at a temperature above 500 ^{o}C. This annealing might change voids and cause a “destructive” effect. We have shown the feasibility to develop a low temperature characterization method by using hydrogenation. In this study, we have studied H diffusion in Si grown at different temperatures by using molecular beam epitaxy growth. This work has used numerical methods to model H diffusion, based on the theory that H prefer to interact with vacancies to form VH_n complexes.

The variable energy positron annihilation spectroscopy were performed to investigate the defects in the as-grown MBE samples (position analysis were done through collaboration with Dr. Luiz Jacobson at Los Alamos National Laboratory). Figure 4 shows the measurement of the line-shape parameter S vs incident energy of positrons for the MBE Si grown at 500 ^{o}C and 650 ^{o}C, respectively. As a comparison, the values of S (in the near surface region) is higher in the 500 ^{o}C MBE grown Si, which means more positrons get trapped and annihilated in open volume defects in this sample. In other words, it shows that 500 ^{o}C MBE grown Si has more vacancies than 650 ^{o}C MBE grown Si.

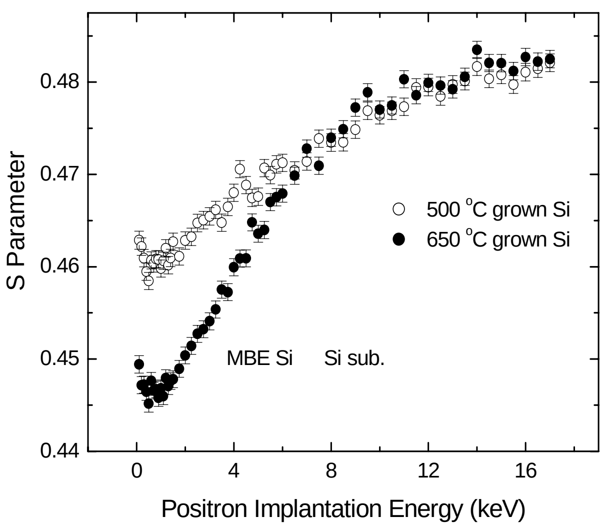


Figure 4 The line-shape parameter S vs incident energy of positrons for the Si grown at 500 C and 650 C, respectively.

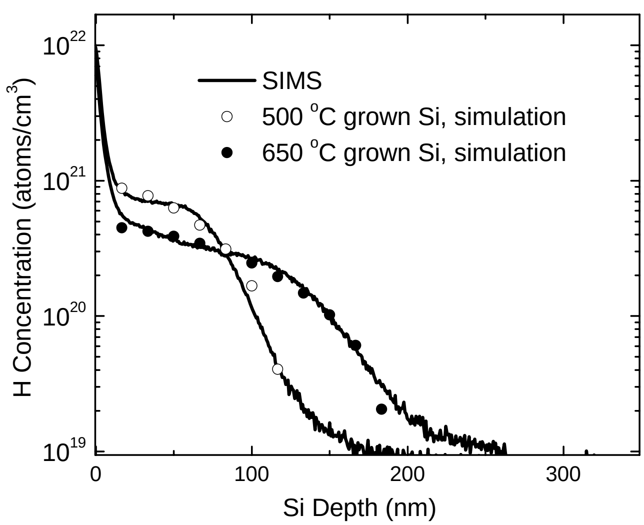


Figure 5 H depth profiles in the hydrogenated Si grown at 500 C and 650 C, respectively.

Figure 5 shows high resolution H depth profiles obtained by using low energy secondary ion mass spectrometry (SIMS). H penetration in the 500 ^{o}C grown Si is shallower than that in the 650 ^{o}C grown Si. Efforts have been made to simulate H penetration. A good agreement can be reached if certain parameters are adjusted. These parameters include vacancy densities in the as grown samples, and the kinetics to form large VH_n complexes. Our preliminary studies suggest that a quantitative analysis of vacancies is feasible. The difficulties arise from the limited knowledge on vacancy hydrogen interactions. Recently, first-principle calculations have been used to examine the possible pathway to form H induced Si platelets [F.A. Reboredo, M. Ferconi, and S.T. Pantelides, Phys. Rev. Lett. 82, 4870 (1999)]. Kinetics predicted from these theories make it possible to develop this low temperate hydrogenation experiment into a low temperate vacancy characterization tool. This effort will be continued in the year 4

Journal Publications:

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