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Investigations of dopant clustering in Si via radial distribution function

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During the formation of Si nano-devices, group III and V dopant atoms – Sb, B, P, As – are introduced into the Si wafer in order to control both the electrical resistivity and the polarity of discrete regions. For dopant atoms to have the intended affect they must become electrically active, implying that the atom occupies a substitutional site *and* contributes/removes a free electron from the conduction band. At low concentrations, < 0.01%, nearly 100% of the dopants are electrically active. As ultra-high concentrations are approached, 0.1. – 1%, the electrical activation process becomes less efficient; for every additional dopant atom only a fraction becomes electrically active.

Clustering of dopant atoms is a suggested mechanism for dopant inactivity at high concentrations. Simulations and electrical tests both agree that dopant clustering does occur and that it does result in a significant fraction of inactive dopant atoms. However, direct experimental verification of clustering has been limited by a gap in characterization systems capable of mapping the location and elemental identity of atoms in a material. The application of the laser atom-probe to the study of Si nanostructures bridges this gap.

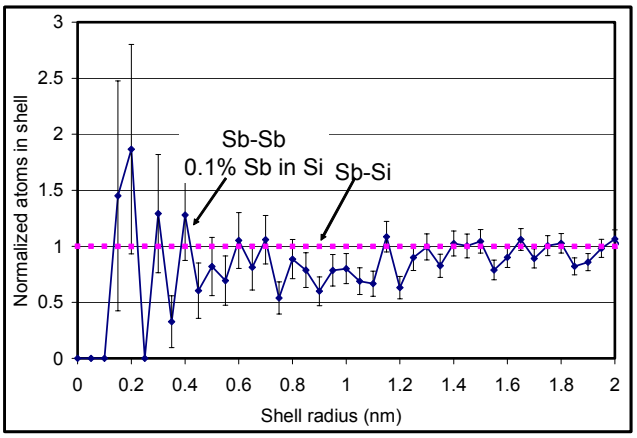
The possibility of clustering was investigated via atom-probe tomography. Results from the atom probe microscope are in the form of atomic positions in space that can reveal subtle gradients in concentration on the nanometer scale. This information is achieved with the controlled field evaporation of individual atoms from the specimen surface and detection thereof on a position sensitive detector. Their sequential detection reveals the third dimension thus resulting in a collection of atoms individually positioned in space. This element specific information allows for the formation of radial distribution functions of the dopant-dopant and dopant-Si interactions [1]. In this case, the radial distribution function is defined by drawing shells at a specific radius around a dopant atom and counting the number and type of atoms within the shell. The thickness of the shell (i.e. delta radius) is 0.1 nm and the radius of the shell is incrementally indexed by 0.1 nm. This is repeated for all dopant atoms in the sample. The number of atoms within each shell is then normalized by the average, or "expected" number of atoms within the shell. In this way, a value of 1 indicates no deviation from the bulk composition, a value > 1 indicates an excess of dopant atoms local to other dopant atoms, and a value < 1 indicates a rarification of dopants.

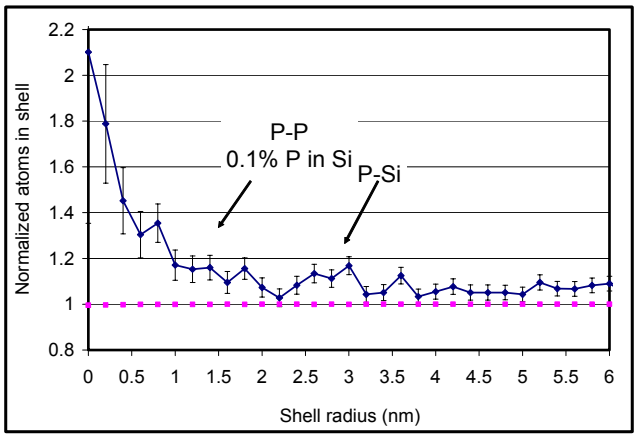
The following systems were investigated: 0.1% Sb in Si, 0.1% P in Si, 0.1% B in Si, and 2% B in Si. Each data set contains at least 10 million Si atoms, and the samples were uniformly doped in all directions. The results are shown in Figs. 1 – 4. As expected, in all cases, the dopant-Si interaction is unity. In Fig. 1, the Sb-Sb interaction is centered around unity with respect to the error bars, indicating no clustering. In contrast to Fig. 1, the P-P interaction, Fig. 2, shows twice the expected number of P atoms within a few nanometers, implying significant P clustering at 0.1%. This difference is not surprising given the difference in electrical activation and solubility of the atoms in Si [2]. At 0.1%, the solid solubility of Sb matches the electrical activity of Sb [1]. The electrical activity of P, however, is ~ 7 times *lower* than the solubility of P in Si. The implication is that while nearly 100% of the Sb atoms are active, only a fraction of the P atoms contribute carriers to the lattice. The B-B interaction at 0.1% B in Si, Fig. 3, is similar to that of Sb-Sb in Fig. 1. Once again,

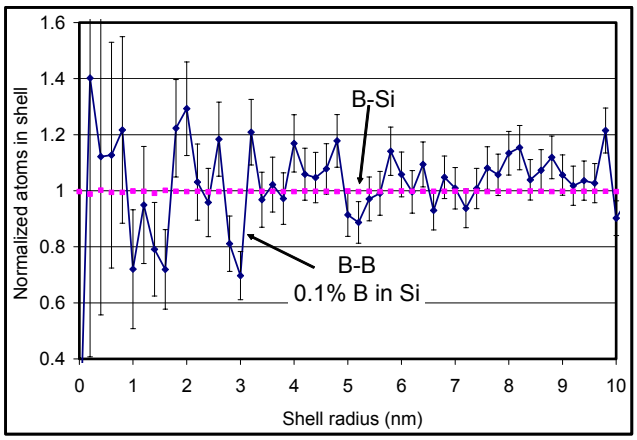
the electrical activity of B in Si, at 0.1% B, matches the solubility of B in Si. Increasing the B concentration to 2% demonstrates a marked change in the B-B interaction. Now, the number of B atoms per shell is 1.7 times the expected amount, indicating definite clustering has occurred.

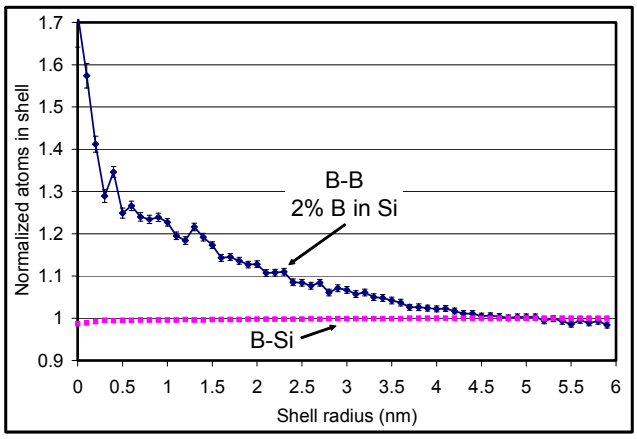
The RDF analysis of datasets collected through 3-D atom-probe tomography enables the investigation of dopant clustering in Si. In this case, clustering occurs when the dopant concentration exceeds the point where the solid solubility and electrical activity of the species in Si are matched.

1. J. Fortner, J.S. Lannin, Phys. Rev. B **39**(8) (March 1989) p. 5527
2. R.C. Jaeger, "Introduction to Microelectronic Fabrication," Addison Wesley Publishing 1993 p. 58









Radial distribution functions for the dopant-dopant and dopant-Si interaction for
Fig. 1. (top left) 0.1% Sb
Fig. 2. (top right) 0.1% P
Fig. 3. (bottom left) 0.1% B
Fig. 4. (bottom right) 2% B

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