

New Opportunities to Study Defects by Soft X-ray Absorption Spectroscopy

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X-ray absorption fine structure (XAFS) can determine the local structure of most atoms in the periodic table. Recently, new opportunities to study dopants and defects in semiconductors have emerged, specifically for those based on low Z (“light”) elements whose absorption edges lie in the soft X-ray range. This progress stems from improvements in the performance of synchrotron radiation sources and related instrumentation and in the development of computational schemes which are able to reliably simulate XAFS spectra.

In this contribution I will report some recent results that demonstrate how semiconductor physics may greatly benefit from such progress. In fact, doping or alloying of semiconductors with light elements is widely employed to tune their physical properties. XAFS investigations on such systems play an important role in knowledge – based materials design and can be crucial to understand and optimize technological processes.

Hydrogen passivation of N-induced effects in GaAsN dilute alloys (“dilute nitrides”) is an intriguing phenomenon with important potential applications. Addition of a few % of N to III-V alloys and subsequent H – irradiation is a powerful method for tuning materials properties (especially the band gap). N incorporation leads to a counterintuitive band – gap reduction of the host lattice. H irradiation induces a restoration of the original band – gap, a change which can be reversibly eliminated by annealing; this represents a new method for materials engineering. The actual defect responsible for this phenomenon was unknown and our XAFS investigations provided a determination of its atomic structure [1 – 3]. A combination of experiment and simulation allowed us to show that the H-N complex which forms is composed by two H atoms bound to the same N atom with C_{2v} symmetry; N is in the neutral charge state. Accurate determination of the H and N concentrations with nuclear techniques indicated that a third H atom is weakly bound and can be eliminated by low temperature annealing, leaving the main defect unaffected. The case of “dilute oxide” alloys, formed by adding a few % of O to II – VI alloys has also been studied [4].

ZnO is a wide band gap, naturally n -type semiconductor with great promise for optoelectronic applications; the main obstacle yet to be overcome is p -type doping. Nitrogen, the most promising candidate currently being pursued as a dopant, has been predicted to preferentially incorporate into the ZnO lattice in the form of a N_2 molecule at an O site when a plasma source is used, leading to compensation rather than p -type doping. We have demonstrated this to be incorrect [5] by using N K-edge XAFS and comparing them with first-principles calculations showing that N, in fact, incorporates substitutionally at O sites where it is expected to act as an acceptor. We also detect the formation of molecular nitrogen upon annealing. These results suggest that effective p -type doping of ZnO with N may be possible only for low-temperature growth processes.

The realization of ultra – shallow junctions with a high dopant concentration and sharp doping profiles is of great current interest. A promising method for B doping in Si is solid phase epitaxy regrowth (SPER): implantation of the dopant in a preamorphized substrate and subsequent activation by recrystallization. An open question is the origin of the limited fraction of electrically active B and in particular the process stage in which inactive B atoms appear. By using B K-edge XAFS we have demonstrated [6] that inactive B-B clusters are formed during the very early stages of recrystallization, when the B atoms are still in the amorphous matrix; these clusters are transferred to the crystalline Si matrix.

F incorporation in Si is able to reduce diffusion deterioration of B doping profiles in ultra – shallow junctions. The common interpretation is that this effect is due to an excess of vacancies (V_s) induced by F, but a precise experimental investigation of atomistic structure of F in Si is still lacking. We have very recently studied this issue [7] and have come to the conclusion that F is incorporated in the form of SiF_4 molecules inside nanocavities, also observed by transmission electron microscopy. Cavities, that can be thought as large aggregates of vacancies, are therefore responsible for the peculiar reduction of B diffusion in this system.

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