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Michael Steger

Transition-Metal Defects in Silicon

New Insights from Photoluminescence Studies of Highly Enriched ^{28}Si

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New Insights from Photoluminescence Studies of Highly Enriched ^{28}Si

Doctoral Thesis accepted by
Simon Fraser University, Burnaby, BC, Canada

Springer

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for dad

Supervisor's Foreword

Devices made from the semiconductor silicon power our ubiquitous computing, communication, information, power, and entertainment technologies. Enormous expenditures have been made in silicon materials and nanofabrication technology, and in the purification and perfection of silicon crystals. It would be surprising if such a thoroughly studied and widely exploited material could reveal novel and unexpected properties at this late date, but that is exactly what this thesis is about.

Silicon, along with almost all other semiconductors, is found in nature as a mixture of stable isotopes, in this case ^{28}Si, ^{29}Si and ^{30}Si. Changing this isotopic composition can have subtle effects on some of the properties of semiconductors, as has been known for some time from studies of isotopically enriched germanium and diamond, but samples of isotopically enriched silicon did not become available until quite recently, as a result of the Avogadro Project, which seeks to redefine the kilogram based on the properties of highly pure and highly enriched ^{28}Si.

Along with the subtle effects previously observed in other enriched semiconductors, the ^{28}Si revealed something completely new: the linewidths of many different optical transitions, spanning the near-gap region to the far-infrared, were found to be much sharper in ^{28}Si than in natural Si. This was an exciting result for semiconductor spectroscopy, since the linewidths even in natural Si were already much sharper than in other semiconductors, due to the purity and perfection of Si. The origins of the inhomogeneous isotope broadening which dominates in natural Si were quickly understood, but until their experimental discovery it had been thought that such effects would be too small to be significant.

Michael Steger's thesis describes in exquisite detail one important aspect of these incredibly narrow spectral lines which can be observed in ^{28}Si. For several decades researchers had been studying deep luminescence transitions (that is, transitions well below the $\sim$1.15 eV band gap energy) and had associated some of these deep luminescence centers with various transition metal impurities. This had practical implications, since transition metals are typically very deleterious for device performance, so detecting small quantities of them in Si was important. Over the years these identifications became well established in the literature, the prime example being the Cu-pair center. This identification was so widely accepted that the Cu-pair center was even used as a test bed for ab initio defect calculations comparing the calculated properties of a defect with its known properties.

Michael discovered finestructure in the luminescence of these centers, which he named isotopic fingerprints. These fingerprints unambiguously identify the type and number of atoms in a complex defect. Beginning with the 'Cu-pair' center, which was shown to actually contain four Cu atoms, it was found that not a single one of the previously studied deep defect centers is actually what everyone up until then thought it to be. This led to consternation in the deep defect community, but the evidence is so convincing that no one has tried to argue with the new identification made using isotopic fingerprints in ^{28}Si. This thesis provides a comprehensive listing of the known properties of these newly identified defects, which comprise sets containing either four or five atoms chosen from among Cu, Li, Au, Ag, and Pt. This information will be invaluable in the much-needed modeling of these centers, in order to understand their formation and properties, and explain why the number of constituents is always four or five. There is little doubt that other, less well-studied deep luminescence centers in Si will reveal new surprises when their isotopic fingerprints are studied in ^{28}Si.

Burnaby, October 2012 Dr. Michael L. W. Thewalt

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