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Highly Enriched ^{28}Si – a New Testbed for Impurity and Defect Structure

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We have recently found that many optical transitions in Si, including those of shallow impurity bound excitons, and the electronic ground state to excited state transitions of shallow donors and acceptors, are remarkably sharper in highly enriched ^{28}Si than in natural Si, due to the removal of inhomogeneous isotope broadening. This work is now being extended to deeper defects, many of which have been studied for decades in natural Si and were until now thought to be well understood. In ^{28}Si, due to the narrowness of the individual transitions, changing the isotopic species of the defect constituents results in well-resolved components, rather than the 'isotope shift' of the broad, unresolved inhomogeneously broadened lines observed in natural Si. This results in an 'isotopic fingerprint' of the defect, revealing not only the participation of a given element in the defect, but also the number of atoms of that element which are involved. We have recently shown [1] that a well known Cu-containing defect with a no-phonon luminescence line at ∼1014 meV, which was thought to be a Cu-pair, and for which ab-initio calculations [2] based on a pair-model appeared to agree convincingly with experiment, in fact contains four Cu atoms. A related center at ∼944 meV, modelled in the past as a different configuration of a Cu-pair [3], was shown to contain three Cu atoms [4]. We have now found that the 944 meV center also contains one Ag atom, and that another defect exists which contains two Cu and two Ag atoms. We will show that high resolution spectroscopy in highly enriched ^{28}Si produces many more surprising results regarding the actual constituents of well known deep centers in Si.

[1] M.L.W. Thewalt et al., Physica B 401-402, 587 (2007).
[2] S.K. Estreicher et al., Phys. Rev. Lett. 90, 035504 (2003).
[3] S.K. Estreicher, D. West and M. Sanati, Phys. Rev. B 72, 121201 (2005).
[4] A. Yang et al., Physica B 401-402, 593 (2007).