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# Unambiguous identification of the split-vacancy configuration of the SnV– defect in diamond

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Point defects in diamond are being intensively investigated for their applications in processing and communication of quantum information, as well as for metrology. So far, the negatively charged nitrogen-vacancy center (NV–) has been the most studied defect [1]. Thanks to its efficient optical spin polarization and spin-state dependent fluorescence, it is being exploited, for example, in the context of high-sensitivity magnetometers [2]. More recently, owing to their superior optical properties, the group-IV-vacancy centers (SiV– [3], GeV– [4], SnV– [5,6], and PbV– [7]) have emerged as one of the leading types of point defects for quantum computing and communication applications. Whereas it is generally accepted that the N atom in the NV– center occupies a substitutional C site, the group-IV atoms in group-IV-vacancy centers are expected to form a so-called split-vacancy configuration where they are centered in between two vacancies. However, experimentally, these structural configurations have so far been only indirectly determined. A detailed, direct and quantitative characterization of the structure of these defects is especially important for the field, since the superior properties of the group-IV-vacancy centers are to a large extent a consequence of the D3d inversion symmetry of the split-vacancy configuration rather than C3v, as in the case of NV–. The D3d symmetry, however, will only be found if the impurity is exactly centered in the double vacancy, which corresponds to the ideal bond-center (BC) position.
We have used the beta- emission channeling method from 121Sn (t1/2=27.1 h) implanted at the low fluence of 2.3E12 atoms/cm2 into natural diamond in order to identify the lattice sites of Sn and hence also possible configurations of SnV defects. Following room temperature implantation ˜60% of the implanted 121Sn occupied substitutional sites, while ˜40% was found on a position that corresponds to a bond-center site and which is attributed to the SnV split-vacancy configuration. While the as-implanted lattice location indicated displacements from the ideal S and BC sites of the order of ˜0.15 Å, following annealing at 920℃ ˜70% of the Sn atoms were found on the ideal substitutional and ˜30% on ideal bond-center positions. The same diamond sample was subsequently implanted with the stable isotope 120Sn and studied by means of confocal photoluminescence (PL) spectroscopy, which, after 920℃ annealing, revealed the characteristic luminescence signal [5,6] of SnV– at a wavelength of 621 nm.
Besides 121Sn, suitable EC probes for further studies of group IV-vacancy centers could be 31Si (157 min), 75Ge (82.8 min), or 209Pb (3.2 h), and ideas for possible future experiments will be outlined.

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