Low-dose 3D Dynamical Characterization of Si-Vacancy Colour Centre in Diamond

Si-vacancy (Si-V) centres in diamond have gained significant interest in recent years (Fig. 1 a&b). These centres have been demonstrated as an effective coherent single photon emitter, unlocking potential application in quantum communications and computing. The structure of these defects plays an important role in defermining optical properties. To enable the engineering of these defects in diamond so that they are created with the desired atomic structures: orientation, location and environment, it is essential to directly visualise their atomic structure and local chemistry at a high spatial resolution in the three dimensions.

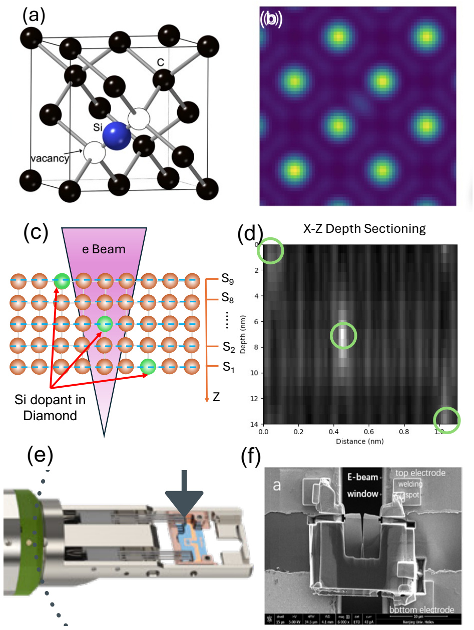

Fig. 1 (a-b) A structural model and simulated ptychographic image of Si-V in diamond; (c-d) Multislice ptychography[2] and its depth sectioning of Si dopant in diamond[2]; (e-f) *In-situ* holder mounted with a FIB sample;

Over the past decade, significant progress has been made in analyzing individual dopant atoms within bulk materials using annular dark field imaging in scanning transmission electron microscopy (ADF-STEM). However, accurately locating dopants or vacancies in 3D materials remains a major challenge. Electron ptychography, enabled by advanced electron detector technologies, offers a promising solution to several imaging challenges. Compared to conventional STEM, ptychography provides significant advantages not only in super-resolution imaging, but also in light-element detection[1], 3D imaging[2,3], coupling to spectroscopic data acquisition[4] and low-dose biological imaging[5,6] as recently demonstrated by our team.

Multiple scattering in crystalline samples presents significant challenges in imaging and structural analysis. These challenges can be mitigated using an advanced multi-slice approach in ptychography (Fig. 1c), which treats the 3D object as a series of 2D slices, each with its own transmittance function, separated by small distances of free-space propagation. By implementing this strategy, our group was the first to demonstrat that electron ptychography can provide phase information from the 3D structure of a thick sample, achieving atomic lateral resolution and depth resolution within 12 nanometers[2]. Recent advancements have improved depth resolution down to 3 nm[7]. These developments suggest that our approaches are highly suitable for studying defects in the crystals, such as diamond colour centres (Fig. 1d)[8]. Therefore, in this proposal, we aim to experimentally implenment 3D multislice ptychography to study local structure around colour centres at the atomic level at low dose. Furthermore, with a range of in-house *in-situ* holders (Fig. 1e &f) at Warwick-capable of applying heat, force, and electricity, we are able to dynamically reveal the microstructure evolution under distinct external stimuli. For example, the evolution, particularly in the formation of these colour centres through the incorporation of Si dopants and vacancies, will be elucidated. It is anticipated that direct imaging of these colour centres in diamond will open new avenues for defect engineering, ultimately allowing for the fine-tuning of diamond's optical and electronic properties.

References:

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