Low-dose 3D Dynamical Characterization of Si-Vacancy Colour Centre in Diamond changing the focus of the focus of the microscope – to microscope – to microscope – to multislice electronical
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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 desired atomic structures. Orientation, location and environment, it is essential to directly v
structure and local chemistry at a high spatial resolution in the three dimensions. S colour centre sidicon doped crystal; red plane denotes S 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 photo information in the set of the set
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Fig. 1 (a-b) A structural model and simulated ptychographic image of Si-V in diamond; (cptychographic mage of 51 -V in diamond, (e-
d) Multislice ptychography² and its depth structure of a thick sample, a sectioning of Si dopant in diamond²; (e-f) \ln -
resolution *situ* holder mounted with a FIB sample;

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Over the past decade, significant progress has been made in analyzing and the simulations were generated using ^(a) (b) individual dopant atoms within bulk materials using annular dark field

individual dopant atoms within bulk materials using annular dark field imaging in scanning transmission electron microscopy (ADF-STEM). However, accurately locating depants or vacancies in 3D materials remains a major challenge. Electron ptychography, enabled by advanced electron detector technologies, offers a promising solution to several Election detector technologies, oners a promising solution to several expressioning inaging challenges. Compared to conventional STEM, ptychography provides significant advantages not only in super-resolution imaging, but provides significant advantages not only in super-resolution imaging, but also in light-element detection¹, 3D imaging^{2,3}, coupling to spectroscopic also in light-element detection¹, 3D imaging^{2,3}, coupling to spectroscopic data acquisition⁴ and low-dose biological imaging^{5,6} as recently demonstrated by our team. $S_{\rm 3D}$ setup to multislice ptychography reconstructions Defocuse optical sections optical sections of the conventions of the convention of the conventio were 0.7 Å despite being also in light-element detection¹, 3D imaging^{2,3}, cou ron detector tecnnologies, offers a promising solution to several
ing challenges. Compared to conventional STEM, ptychography recorded on During the convention of dopation of dopants in the convention of the conventions. $\frac{1}{2}$ and $\frac{1}{2}$ a $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ $\frac{1}{2}$ data acquisition⁴ and low-dose biological imaging^{5,6} as recently ig challenges. Compared to conventional STEM, ptychography a ac
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Multiple scattering in crystalline samples presents significant challenges
in imaging and structural analysis. These shallenges can be mitigated using in imaging and structural analysis. These challenges can be mitigated using Schematic of 4D-STEM setup to multislice ptychography reconstruction pixelated detector Reconstructed Slice at Different Depth 21.4mrad 30mrad is clearly visible at each depth in the sample. Scale bar is 2 Å ADF 7 Å 2 Å Slice at depth of 0 Å Slice at depth of 3.5 Å Slice at depth of 7 Å 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 Individual slips** function, separated by small distances of free-space propagation. By $\frac{1}{2}$ implementing this strategy, our group was the first to demonstrat that Fig. 1 (a-b) A structural model and simulated electron ptychography can provide phase information from the 3D $\frac{1}{\text{pt}}$ $\frac{1}{2}$ and $\frac{1}{2}$ (c. Electronic profile profile provide primes information from the 3D
d its depth structure of a thick sample, achieving atomic lateral resolution and depth resolution within 12 nanometers². Recent advancements have improved resolution within 12 nanometers . Recent advancements have improved
depth resolution down to 3 nm⁷. These developments suggest that our $\frac{1}{2}$ Comparison of Optical Section recorded by our team.
All corrections of the samples presents significant challenges $\frac{1}{2}$ gated using
[,]hich treats Individual slice reconstructions of the scribing of the scattering in crystalline samples presents sign 21.4mrad 30mrad Comparison of Optical Sectioning Methods is clearly visible at each depth in the sample. Scale bar is 2 Å ADF 7 Å 2 Å

approaches are highly suitable for studying defects in the crystals, such as diamond colour centres (Fig. 1d)⁸ approaches are highly suitable for staaying acreats in the orystals, such as alament soletal centres (Fig. 20, structure around colour centres at the atomic level at low dose. Furthermore, with a range of in-house *in-situ* of actare around colour centres at the atomic rever at low acse. Furthermore, with a range of immodes *in site*
holders (Fig. 1e &f) at Warwick-capable of applying heat, force, and electricity, we are able to dynamically r the microstructure evolution under distinct external stimuli. For example, the evolution, particularly in the \blacksquare In the control 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.
Pa£a was ∞ References: imaging of these colour centres in diamond will open new avenues for defect es critough che i silican communities in an
the incornoration of Sildo $\begin{bmatrix} \text{C} & \text{C} & \text{C} \\ \text{C} & \text{C} & \text{C} \end{bmatrix}$ $\begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$ α evolution under atstrict external stimuli. For example, the evolution, ρ resolution is increased by increasing semiangle, but the intensity of the intensity of the intensity of the in
Intensity of the intensity at unect maging or the . DIOUT CENTES AT THE ATOMIC TEVEL AT TOW UP is anticipated that direct imaging of these colour centres in diamond will open new avenues for defect each Si dopant. resolution is increased by increasing semiangle, but the intensity of the ts in the crystals, such as dia nt,, not
le the e the microstructure evolution unde

t **Wang*, P**., *et al* Electron Ptychographic Diffractive Imaging and Straw, L., Song, J.,..., **Wang*, P.** Low-do of Boron Atoms in LaB₆ Crystals. Scientific Reports 7, 2857, biological specimens using cryo-elect (2017). (2017).
 Each Si dopant. The intensity of the inte angle of bottom victing in cab_b crystals. Scientific hepotes r, 2001, and Stemspear
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2 Gao, S., **Wang*, P.**, et al Electron ptychographic microscopy 6 Pei#, for three-dimensional imaging. *Nature Communications* **8**, 163, single par (2017). transfer. *Nature Communications* **14**, 3027, (2023). [4] and spatial resolution is calculated as ∆ = 0.612/ [5], Spatial and depth resolution is improved by increasing convergence begins to decrease with larger convergence angles. limited by the largest scattering angle on the detector. This is ., et al Electron ptychographic microscopy and both Pei#, X.,..., **Wang*, P.** Cryogenic electron of person

(2017).
3 Ding, Z.,..., **Wang*, P.** Three-dimensional electron 7 Chen, Z., et al, Electron ptychograpl
2 problems the serve is associated and the bottom of a server is believed as a server than the server of a server is th ptychography of organic-inorganic hybrid nanostructures. The resolution limits set

Nature Communications 13, 4787, (2022). (2021). (2021). *Nature Communications* **13**, 4787, (2022). depth resolution. In contrast, the resolution of ptychography is [4] and spatial resolution is calculated as ∆ = 0.612/ [5], observed in our results, but we find that the signal from the dopant

Nature Communications 13, 4787, (2022).
4 Song, B., Ding, Z.,,..., **Wang*, P.** Hollow Electron 8 Horne, A., ,..., Gr Ptychographic Diffractive Imaging. *Physical Review Letters* 121, and paracterisation of pricing, the resolution of pricing as a solution of pricing as a solution is calculated as $\frac{1}{2}$, and $\frac{1}{2}$, characterisatio 146101, (2018). $\overline{}$

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Angle transfer Nature Communications 14, 2027 (2023) $\frac{1}{100}$ o rest, $\frac{1}{100}$, waig, r. Clyogenic electron prychographic
nos **8** 163 cingle particle analysis with wide bandwidth information Depth profiles of each imaging technique, normalised to the

7 Chen, Z., et al, Electron ptychography achieves atomicrince dimensional electron resolution inits set by lattice vibrations. Science 372, 826-831, (2021). intensity of a carbon atom. Very little information is retrievable in

Wang^{*}, P. Hollow Electron 8 Horne, A., , ..., Green, B, Wang, P. High resolution structural and the detector. This is in the detector of silicon vacancy colour contros in diamond zing. Physical Review Letters 121, and that acterisation of silicon-vacancy colour centres in diamond that the signal from the 146101, (2018).
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 10 22443/rms mmc2023 88 (2023) 10.22443 /rms.mmc2023.88, (2023). irai
not intensity of a carbon atom.
123 observed in the signal from th
In the signal from the dopanties of the signal from the dopanties of the signal from the signal from the signa intensity of a carbon atom. $\mathbf 1$ Both visually and the profile, A., μ , μ , **views**, b, wang, respective profile and the profile profile profile profile profile and the profile profile profile profile profile profile and the profile profile profile p Letters 121, letters and a much-improved and setters in diamond
using 4D-STEM and ptychography. *EMAG Conference 2023* C *C* 20 *Z* 3.88 , (2023).