

Supplementary information

Direct imaging of boron segregation at dislocations in B:diamond hetero-epitaxial films

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S1. Characterisation of the Burgers vectors of [001] dislocations using weak-beam dark field TEM.

The following WBDF-TEM images have obtained in [110] oriented FIB foil. In this orientation, all the dislocations can be identified except the edge dislocations with Burgers vector $\vec{b} = \frac{a}{2}[110]$. Indeed, all the diffraction vectors offered by the [110] zone axis are perpendicular to this Burgers vector leading to the invisibility of this family of dislocations. The WBDF image of Figure S1 was obtained with $g = 220$ in the same region shown in Figure 2 in the main manuscript. It exhibits dislocations parallel to the [001] direction. In the WBDF image of Figure S2 obtained with $g=004$, some dislocations indicated by ‘E’ in Figure S1 vanished. This confirms that these dislocations are edge dislocations of type $\vec{b} = \frac{a}{2}[110]$. The WBDF image of Figure S3 has been obtained using the diffraction vector $g = 1\bar{1}1$. In this image, the dislocations labelled ‘M1’ in Figure S1 are invisible even though they present a small residual contrast due to the presence of Boron at the dislocation core which can affect the diffraction contrast and the extinction conditions. This indicates that these dislocations are 45° mixed dislocations with Burgers vector of type $\vec{b} = \frac{a}{2}[10\bar{1}]$ or $\vec{b} = \frac{a}{2}[011]$. Indeed, these two vectors make an angle of 45° with the line of the dislocations ([001]). Figure S4 exhibits WBDF image obtained with $g = \bar{1}11$. In this image, the dislocations labelled ‘M2’ in Figure S1 vanished. They are 45° dislocations with Burgers vector $\vec{b} = \frac{a}{2}[101]$ or $\vec{b} = \frac{a}{2}[0\bar{1}1]$. Here again, a small residual contrast due to Boron segregation can be observed.

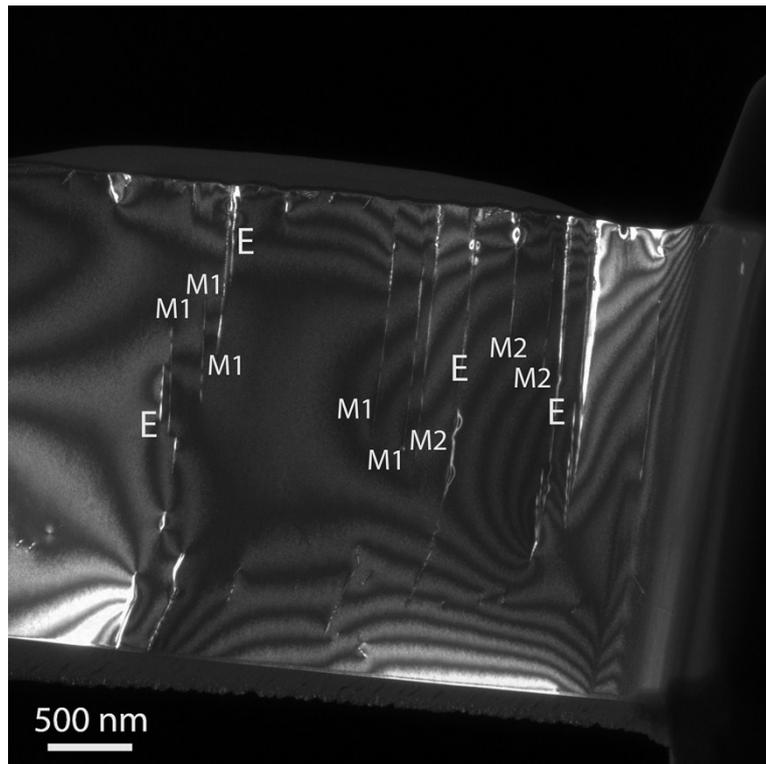


Fig. S1 : WBDF image obtained with $g = 220$. Edge dislocations are indicated by 'E' while 45° mixed dislocations are labelled 'M1' and 'M2'.

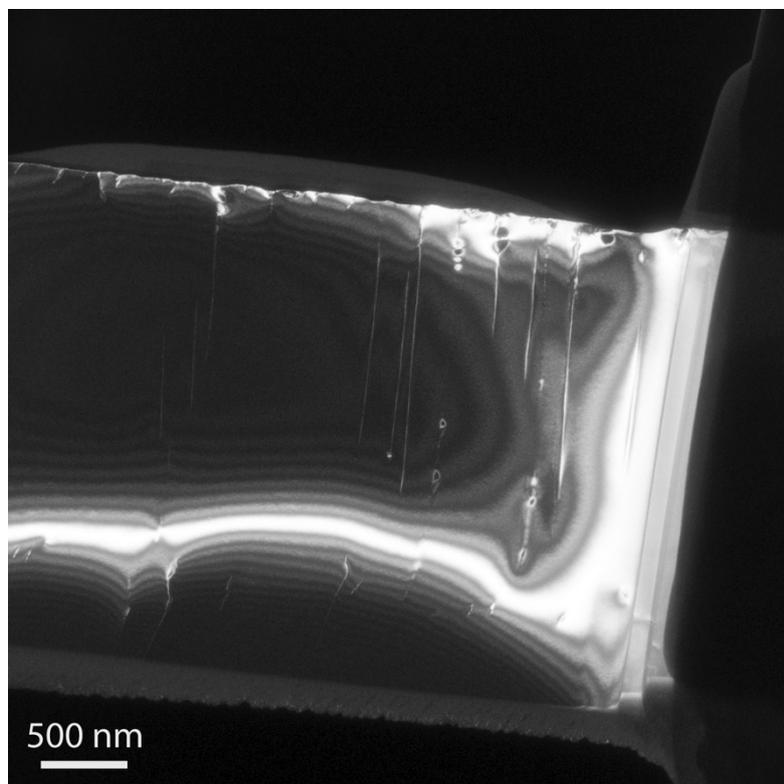


Fig. S2 : WBDF image obtained with $g=004$

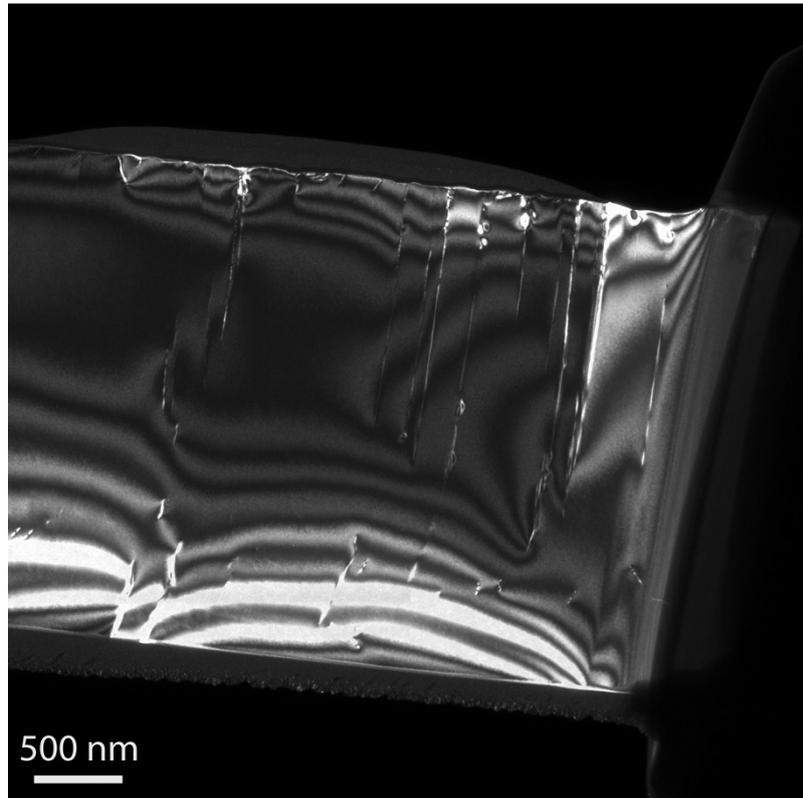


Fig. S3 : WBDF image obtained with $g = 111$

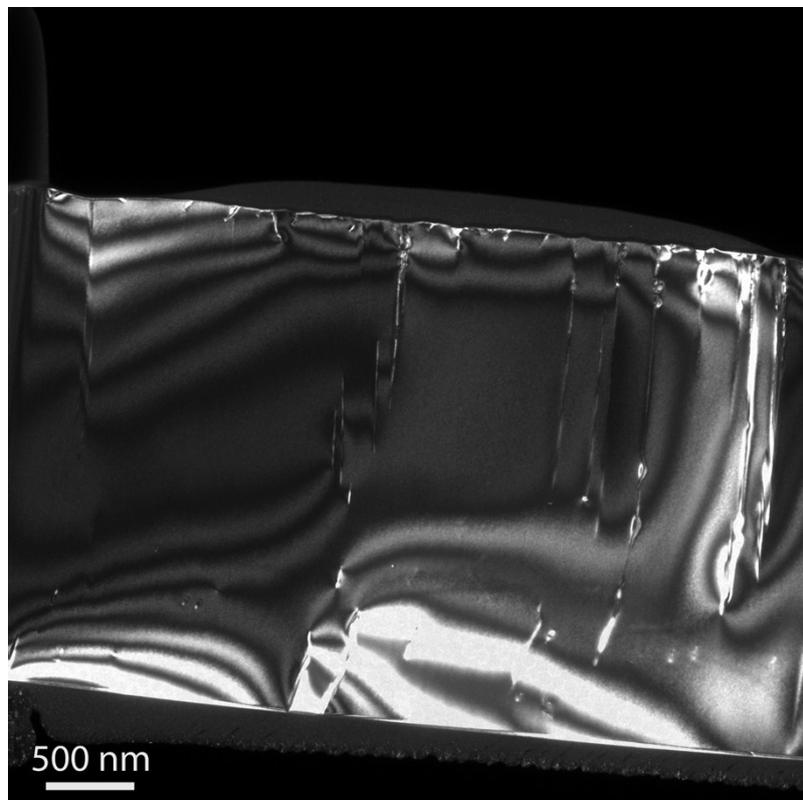


Fig. S4 : WBDF image obtained with $g = 111$

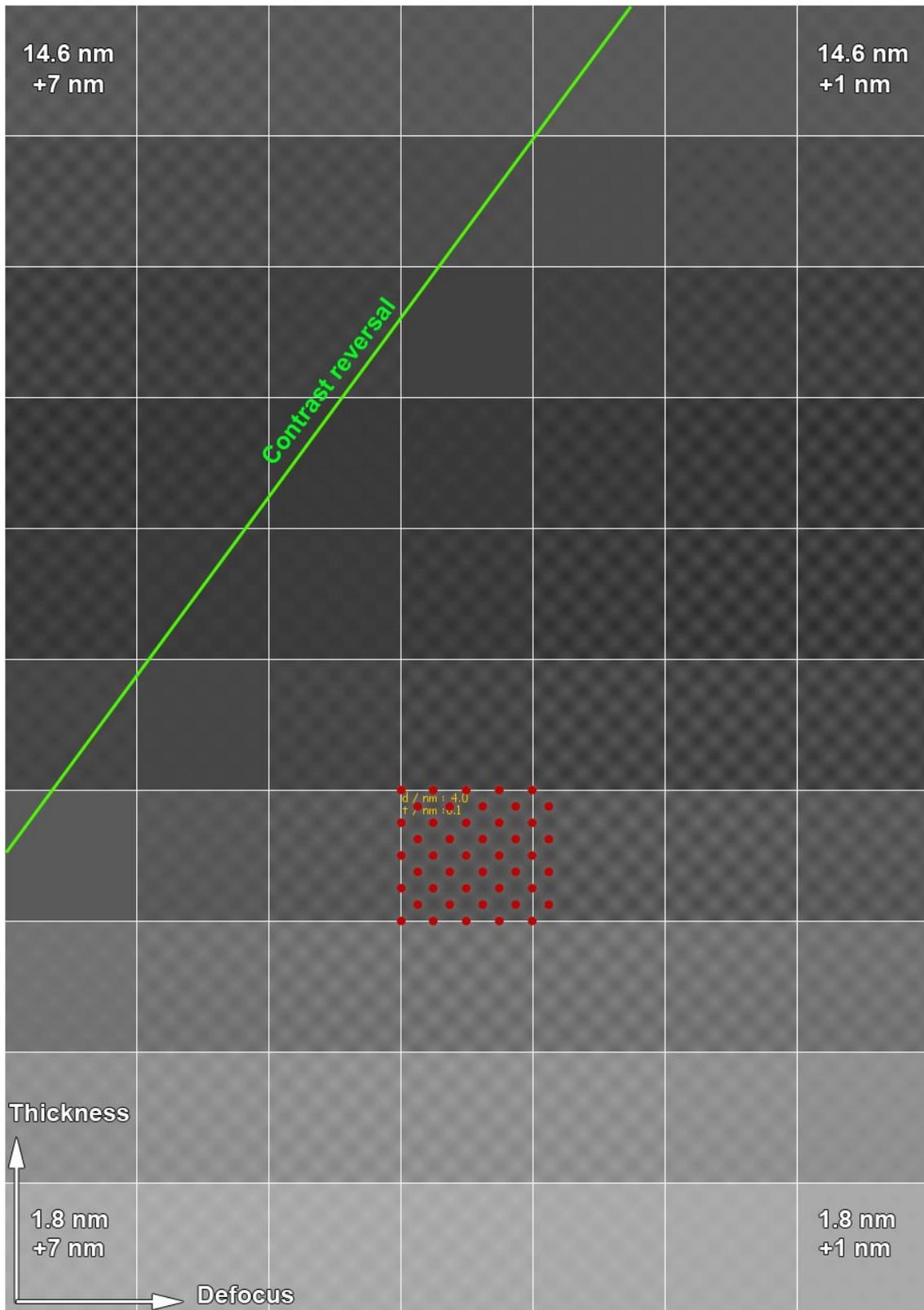


Fig. S5 : HRTEM image simulations for diamond along the [001] zone axis orientation. Image simulations were performed for a microscope operated at 300 kV, with the C_s value tuned to $-12 \mu\text{m}$. At slight overfocus conditions, in thin samples, the atomic C columns are imaged as white image contrast. The red dots represent the true atom column positions.