Novel bending phenomena in van der Waals materials

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2D materials such as graphene, hexagonal boron nitride and transition metal dichalcogenides have been thoroughly characterised by high resolution TEM imaging typically down their surface normal, i.e. the [0001] zone axis. This is excellent for looking at the structure and mobility of point defects and dopants in atomically thin sheets[1]. However, 2D materials are only useful as part of 3D structures, such as transistor devices[2], polymer composites[3] and surface coatings. Cross sectional TEM yields this missing dimension[4], and here we present exciting new bending and folding phenomena in van der Waals materials, revealing how geometries unique to this structure family change the further we go from the crystal surface.

Different bending phenomena in graphene, hexagonal boron nitride and $MoSe_2$ kink bands were captured in cross section by high resolution scanning TEM and analysed carefully to recover quantitative information via image processing and segmentation. Bend geometries were found to fall into 3 categories: Nanotube-like bending, a novel crystallographic twin boundary, and a mix between these two which induces sub-surface delamination.

The type of bend geometry adopted is found to depend upon the bending angle and the thickness of the crystal. Nanotube-like bending is adopted by very thin crystals at any bend angle. Novel twin boundaries with extended regions of incommensurate curvature are found in thick crystals above a threshold twinning angle. Mixed bending is found only in thick crystals with large bend angles. We hypothesis that mixed bending may be a key mechanism for exfoliation routes from bulk to 2D materials as large delaminations are frequently seen in the body of the crystal far below its surface. Finally, the strain induced by bending is incredibly localised and as such we anticipate bending and folding to be a new avenue for reliably engineering the electronic band structure of 2D materials.

References:
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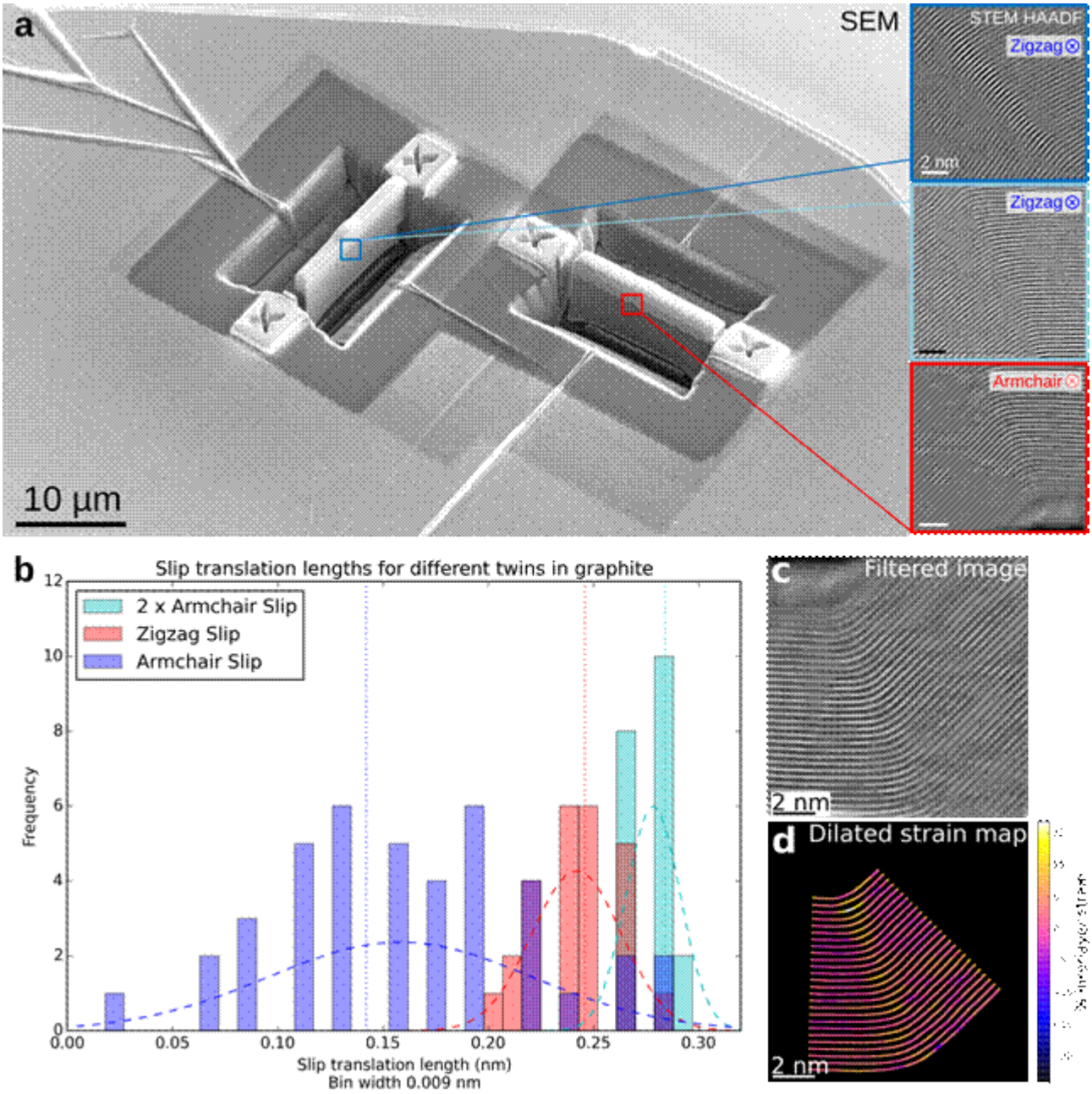
The authors would like to thank the UK Engineering and Physical Sciences Research Council (EPSRC) (grant numbers EP/K016946/1 and EP/M010619/1), the US Defense Threat reduction agency (grant HDTRA1-12-1-0013), and the EPSRC NowNano EPSRC doctoral training center.



TEM cross section analysis of novel twin boundaries in graphite. a) SEM of two lamellae, prepared by ion beam milling, intersect two kink bands. The left (right) kink band follows the zigzag (armchair) direction of the crystal. The insets rightmost show high resolution STEM images of different twin structures. b) Analysis of the insets in a) demonstrates the deviation from perfect twinning. In each case, the crystallographic slip follows a normal distribution about a mean. The standard deviation decreases as the crystal bends to higher angles, attributed to strain. c) and d) demonstrate how interlayer strain can be extracted for each graphene sheet across the twin boundary.