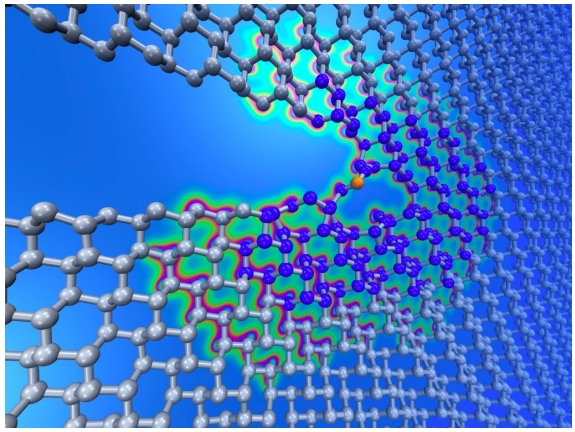
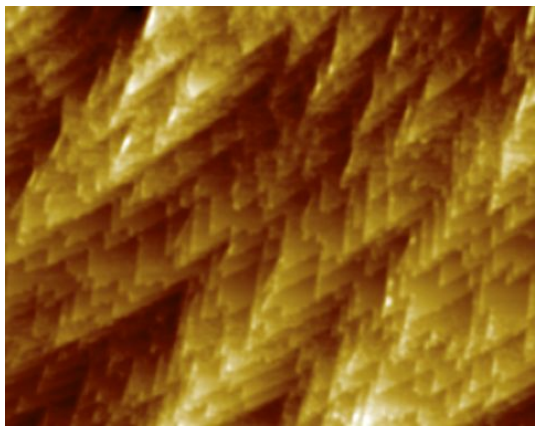
Multiscale Modelling of the Effect of Defects on the Mechanical Properties of Diamond

Failure by crack propagation is the major lifetime limiting factor for diamond drill bits. Both naturally occurring and synthetic diamond specimens always contain defects, but the effects these have on crack propagation are currently poorly understood.

Recent work has shown that a single defect can be enough to deflect a crack as it travels through a crystal according to recent quantum mechanical simulations (above left, Ref. [1]), leading to microscopic ridges on the surfaces of the broken material (above right). This PhD project will extend the modelling approach to study the effect of defects in diamond on its mechanical properties. The project will involve combining existing classical interatomic potential models for diamond with a density functional theory model for defect sites using the "Learn on the Fly" multiscale modelling approach [2].

The four year PhD position is funded through the Diamond Science and Technology CDT. The successful candidate will be required to undertake the MSc taught component at Warwick and then two associated mini-projects at partner universities Imperial College London (with Dr Finn Giuliani, Mechanical Engineering/Materials) and Newcastle (with Dr Jonathan Goss, Electrical Engineering). The student will benefit from being part of a supportive network, and from being taught by experts from eight different universities which they can tap into in future years.

[1] J. R. Kermode, L. Ben-Bashat, F. Atrash, J. J. Cilliers, D. Sherman, and A. De Vita, Nature Commun. **4**, 2441 (2013).

[2] J. R. Kermode, T. Albaret, D. Sherman, N. Bernstein, P. Gumbsch, M. C. Payne, G. Csányi, and A. De Vita, Nature **455**, 1224 (2008).

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