Grain boundaries in chemical vapor deposited hexagonal boron nitride

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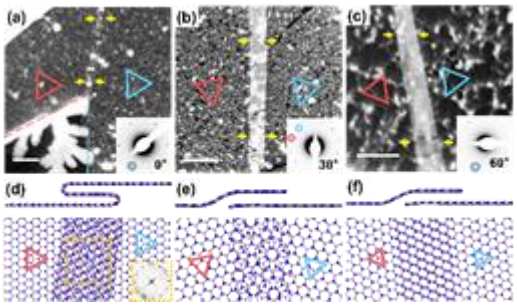

Figure: Grain boundary structures of three typical misorientation angles

Hexagonal boron nitride (h-BN) is a two-dimensional (2D) crystal which has similar lattice structure as graphene, while with a large band gap of around 5.9 eV[1].The atomic thin h-BN layer has very high mechanical strength and good thermal conductivity, as well as excellent chemical and thermal stability[2]. While CVD grown films are typically poly-crystalline and therefore result in grain boundaries (GBs)[3]. It is essential to explore the GB structures to evaluate the influence of these interfaces on the properties of h-BN sheets, such as mechanical, thermal and electronic properties[4].

Here we give a full picture of GB structures in CVD grown h-BN by using Dark-filed imaging which provides a nanometre- to micrometre-scale grain analysis, combined with aberration corrected TEM imaging method to get the detailed structures. Unlike the covalently bonded GB (CBGB) which are commonly seen in graphene, the overlapping GB (OLGB) are dominated in CVD grown h-BN based on our statistical analysis while play a finite part in other 2D materials. And we also explored the structure of GBs in two rotationally aligned grains, which differs from it in CBGB and OLGB. To have a better understanding on the formation mechanism of OLGB in h-BN, we carried out density functional theory (DFT) calculations which reveal the role of hydrogen and the energetic competition between CBGB and OLGB in formation process.

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