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Dynamics of Triangular Hole Growth in Monolayer Hexagonal Boron Nitride under Electron Irradiation

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Defects are known to influence the intrinsic properties of materials. In graphene, topological defects have been shown to alter its chemical and physical properties and these have been extensively investigated. [1], [2] Such defects in hexagonal boron nitride (hBN) have been reported, but the formation mechanism of defects is not fully understood. Indeed, most reports have focused on defect formation and characterization [3], [4], [5] in localized regions of exfoliated hBN. At present, it is known that the edges of holes in hBN layers usually adopt zigzag and armchair-type configurations, with the former being more common. [3] Moreover, the zigzag configuration contains two different types of terminated edges due to the intrinsic heterogeneity of hBN, factors that have been shown to affect the material's intrinsic electrical properties.[7] However, the growth mechanisms of hBN defects are also not well established.

The dynamics of triangular defects induced by electron beam irradiation were analyzed using aberration corrected TEM with a monochromator to elucidate the mechanism of defect growth in hBN monolayers. A large area monolayer of hBN grown by chemical vapor deposition at atomic resolution is shown in Figure 1. Figure 1a shows initial formation of triangular holes. After prolonged electron beam irradiation, grown triangular holes can be conformed as shown in Figure 1b.

The hBN defect growth process was subsequently investigated. Efforts were then directed towards assessing whether the defects maintained their triangular shape after prolonged periods of electron beam irradiation. As summarized in Figure 2, the growth of a triangular hole appeared to be initiated by the removal of B and N atoms near the centers of the defect edges. This experimental observation indicated that triangular defects featuring edges with missing B and/or N atoms are more stable than those with atoms missing near a vertex. Regardless, under prolonged electron beam irradiation, the B and N atoms next to the vacancies were subsequently ejected in a manner that ultimately restored the overall triangular shape of the defect. Moreover, the triangular shape of the defects was maintained even after two holes merged together.

In this study, the growth of triangular holes in hBN monolayers was observed using sequential TEM imaging. When a monolayer of hBN was subjected to electron beam irradiation, a vacancy formed initially and grew while maintaining a triangular shape. Such shapes were observed even when such holes merged. This mechanism for the growth of these defects appeared to involve the ejection of B and N atoms near the centers of the defect edges and also the ejection of bundles of atoms.

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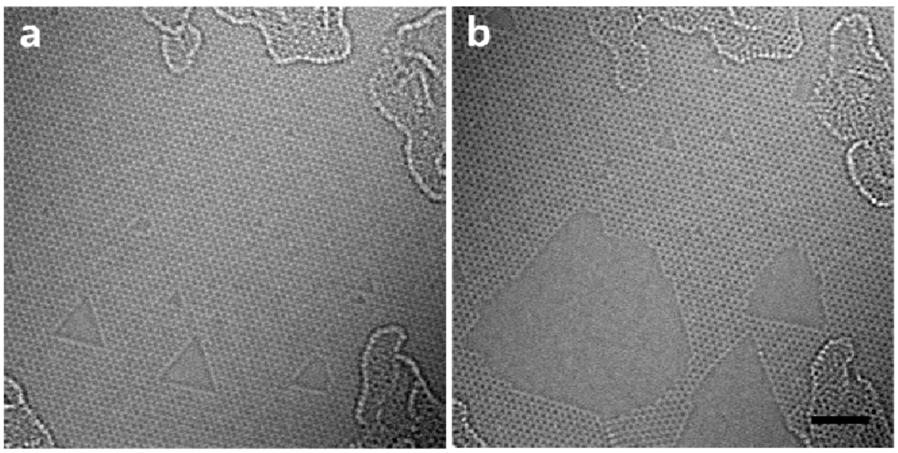

Figure 1. Formation and growth of large triangular holes in monolayer hBN by electron beam irradiation. The TEM images show (a) the initial defects and (b) an enlarged area of the same region. The scale bar is 2nm.

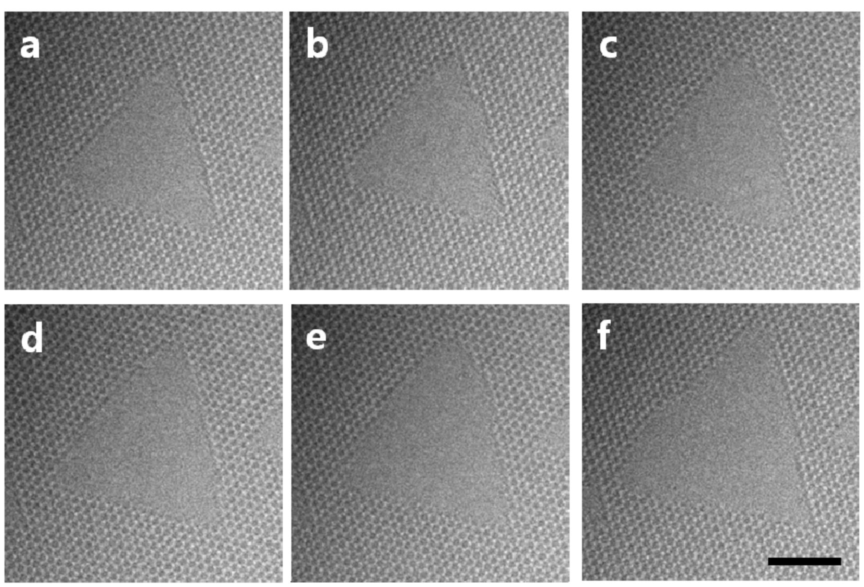

Figure 2. Sequential atomic resolution images of monolayer hBN showing how the shape and orientation of the defects are maintained upon further growth. The scale bar is 2 nm.