Atomic and Electronic Structures of the {111} Diamond/Cubic Boron Nitride Interface

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Diamond and cubic boron nitride (c-BN) are the top two hardest materials on earth. Their superhardness can be attributed to the extremely strong covalent bonds between atoms with an sp^3 configuration [1]. For decades, extensive effort has been devoted to fabricating diamond and c-BN with high quality and discovering novel properties and applications [2]. However, most of these studies are concentrated on each individual. The issues, how diamond and c-BN can actually join at the heterojunction and accommodate the lattice misfit at their interface, are still unclear. Understanding these issues is of fundamental importance for combining these two materials for enhanced properties, which takes on practical significance in electronics and mechanical engineering.

Misfit dislocations are often formed at the interface between two materials with different lattice constants to relieve strains. The interfacial misfit dislocations and their associated impacts on the properties of materials have attracted continuous and remarkable interest, especially in those systems with deformable crystal lattices, such as metals, semiconductors, and so on. However, our knowledge on the misfit accommodation mechanism of two superhard materials with rigid lattices remains very limited due to the extreme difficulty in preparing one superhard material on the other. In this study, we successfully grow the c-BN single crystals on diamond via the temperature gradient method at high pressure and temperature [3]. By transmission electron microscopy, we reveal a novel misfit accommodation mechanism for a {111} diamond/c-BN interface, that is, lattice misfit can be accommodated by continuous stacking fault networks, which are connected by periodically arranged hexagonal dislocation loops. The loops are constructed by six 60° Shockley partial dislocations. Atomically, the carbon in diamond bonds directly to boron in c-BN at the interface, inducing a two-dimensional electron gas that has never been realized in either of the bulk materials alone. Our findings point to the existence of a novel misfit accommodation mechanism associated with the superhard materials. The new electronic states could find applications for advanced electronic devices.

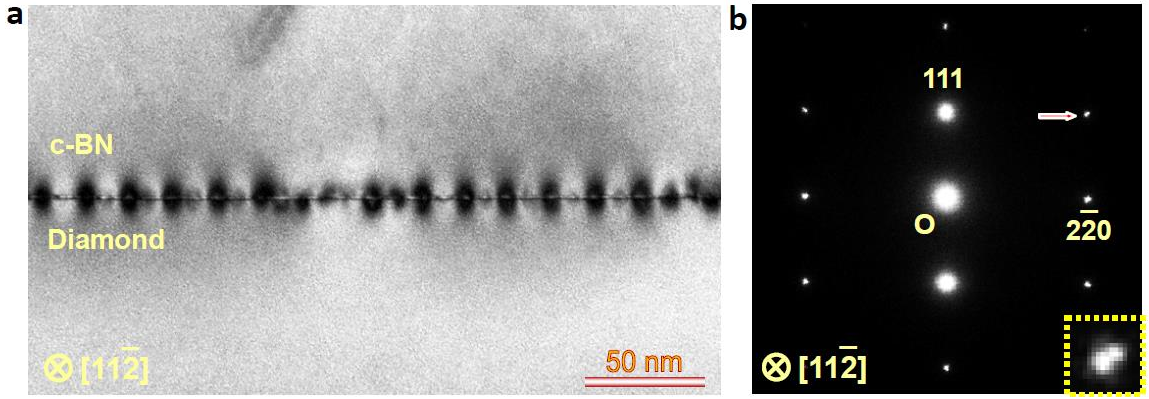

Fig. 1. Microstructure of the {111} diamond/c-BN interface. (a) Bright field TEM image and (b) corresponding diffraction pattern.

References

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