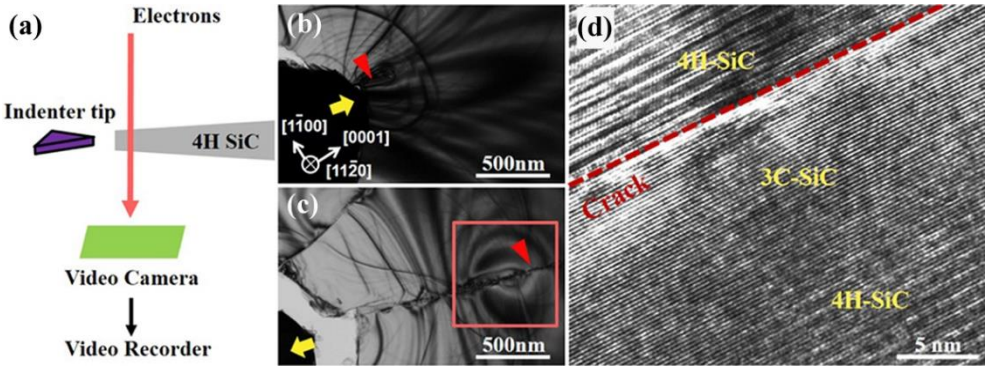
Nanoindentation-induced phase transformation between SiC polymorphs

Yao, T.[1]

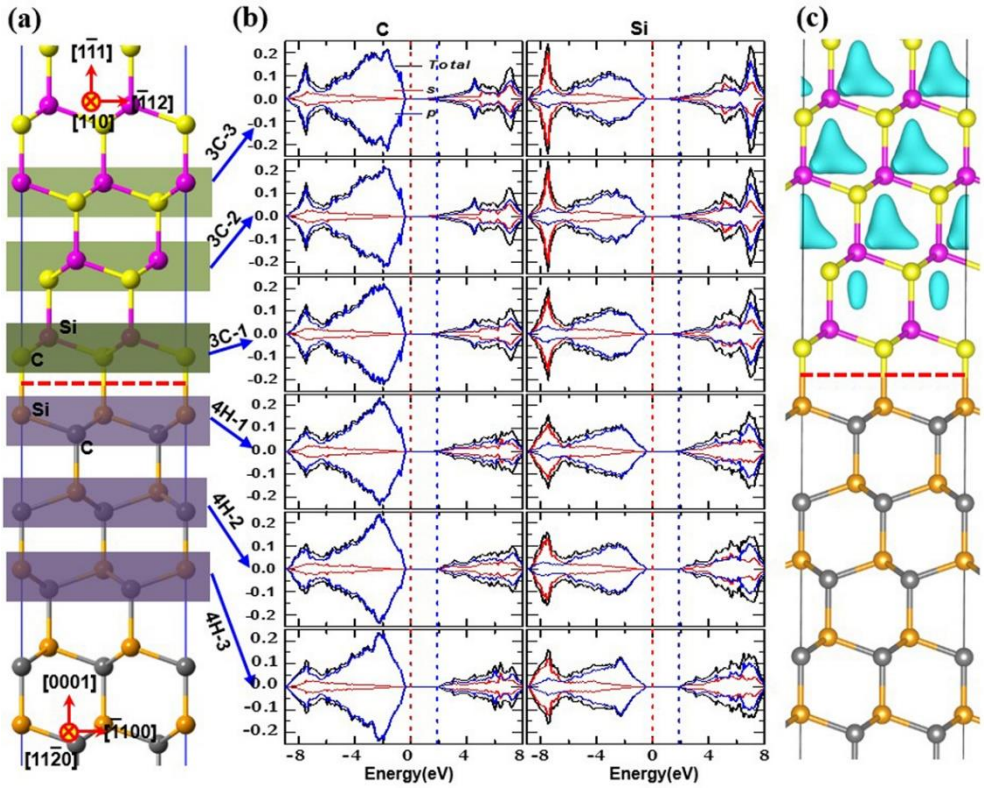
[1] Institute of Metal Research, China

Deformation and fracture dynamics of 4H silicon carbide (SiC) were investigated by in situ nanoindentation experiments, which were performed through moving the transmission electron microscopy (TEM) specimen toward a fixed wedge-shaped diamond indenter tip, as illustrated in Fig. 1a. Microcracks formed easily and propagated with the loading increased. The detailed TEM analyses of the residual crack (Fig. 1d) revealed the nanoindentation-induced phase transformation from 4H SiC to 3C SiC, which may contribute to the retard of the propagation of cracks to a certain extent.



Furthermore, to evaluate the driving force and energy barrier for the phase transformation, we calculated the energies and electronic structures of the 4H-SiC, 3C-SiC, and their interface. The most stable interface, as shown in Fig. 2a, was confirmed by the largest adhesion energy of the interfaces. The very smooth structural transition across the interface, of which C atoms of 3C-1 layer could be recognized as the extension of 4H-SiC, formed a coherent interface with low energy. Furthermore, the partial density of states of both C and Si in 3C-SiC near the interface (i.e. 3C-1 and 3C-2 layers) were very similar to

those in 4H-SiC (Fig. 2b), suggesting a negligible transition of electronic structures across the interface. The first principles calculations pointed out an extremely low energy barrier for this phase transformation, which could be attributed to the very smooth transition in the atomic and electronic structures across the 3C/4H interface. The phase transformation from 4H to 3C may reduce the band gap of SiC from 2.326 ev to 1.407 ev, implying a significant variation of electronic properties.



Acknowledgements

This work is supported by the Key Research Program of Frontier Sciences, CAS (No. QYZDY-SSW-JSC027), "Thousand Youth Talents Plan" of China, and the National Natural Science Foundation of China (Grant No. 51771200 and No.11332013). We thank Prof. Yuichi Ikuhara for valuable discussion.