Multiple twinning is widespread in both natural and synthesis matter. The two types of multiple twinning, lamellar and cyclic, have attracted much attention due to their unique structures and properties. Lamellar twinning was shown to give a combination of high strength and toughness in copper [1], and highest creep resistance in titanium aluminide alloys [2]. Cyclic twinning, as another type of multiple twinning, occurs in an even wider range of materials, including not only inorganic small particles and thin films, but also proteins and virus [3]. The fivefold twinning is the most common form for multiple cyclic twinning [3].

The fivefold twinning has also attracted attention from the viewpoint of symmetry, which is an important concept in modern science. In fact, the fivefold rotational symmetry is geometrically forbidden in periodic crystals, although widely found in quasicrystals. Due to the geometrical incompatibility, the fivefold twins have to be strained relative to the single-crystalline counterpart. Various models for the strain distribution have been proposed, including the linear homogeneous strain, angular and radial homogeneous strain, and the inhomogeneous strain models.

In this work, the atomic structure of the fivefold twins in diamond and silicon have been investigated by combining aberration-corrected transmission electron microscopy and first-principles calculations. In contrast to the strain distribution in metallic systems, which has small inhomogeneity, the strain in the fivefold twins of semiconductors depends significantly on the Pugh’s ratio of shear modulus to bulk modulus. For diamond with very high Pugh’s ratio, the strain is highly concentrated at the twin boundaries. Correspondingly, the frontier orbitals are located at the surfaces, in contrast to the case of silicon, where the frontier orbitals are close to the center.

References:

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Fig. 1: (a) Aberration-corrected TEM image of and (b) strain distribution in diamond five-fold twins.