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The boundaries of 2D Mo₂C superconducting crystals

Domain (grain) boundaries have significant influence on the electrical, thermal, optical, mechanical properties of 2D materials. Ultrathin transition metal carbides (TMCs), known as MXenes, have attracted increasing attentions due to their promising applications in energy storage, electromagnetic interference shielding, water purification, sensors, and catalysis [1-4]. In this talk, we used aberration-corrected scanning transmission electron microscopy (STEM) to study the domain (grain) boundary structure of chemical vapor deposited high-quality 2D Mo₂C superconducting crystals [5,6]. For different regular shapes including triangles, rectangles, hexagons, octagons, nonagons, and dodecagons, the Mo atom sub-lattice in all these crystals has a uniform hexagonal closely-packed arrangement without any boundaries. However, except for rectangular and octagonal crystals, the C atom sub-lattices are composed of three or six domains with rotational-symmetry and well-defined line-shaped domain boundaries. We found that there is very small lattice shear strain perpendicular to a domain boundary. In contrast to the single sharp transition observed in single-domain crystals, transport studies across domain boundaries show a broad resistive superconducting transition with two distinct transition processes due to the formation of localized phase slip events within the boundaries, indicating a significant influence of the boundary on 2D superconductivity. We also studied the grain boundaries (GBs) of 2D Mo₂C crystals, which show dislocation structure or unique sawtooth pattern depending on the tilt angle. Moreover, we found two new $\Sigma 7$ GBs with different periodic structure and crystallographic orientation at tilt angle of $\sim 22^\circ$. These findings provide new understandings on not only the defect structure of 2D TMCs but also the influence of boundaries on 2D superconductivity, which would be helpful for tailoring the properties of TMCs through boundary engineering.

References

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