Visualization of Confined Electrons at Grain Boundaries in a Monolayer Charge-Density-Wave Metal

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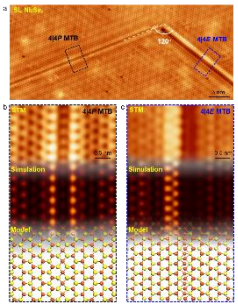
The properties of atomically thin 2D materials are extremely sensitive to structural imperfections including defects, edges, wrinkles, and grain boundaries. In the past decade, diverse structural imperfections have been widely studied in graphene, which are confirmed to realize rich physical phenomena, such as magnetic moments and topologically protected state. Structural imperfections in transition metal dichalcogenides (TMDs) have been explored to a lesser extent, but are ubiquitous and supposed to generate more plentiful physics. One-dimensional grain boundaries in TMDs are ideal for investigating the collective electron behavior in confined systems. However, clear identification of atomic structures at the grain boundaries, as well as precise characterization of the electronic ground states in charge-density-wave (CDW) metals, have largely been elusive.

Here, using molecular beam epitaxy, we successfully synthesize two types of mirror twin boundaries (MTBs) in monolayer $NbSe_2$, that is, 4|4P and 4|4E MTBs. With high resolution scanning tunneling microscopy observations, we provide direct experimental evidence for confined electronic states and charge density modulations at MTBs in CDW metals. Our measurements show that both MTBs can introduce local band bending effects and additional resonance peaks. Moreover, the intrinsic CDW signatures of monolayer $NbSe_2$ are efficiently suppressed as approaching an isolated MTB, but can be either enhanced or suppressed in MTB-constituted confined regions, depending on the electron energies. Such a phenomenon is well explained by the MTB-CDW interference. Our results reveal the significance of MTB-CDW interference in CDW metals, paving the way for the investigation of collective electron behavior in confined systems.



Pic.1 a) Large-scale STM image of monolayer $NbSe_2$. There are two types of MTBs, that is, 4|4P and 4|4E, with their intersection angle of 120°. b,c) Zoomed-in STM images of 4|4P and 4|4E MTBs from panel a, as well as the corresponding STM simulations and atomic structures.

Bibliography

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[2] Chen, Y.; Zhang, Y.; Huang, Z. P.; Wang, Y. *Adv. Quantum Technol.* **2023**, **6(7)**: 230087.