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ABSTRACT:

Dislocation Annihilation in Epitaxial Silicene

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Epitaxially-formed two-dimensional (2D) materials can have stress domains originating from lattice mismatch between the 2D lattice and the single-crystal substrate surface. Epitaxial silicene sheet spontaneously formed on ZrB₂ thin film grown on Si(111) substrate by surface segregation of Si atoms diffusing from the substrate through the film [1] have a characteristic domain structure which also exists in those formed by Si deposition on ZrB₂(0001) single crystal surface [2]. Scanning tunneling microscope (STM) observations reveal stripe domains with approximately 3 nm width [1]. The domain boundaries running along arm-chair directions in silicene honeycomb lattice are the part of the continuous honeycomb lattice which contain partial dislocations [3]. The transformation process of this domain structure into a single-domain through adsorption of a small amount of silicon atoms [4] was observed by in-situ real time STM at room temperature to investigate how dislocations react and eventually annihilate. Stepwise reactions of partial dislocations lead to the nucleation of a single-domain island, and this island extends by the propagation of edge dislocations at its frontiers. The identification of this dislocation annihilation process in epitaxial silicene sheet provides insights into how crystallographic defects can be healed in 2D materials.

[1] A. Fleurence et al., Phys. Rev. Lett., 108, 245501 (2012).

[2] T. Aizawa, S. Suehara, and S. Otani, J. Phys.: Condens. Matter, 27, 305002 (2015).

[3] A. Fleurence and Y. Yamada-Takamura, 2D Mater., 8, 045011 (2021).

[4] A. Fleurence et al., App. Phys. Lett., 108, 151902 (2016).