Point defects in epitaxial silicene on Ag(111) surface

Hongsheng Liu[1], Haifeng Feng[2], Yi Du[2], Jian Chen[3], Kehui Wu[3], Jijun Zhao[1,4]

[1] Key Laboratory of Materials Modification by Laser, Ion and Electron Beams (Dalian University of Technology), Ministry of Education, Dalian 116024, China
[2] Institute for Superconducting and Electronic Materials (ISEM), University of Wollongong, Wollongong, New South Wales 2525, Australia
[3] Beijing National Laboratory for Condensed Matter Physics and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China
[4] Beijing Computational Science Research Center, Beijing 100084, China
Corresponding authors. Email: zhaojj@dlut.edu.cn (J. Zhao), ydu@uow.edu.au (Y. Du)

Abstract

Silicene, a counterpart of graphene, has achieved rapid development due to its exotic electronic properties and excellent compatibility with the mature silicon-based semiconductor technology. Its low room-temperature mobility of ~100 $cm^2 \cdot V^{-1} s^{-1}$, however, inhibits device applications such as in field-effect transistors. Generally, defects and grain boundaries would act as scattering centers and thus reduce the carrier mobility. In this paper, the morphologies of various point defects in epitaxial silicene on Ag(111) surfaces have been systematically investigated using first-principles calculations combined with experimental scanning tunneling microscope (STM) observations. The STM signatures for various defects in epitaxial silicene on Ag(111) surface are identified. In particular, the formation energies of point defects in Ag(111)-supported silicene sheets show an interesting dependence on the superstructures, which, in turn, may have implications for controlling the defect density during the synthesis of silicene. Through estimating the concentrations of various point defects in different silicene superstructures, the mystery of the defective appearance of $\sqrt{,13} \times \sqrt{,13}$ silicene in experiments is revealed, and 4×4 silicene sheet is thought to be the most suitable structure for future device applications.