

New One-Dimensional Structure of Si Allotrope on Ag(111)

GSFS, The Univ. of Tokyo¹, ISSP, The Univ. of Tokyo²

°Lingyu Feng¹, Akitoshi Shiotari¹, Keisuke Yabuoshi¹, Masahiro Fukuda²,

Taisuke Ozaki², Yoshiaki Sugimoto¹

E-mail: fenglingyu0819@g.ecc.u-tokyo.ac.jp

In recent years, the progress of high-functionality and miniaturizing of electronic devices stimulates a growing interest in one-dimensional materials. Graphene nanoribbons are the most famous and widely-researched one-dimensional materials. Depending on the crystallographic orientation of the edges, graphene nanoribbons have different electronic and magnetic behaviors [1-2]. Besides graphene nanoribbons, silicon nanoribbons (SiNRs) have also attracted much attention. SiNRs have the potential to apply to future electronics devices because its compatibility with current silicon-based electronics and the theoretical outstanding electronic properties such as size-dependent band gap [3].

Here, we report the atomic structure of SiNRs on Ag(111) [4]. We found SiNRs on Ag(111) by depositing Si on the Ag(111) substrate. We investigated SiNRs on Ag(111) with a combination of scanning tunneling microscopy (STM), AFM and density functional theory (DFT) calculations. We obtained the atomic resolution STM images (Fig. 1(a)) and AFM images (Fig. 1(b)) of SiNRs on Ag(111). They reveal that SiNRs have the same width and align along the equivalent orientations of Ag(111). The main body of SiNRs was found symmetric about the long axes of ribbons, but the

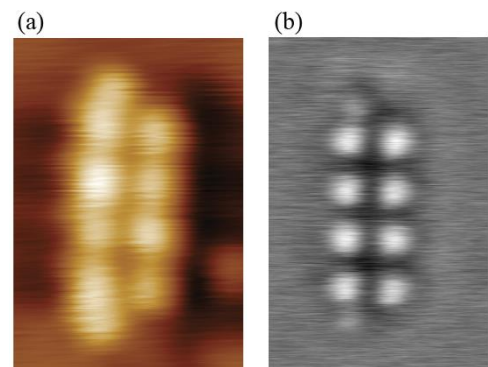


Figure 1: STM image (a) and AFM image (b) of a SiNR on Ag(111).

terminals of SiNRs break the symmetry. The observations indicate that SiNRs are stable under room temperature. In order to determine the detailed atomic structure of SiNRs, we performed the DFT calculations. The calculation results reveal the buckled single-layer structure of SiNRs, which agrees well with the STM and AFM observation results. In our proposed atomic structure, SiNRs have the unique structure that are composed of Si hexagonal and tetragonal rings.

Reference

- [1] Y.-W. Son *et al.*, Nature **444**, 347 (2006).
- [2] P. Koskinen *et al.*, Phys. Rev. Lett. **101**, 115502 (2008).
- [3] S. Cahangirov *et al.*, Phys. Rev. Lett. **102**, 236804 (2009).
- [4] L. Feng *et al.*, Phys. Rev. Mater. **5**, 034002 (2021).