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Quintuple-period Si atomic wires with alternative double and triple modulations by metal: Mg/Si(557)

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ABSTRACT

The formation of Mg-induced quasi-one-dimensional atomic wires on a Si(557) surface was studied by low energy electron diffraction (LEED), scanning tunneling microscopy (STM), and first-principles calculations. The atomic wires were produced on the Si(557) surface without faceting when heated to 330 C. The atomic wires had a ×5 period along the wires, as observed by LEED. STM images showed the existence of three kinds of atomic wires in a unit cell: an atomic wire located at the step edge and the others on the terrace. Interestingly, alternative double and triple modulations resulting in the ×5 period was observed at the atomic wire located at the step edge. Among the variety of atomic structure models available, the one based on a honeycomb-chain-channel model, which is that of a metal/Si(111)-(3×1) surface, reproduced the STM images well and was relatively stable energetically.

1. Introduction

Recently, vicinal Si(111) surfaces have been studied extensively to fabricate one-dimensional (1D) structures efficiently and to understand their underlying phenomena. Among the vicinal Si(111) surfaces, quasi-1D wires with a highly anisotropic electronic structure were first found on a Au/Si(557) surface [1–7]. A metallic Au/Si(553) surface with multiple quasi-1D metallic energy bands was discovered next [7–9]. The interesting quasi-1D metal-insulator transition, which was originally suggested to be due to quasi-1D charge density wave, is still under debate. An order–disorder transition and magnetic ordering were also suggested to be its origin [5,9–19]. More recently, quasi-1D transport and strong lateral coupling were observed on a Pb/Si(557) surface [20–22] and a triple-period atomic wire was reported on a In/Si(557) surface [23].

The reactions of alkali metals (AM) and alkaline earth metals (AEM) with surfaces have been studied as a fundamental reaction on both metal and semiconductor surfaces and many interesting phenomena in surface science have been reported [24–30,34]. On a Si(111) surface, one of intensively-studied systems was the metal(AM, AEM)-induced Si(111)-(3×1) surface with an anisotropic two-dimensional atomic structure [31–42,44–46]. Here, we report how the atomic structure of the Si(557) surface is reconstructed one-dimensionally by a metal with a simple electronic structure, where Mg was chosen as a prototype. Interestingly, Mg produced quintuple-period Si atomic wires with alternative double and triple modulations, as shown in Fig. 1, maintaining the same terrace width as the bulk-terminated Si(557) surface, whereas only double and triple spacing have been observed. An atomic structure model with a honeycomb-chain-channel (HCC) structure, which was the building block of the metal/Si(111)-(3×1) surface, reproduced most of the features of the scanning tunneling microscopy (STM) images and was energetically stable compared to other atomic structure models [31,34,36,42,47–50,52]. Moreover, since most of the atomic structures of other metal-induced vicinal Si(111) surfaces were similar to the relaxed bulk-terminated Si(111) surfaces, it is interesting that two honeycomb chains separated by an empty channel can be stabilized on a Si(557) surface.

2. Methods

The experiments were performed in an ultrahigh vacuum chamber equipped with commercial variable-temperature STM (Omicron, Germany) and low energy electron diffraction (LEED) (Omicron, Germany). An *n*-type Si(557) wafer (9.45° offcut from the [111] orientation toward the [1 12] direction) was used. A clean Si(557) surface was prepared by repeated resistive heating, where an electric voltage was applied along the step edge direction [58,59]. Mg was evaporated by heating a tungsten wire wrapping a Mg rod. The Mg coverage of the Mg/Si(557)-(5×1) surface was approximately 0.2 ML, where the Mg coverage was roughly calibrated based on that of the Mg/Si(111)-(3×1) surface [43,44]. First-principles calculations were performed using VASP based on the density functional theory [60]. For the total

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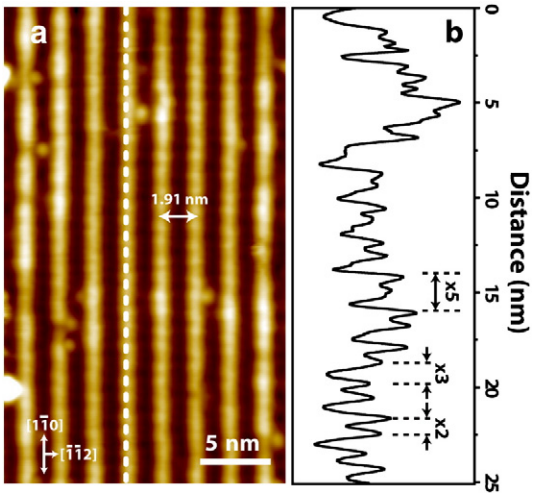

Fig. 1. (a) A filled-state STM image ($V_s = -2.5$ V) of the Mg/Si(557)-(5×1) surface produced at $T_s = 330$ °C. (b) The line profile along the dotted line in (a).

energy and force calculations, ultrasoft pseudopotentials provided with VASP were used within the generalized gradient approximation for the exchange-correlation energy [61,62]. The plane-wave cutoff energy was 250 eV. For surface Brillouin-zone integration, a 2×2 grid in Monkhorst–Pack special $\vec{k}$-point scheme including Γ-point was used [63]. The calculations were performed in a slab geometry with three Si bilayers and a vacuum region of approximately 18 Å. Si atoms at the bottom were saturated with H. All atomic positions were determined by minimizing the total energy until the residual forces on each atom were smaller than 0.04 *eV/Å* with the bottom Si and H layers kept fixed. STM images were simulated using the method reported by Tersoff and Hamann [64].

3. Results and discussion

3.1. LEED and STM experiments

The phase transitions of the Si(557) surface were investigated as a function of temperature and Mg coverage by LEED. A (5×1) LEED pattern began to appear when the sample was heated to 300 °C, as shown in Fig. 2. The (5×1) LEED pattern was optimized at temperatures ranging from 300 to 400 ?°C. When heated to 450 °C, the (5×1) LEED pattern became blurred. The (5×1) LEED pattern disappeared and a (7×1) LEED pattern of the clean Si(557) surface reappeared when heated above 500 °C. STM images of the Mg/Si(557)-(5×1) surface [hereafter Mg-(5×1)] were acquired to understand its real space morphology. Fig. 3 shows filled-state STM images of the Mg-(5×1) surfaces produced at 330 and 400 °C, respectively. The Mg-(5×1) LEED patterns were similar in the temperature range from 330 to 400 °C. On the other hand, uniformity of the Mg-(5×1) surface was quite different in the STM images. When the temperature of the sample (T_s) was near 330 °C, atomic wires were aligned uniformly with minimal atomic defects, as shown in Fig. 3(a)–(c). In contrast, when T_s ~400 °C [see Fig. 3(d)–(g)], atomic and line defects developed, which might be due to Mg desorption.

The filled-state STM image of the Mg-(5×1) surface shows that the distance between the wires is 1.91 nm which is the same length of the single terrace of the bulk-terminated Si(557) surface, as shown in Fig. 1(a). The line profile along the wire shows that the ×5 period along the wire is made up of alternative double and triple modulations

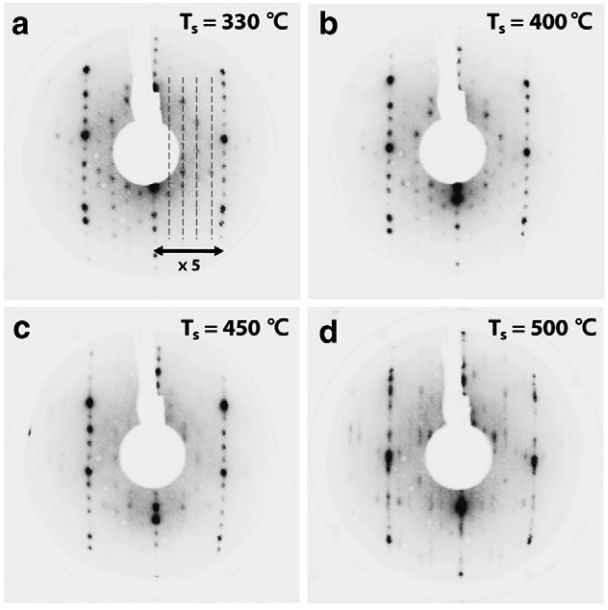

Fig. 2. LEED patterns of the Mg/Si(557)-(5×1) surface produced at T_s = (a) 330, (b) 400, (c) 450, and (d) 500 °C, respectively.

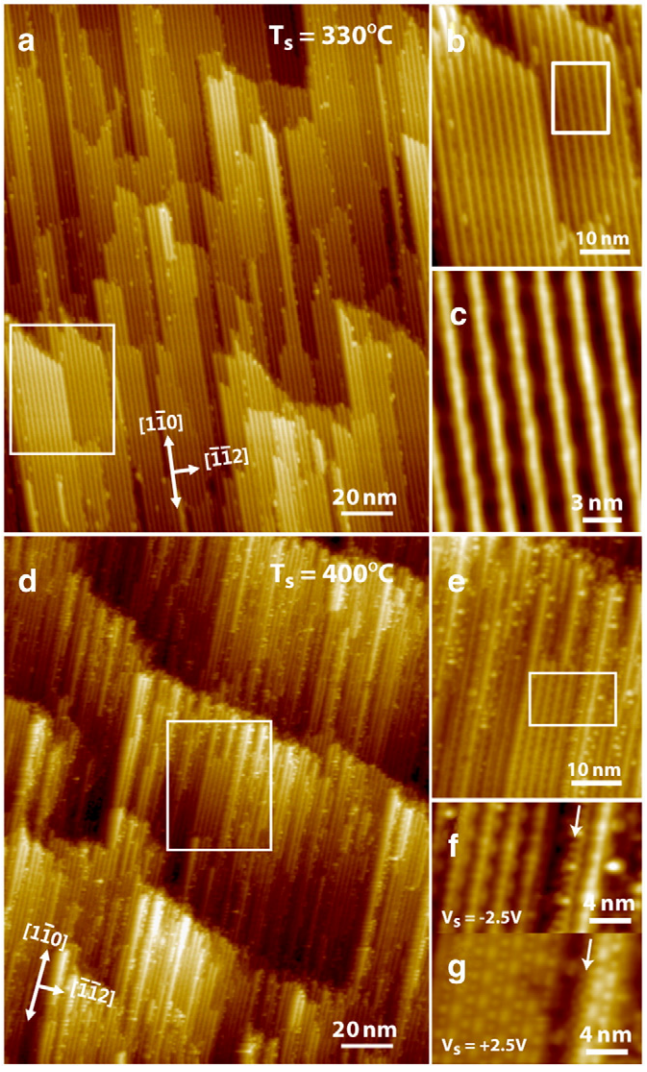

Fig. 3. Filled-state STM images ($V_s = -2.5$ V) of the Mg/Si(557)-(5×1) surface produced at T_s = (a)–(c) 330 and (d)–(f) 400 °C, respectively. Panels (b) and (c) are the enlarged images of the regions outlined by the rectangles in (a) and (b), respectively. Panel (e) is the enlarged image of the region outlined by the rectangle in (d). Panels (f) and (g) are the enlarged filled- and empty-state STM images of the region outlined by the rectangle in (e). The arrows in (f) and (g) indicate a clean Si(557) surface.