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# Quasi-one-dimensional structures on the Si(1 1 1) surface induced by Ba adsorption

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ABSTRACT

Ba-induced quasi-one-dimensional reconstructions of the Si(1 1 1) surface have been investigated by low energy electron diffraction (LEED) and scanning tunneling microscopy (STM). While the 3 × '2' surface shows double-periodicity along the stripes in STM images consistent with half-order streaks observed in LEED patterns, no sign of the double-periodicity along the chain direction was detected for the 5 × 1 surface. The 5× stripes in STM images show internal structures with multiple rows. The two rows comprising the boundaries of a 5× stripe in the filled-state STM image are found to have $3a \times \sqrt{3}/2$ spacing across the stripe. The observation of the successive 3× and 2× spacings between the boundary rows supports a structural model proposed for the Ba-induced 5 × 1 Si reconstruction composed of honeycomb chains and Seiwatz chains. The highest coverage 2 × 8 surface does not reveal a quasi-1D row structure in STM images.



## 1. Introduction

Adsorption of metal atoms on a Si(1 1 1) surface has been known to induce various reconstructions. Some of them form quasi-one-dimensional (quasi-1D) structures. The metal-induced quasi-1D structures on the Si surface have been the subject of extensive studies due to their fundamental and technological interest. Adsorption of divalent metal atoms such as Ca (alkaline-earth) [1–4] and Yb [5], Sm [6], and Eu [5] (rare-earth) has been known to induce a series of quasi-1D reconstructions $n \times 1$ ($n$ = 3, 5, 7, 9, and 2) with increasing coverage. For the Ba adsorption, reconstructions with 3 × 1, 5 × 1 and 2 × 8 low-energy electron diffraction (LEED) patterns were found to form with increasing the coverage [7]. Among these, the 3 × 1 phase, the smallest coverage phase, has been mostly investigated [8–10]. Its Si reconstruction was proposed to have a honeycomb chain-channel (HCC) structure, which was originally proposed for the alkali-metal-induced Si(1 1 1)surfaces [11,12]. The HCC structure with a Ba coverage of 1/6 ML was found to well explain the semiconducting property of this surface [8–10]. The same structural model was subsequently found to well account for the 3 × 1 surface induced by other divalent metals (Ca [4], Yb [13], Sm [14], Eu [13]). Compared with the 3 × 1 phase, the higher coverage phases have been much less studied.

In this work, the Ba-induced quasi-1D reconstructions of the Si(1 1 1) surface were studied by using LEED and scanning tunneling microscopy (STM) at room temperature (RT). The 3 × 1 phase shows double-periodicity along the stripes in STM images consistent with half-order streaks in LEED patterns. For the 5 × 1 phase, no sign of the double-periodicity along the chain direction was detected either in LEED patterns or in STM images. The 5× stripes in the empty- and the filled-state STM images appear to have internal structures comprised with multiple rows. The stripes in the filled-state STM image, in particular, reveal boundary rows at either sides with $3a \times \sqrt{3}/2$ spacing. The observation of both 3× and 2× spacings is compatible with a structural model with a simple combination of a honeycomb chain and a Seiwatz chain proposed for the Ca-induced 5 × 1 Si reconstruction [2,3]. The 2 × 8 LEED phase does not reveal a quasi-1D row structure in STM images. Instead it appears to have two-dimensional (possibly 8 × 8) structure.

## 2. Experimental

The experiments were performed in an ultrahigh vacuum chamber (base pressure ~$2 \times 10^{-8}$ Pa) equipped with LEED and a homemade STM system. The Si(1 1 1) substrate was cut from a commercial p-type Si (1 1 1) wafer (B doped, Virginia Semicon.) with a resistivity of 1–10 Ω cm. The Si(1 1 1) sample was first outgassed at 600 °C for 10 h, then flashed several times at 1200 °C until a clean (7 × 7) surface was obtained. Ba was evaporated from

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a thoroughly outgassed commercial getter source (SAES Getters Inc.) and deposited onto the Si substrate. During the evaporation, the chamber pressure was maintained in the low $10^{-9}$ mbar region. Depending on the Ba deposition time and the Si(1 1 1) substrate temperature, several different phases with 3 × 1, 5 × 1, and 2 × 8 LEED patterns were formed with increasing coverage, as shown in Fig. 1. STM images were taken at room temperature employing an electrochemically etched tungsten tip cleaned by *in situ* electron bombardment heating.

## 3. Results and discussion

Fig. 1 show LEED patterns of the three Ba-induced phases, (a) 3 × 1, (b) 5 × 1, and (c) 2 × 8 taken at RT. These three phases were prepared subsequently starting from the high-Ba-coverage phase. Specifically, the phase with the 2 × 8 LEED pattern was prepared by depositing some enough amounts of Ba on the Si substrate at 550 °C, followed by postannealing at 670 °C for 3 min. Then the surfaces with 5 × 1 and 3 × 1 LEED patterns were sequentially obtained by heating the surface additionally at 750 °C for 4 min, and 800 °C for 2 more minutes, respectively. Very weak and faint half-order streaks are visible in the 3 × 1 LEED. Considering these streaks, we will denote the 3 × 1 phase as 3 × '2' hereafter. In contrast, no half-order streaks or spots are visible in the 5 × 1 LEED at RT, similar to the cases of other divalent-metal-induced 5 × 1 surfaces [2,3,5,6]. For the 3 × '2' and the 5 × 1 phases, one-dimensional LEED patterns with a dominating single domain could result from certain preparation procedures (see Fig. 1(a) and (b)). However, the 2 × 8 LEED pattern always appeared as being two-dimensional. The 2 × 8 surface with 1D LEED pattern has never been made either in this work or in previous studies. Alternatively, the LEED pattern may be considered as 8 × 8 with many missing spots (except for the 1/2 and 1/8-th order spots).

Fig. 2 shows empty-state STM images of the three Ba-induced Si(1 1 1) reconstruction surfaces, taken at RT. The 3 × '2' (Fig. 2(a)) and 5 × 1 surfaces (Fig. 2(b)) consist of stripes running in the $[1\bar{1}0]$ direction. The separation between the stripes is $na$ ($n = 3$ for 3 × '2' and 5 for 5 × 1), where $a = a_0 \sin 60^\circ = 0.333$ nm [$a_0 = 0.384$ nm, a unit lattice spacing on a bulk-terminated Si(1 1 1)-1 × 1 surface]. In the case of 3 × '2' surface, the double-periodicity ($2a_0$) modulation along the stripes is clearly recognizable despite the presence of many defects, as already reported previously [8,9]. The lack of correlation of the phases in this double-periodicity between the neighboring stripes is consistent with the half-order streaks, instead of spots, in LEED patterns [9,10]. For the 5 × 1 surface, however, neither ×1 nor ×2 periods is resolved in the image. Each stripe on the surface takes a wavy appearance, suggesting the presence of double rows within a stripe. The bright protrusions on the stripes, mostly located on either sides of the stripes, may also indicate the possibility of this double-row structure.

The failure to observe the ×2 periodicity along the stripes in STM images of the 5 × 1 surface is consistent with the absence of the half-order streaks in LEED patterns, observed at RT. In the case of Ca, half-order spots or streaks were recently observed in the 5 × 1 LEED taken at 100 K [4]. Therefore, the double-periodicity in the Ca-induced 5 × 1 phase is believed to exist, although it has not been resolved in STM images as yet. Assuming the similarity with the Ca-induced surface, it is speculated that the Ba-induced 5 × 1 surface also has double-periodicity which is not yet detected. This assumption of the double-periodicity along the stripes in the Ba-induced 5 × 1 surface was justified by the compatibility with the core-level photoemission data [15].

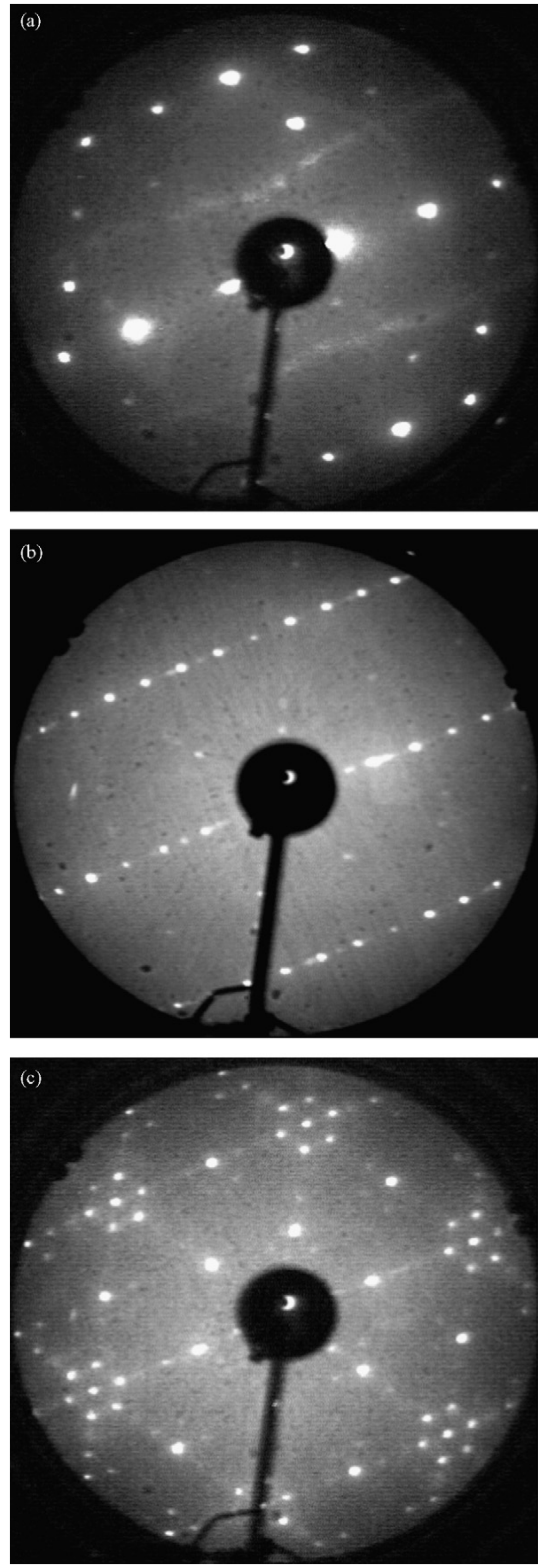


**Fig. 1.** Representative LEED patterns of the (a) 3 × 1-Ba, (b) 5 × 1-Ba, and (c) 2 × 8-Ba surfaces, observed at RT. Note that very weak half-order streaks are visible in the LEED of the 3 × 1.