

## Surface Structures of GaAs(001) with Selenium Adsorbate Studied by Scanning Tunneling Microscopy

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Under the low chemical potential condition, new structures other than the 2x1 and 2x3 structures were found on the Se-treated GaAs(001) surface. These structures consist of elliptical protrusions with 0.6 nm periodicity in the [110] direction, similarly to the STM images obtained for the 2x3 surface. Their axes, however, are in directions different from [110].

In the study of the initial growth of CdTe films on the GaAs(001) surface, Feldman and Austin found a new structure with  $\sqrt{3} \times \sqrt{3}$  periodicity [1]. Atomic orientation direction of the surface was found to be different from the crystal axis; however, the atomic structure has not been elucidated to date.

Recently, by means of state-of-the-art total energy calculation [2], attractive interaction between the As dimers and relaxation of the As dimer block were shown to be essential to the stability of the As-rich GaAs(001) surface. On the other hand, adjacent chalcogen dimers of the passivated GaAs(001) surface are expected to interact repulsively due to the excess electrons, one electron per dimer, and dimer reconstruction differing from that on the surface of As/GaAs(001) is expected. Stability of the 2x1 chalcogen dimer structures commonly appearing on the chalcogen-treated surfaces [3] is a possible result of the repulsive interaction.

Therefore, in addition to the clarification of the passivation mechanism, an understanding of the surface stabilization mechanism of chalcogen-passivated compound semiconductor surfaces is very important from both fundamental and practical points of view. Among the chalcogen passivated GaAs(001) surfaces, the Se/GaAs(001) structure is the most interesting because the atomic radius of Se

is closest to that of As.

Under the low chemical potential condition, new structures other than the 2x1 and 2x3 structures were found on the Se-treated GaAs(001) surface. These structures consist of elliptical protrusions with 0.6 nm periodicity in the [110] direction, similarly to the STM images obtained for the 2x3 surface [3]. Their axes, however, are in directions different from [110], which is similar to the structure of the  $\sqrt{3} \times \sqrt{3}$  structure observed for the Te/GaAs(001) surface [1, 4]. In this paper, we report the newly observed atomic structure for the Se-treated GaAs(001) surface using scanning tunneling microscopy (STM).

GaAs(001) surfaces, oriented to within 0.5 degrees of the [001] direction and Si-doped at a dose of  $\sim 1 \times 10^{18} \text{ cm}^{-3}$ , were prepared by thermal cleaning. After observation of the 4x2 RHEED pattern, selenium of up to 100-300 nm thickness was evaporated onto the GaAs(001) surface at room temperature. Then, the samples were flash-heated under RHEED observation. The back-pressure was kept lower than  $\sim 1 \times 10^{-10}$  Torr throughout the heat treatment in order to suppress the readsorption of desorbed Se atoms. Thereby, 2x3 RHEED pattern was obtained by lower-temperature heat treatment around  $\sim 400$  to  $\sim 500$  °C and was stable even after the samples were cooled.

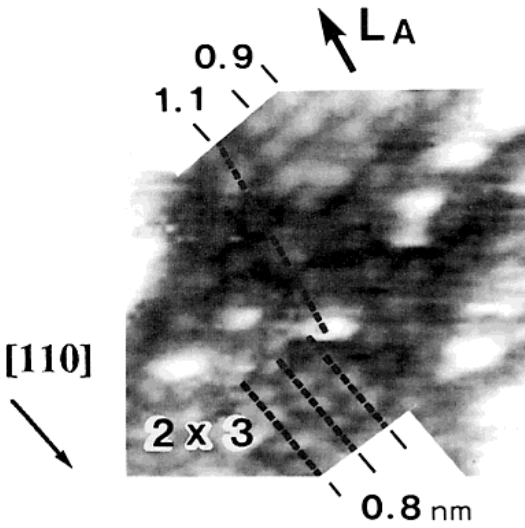


Figure 1. STM image of Se/GaAs(001) where the 2x3 structure and a new structure with axis  $L_A$  exist.

Figure 1 shows an STM image of the Se-passivated surface treated at  $\sim 500^\circ\text{C}$ . The sample bias was  $-2.0$  eV. STM imaging was performed in the constant-current mode (setting current:  $I_s = 20$  pA). In addition to the 2x3 structure, a domain with a different structure, the axis of which is indicated by  $L_A$ , is shown in the figure. Figure 2 shows two

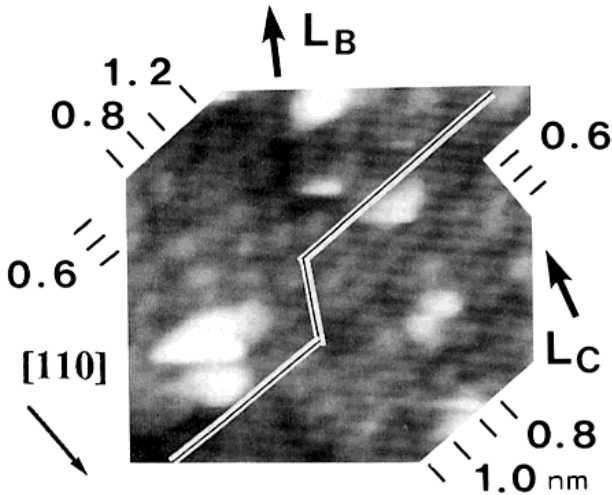


Figure 2. STM image of Se/GaAs(001) surface consisting of two domains with axes  $L_B$  and  $L_C$ .

other domains with different structures observed on the surface. Here, two different structures, the axes of which are indicated by  $L_B$  and  $L_C$ , are shown.

Since As dimer interaction is an attractive one and surface reconstructions occur at the 2x4 As dimer units [2], symmetric structures observed along the dimer row axes are thought to be caused by the repulsive interaction between the Se dimers due to the excess electrons remaining on the Se dimers. These structures were then analyzed by reconstructions of dimers with repulsive interaction. A model to explain the structure in Fig. 1 is shown in Fig. 3, where the label of  $L_{4.5}$  represents the

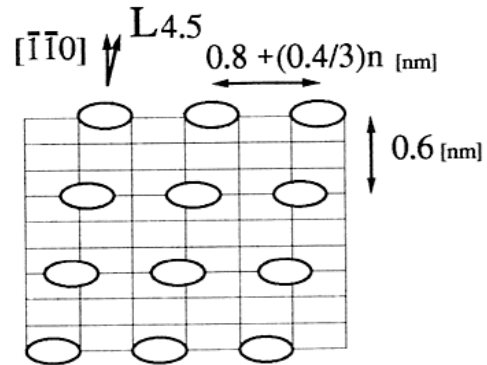


Figure 3. Structural model for the Se/GaAs(001) surface observed in Fig. 1.

orientation angle of dimers from the  $[\bar{1}10]$  direction;  $\theta = \tan^{-1}(4.5)$ . Observed distances between the dimer rows agreed well with the values for the model. Similar agreements were obtained for the structures shown in Fig. 2 by the models of  $L_B=L_{1.5}$  and  $L_C=L_3$ .

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