CONTROL OF SEMICONDUCTOR INTERFACES
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Dimer Model for Comprehensive Interpretation of Selenium-Passivated GaAs(001) Surface Structures

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A mechanism to explain Ga_2Se_3-like structural formation on a selenium treated GaAs(001) surface was proposed through the analysis of the selenium-treated GaAs(001)-2x3 surface by scanning tunneling microscopy, where ordered 1/3 ML Ga vacancies in the second layer and replacement of As atoms in the third layer can be introduced through the phase transition between 2x1 and 2x3 structures upon heat treatment.

Since S/Se treatments are beneficial to the structural and electronic properties of compound semiconductors, they have been considered to be one of the most promising techniques for the atomic control of compound semiconductor surfaces and interfaces [1]. The dimer model has been successfully used to explain many experimental results; however, recently, the Se-treated surface has been found to have a more complicated structure: Ga_2Se_3-like structure with ordered Ga vacancies [2]. On the other hand, upon heat treatment, a 2x3 structure was observed at higher temperature, and changed reversiblly into the 2x1 structure when the samples were cooled again [3]. Change in the number of Ga vacancies during the heat treatment is also revealed by photoemission study [3]. Therefore, from the standpoint that the Ga_2Se_3 structure is formed from the original 2x1 dimer structure through phase transition upon heat treatment, the Se-treated GaAs(001)-2x3 surface was studied using scanning tunneling microscopy (STM).

GaAs(001)-2x4 and 4x2 surfaces show a similar 2x1 diffraction pattern after Se treatment. As-rich 2x4 surface may give a flatter surface, however, As atoms in the top layer are easily replaced by Se atoms, and are considered not to affect the structural formation. Therefore, in order to prevent Se atoms from diffusion during heat treatment as much as possible, Se atoms were evaporated onto the thermally cleaned GaAs(001)-4x2 surface at room temperature. Then the samples were flash-heated in the STM chamber with the back pressure kept lower than $\sim 1\times10^{-10}$ Torr throughout the heat treatment in order to suppress the readsorption of desorbed Se atoms. As a result, a 2x3 RHEED pattern was obtained by lower-temperature heat treatment of around ~400 to ~500 ℃, and was stable even after

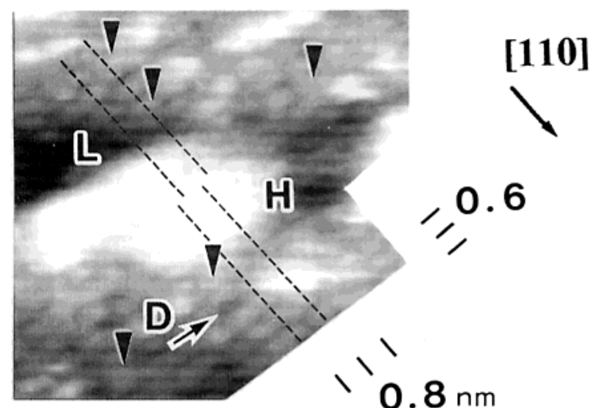

Figure 1. STM image of Se-treated GaAs(001) (V_s= - 2.0V, I_t=20pA).

the samples were cooled. When the back pressure was higher, a 2x1 pattern was observed, as expected.

Figure 1 shows an STM image taken after observation of the 2x3 RHEED pattern, where a step with two terraces indicated by H and L exists. The distance between the arrays oriented in the [110] direction is ~0.8 nm. and the axes of the rows on both terraces are shifted by about ~0.2 nm, as shown in Fig.1. The structure agrees well with the double-layered structure of the dimer model [1]. In addition to the 2x3 structure consisting of the protrusions with ~0.6 nm periodicity in the [110] direction, clusters with ~0.4 nm periodicity which correspond to the 2x1 structure were observed in some parts, as indicated in Fig. 1 by arrows. Apparent defects on the flat area consist of dimer units, as indicated in Fig. 1 by D. Some 2x1 clusters have enough space to form the 2x3 structure, as shown in Fig. 1, around the defect D, which suggests the existence of some potential barrier for the structural change from 2x1 to 2x3. A possible model for the 2x3 structure is shown in Fig. 2(a). Here, Ga atoms form dimers in the second layer following Se-dimer desorption. The Ga-Se bonds on the other sides of the Ga dimers, indicated by dashed lines in Fig. 2(a), tend to

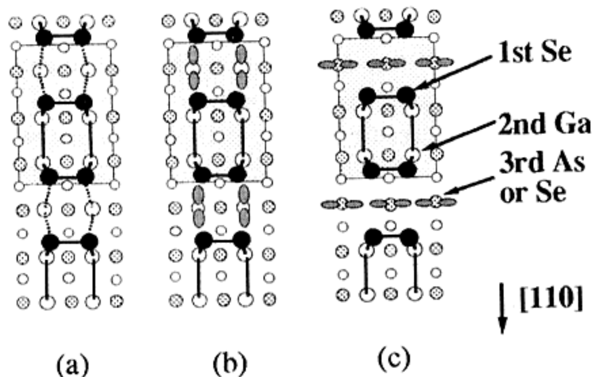

Figure 2. Structural models of the Se/GaAs(001)-2x3 surface.

break because of the excess electrons existing in the antibonding state, and the structure is expected to be stabilized by the transfer of these excess electrons into the Ga dangling bond states produced by bond breaking (Fig.2(b)). Such charge transfer explains the Se 3d core level shifts appearing in the 2x1 and 2x3 structures well [3]. In this model, some Ga atoms in the second layer are exposed to the atmosphere, therefore, if samples are heated at higher temperatures, the removal of the arranged Ga atoms, 1/3 ML at maximum, becomes possible without disturbing the structure (Fig. 2(c)), the amount of

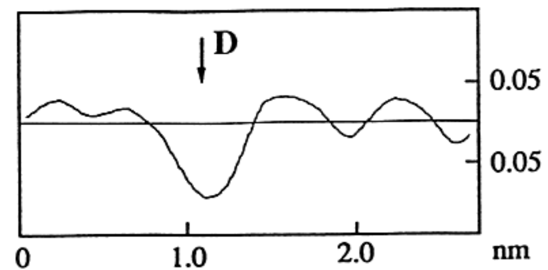

Figure 3. Cross section of the Se defect D shown in Fig. 1.

which is close to the value obtained from the analysis of the photoemission spectra (1/4ML) [2]. Since the 2x1 clusters still remained after the samples were flash-heated, the phase transition possibly remains at the initial step, as shown in Fig. 2(a). Actually, corrugations at the defects are ~ 0.15 nm, as shown in Fig. 3 for defect D, which is close to the height of one GaAs (001) layer. When As atoms in the underlayer are replaced by Se atoms following Ga atom desorption (Fig. 2(c)), the surface becomes closer to the Ga_2Se_3-like structure which has been proposed in recently [2].

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REFERENCES

1. M. Katayama, M. Aono, H. Oigawa, Y.Nannichi, H. Sugahara and M. Oshima, Jpn. J. Appl. Phys., 30 (1991) L786.
2. S. Takatani, T. Kikawa and M. Nakazawa, Phys. Rev. B, 45, (1992) 8498.
(1992) 181.
3. F. Maeda, Y. Watanabe, T. Scimeca and M. Oshima, Phys. Rev. B, 48, 4956 (1993).