Extended Abstracts of the 21st Conference on Solid State Devices and Materials, Tokyo, 1989, pp. 497-500

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Semiconductor Interface and Surface Structure Studies by Means of Grazing Incidence X-Ray Diffraction

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Surface superstructures (reconstructed structures) have been observed by many techniques. However, it was not easy to confirm that a superstructure does exist at an interface between two solid layers. This paper reports a direct observation of superstructures at the interface by grazing incidence X-ray diffraction with use of a synchrotron radiation. Firstly, we describe a design of a MBE apparatus for in-situ grazing incidence X-ray diffraction studies and show in-situ studies of a structure change from the surface 7x7 structure of the Si(111) to the interface 7x7 structure of the a-Si/Si(111). Secondly, the observation of superstructures at metal/semiconductor interfaces has been performed and the relation between the interface structures and Schottky-barrier heights will be discussed.

1. Introduction

There are many observations of superstructure (reconstructed structures) on semiconductor or metal surfaces. These superstructures are mostly believed to exist only on a clean surface fabricated under the condition of ultra high vacuum. Recently, however, superstrucures have been successfully observed at interfaces by means of transmission electron diffraction (TED) [1] and grazing incidence X-ray diffraction (GID) [2,3]. Almost all techniques for surface studies , such as low energy electron diffraction (LEED), reflected high-energy electron diffraction (RHEED) and scanning tunneling microscopy (STM) are not applicable to study buried interface structures. However, the technique of grazing incidence X-ray diffraction with use of a synchrotron radiation has much power for studying a buried interface structure. From technological and scientific points of view, the investigation of the interface structure is very important not only to understand the electronic properties of semiconducting materials, but also to develop new electronic devices.

Firstly, we describe a design of a MBE apparatus for in-situ grazing incidence X-ray diffraction studies and show in-situ studies of a structure change from the Si(111)-7x7 surface structure to the a-Si/Si(111)-7x7 interface structure. Secondly, we will show superstructures at the Yb/ GaAs(100) interface and will discuss the interface structure in relation to Schottky-barrier formation.

2. In-situ grazing incidence X-ray diffraction [4]

A molecular beam epitaxy (MBE) technique, for example, has become one of the popular techniques to grow and control the sophisticated materials. We constructed a MBE apparatus for in-situ grazing incidence X-ray diffraction studies.

Figure 1 shows an overview of the apparatus. In our work, a sample (5) is mounted horizontally, and then the surface normal is nearly perpendicular to the X-ray polarization direction. In this geometry, a large active sample area is irradiated because of the shape of the incident synchrotron X-rays at BL-9C of the Photon Factory, National Laboratory for

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High Energy Physics. This geometry also allows that the entire UHV chamber (318.5 mm in diameter and 300 kgw) is rotated simply with using a spring (26) of constant force (200 kgw) without compromising precision of the diffractometer (10,12). The UHV chamber is placed on a vertical two-axis goniometer (12). A two-theta arm (13) is used for moving the counter (9). The two-axis goniometer (12) is set on a horizontal one-axis goniometer (10) for adjusting the grazing incidence angle. These goniometers (10,12) and the UHV chamber are installed on the Z-table (11), which can be moved along a vertical direction. Two 200 μm thick Be windows (4) are located on the chamber walls for the incident beam. The diffracted beam is collected by a scintilation counter (9) through the Be window (7) and the 0.17° Soller slits (8). By the combination of three Be windows, two-theta angle can be changed from 0° to 126° without any blind angles. The sample, which can be heated up to 1000 ℃ by a Ta heater (6), is mounted on the top of the rotating manupilator (17) with a precisely tilting mechanism (14). The chamber is equipped with the RHEED apparatus (24). For the crystal growth or evaporation, two 2cc PBN Knudsen cells (21) and two E-gun evaporation sources (22) are prepared so as to make in-situ X-ray diffraction measurements without changing the sample position. The sample is transferred by the magnetic transfer rod (25) from a preparation chamber (20). The base pressure in the MBE chamber is 2×10^{-10} Torr.

Using this apparatus, a chemically pre-cleaned (111)Si wafer was heated up at 850 ℃, on which we observed the 7x7 superstructure by RHEED and X-ray diffraction. Fig. 2(a) shows the observed diffraction intensities of clean 7x7 surface. The diagram (Fig. 2(a)) illustrating the observed intensity distribution has a resemblance to that observed by TED [8]. Subsequently, in the same chamber without changing the sample position, a-Si layer of 10 nm in thickness was deposited on the sample. Fig. 2(b) shows the observed diffraction in-

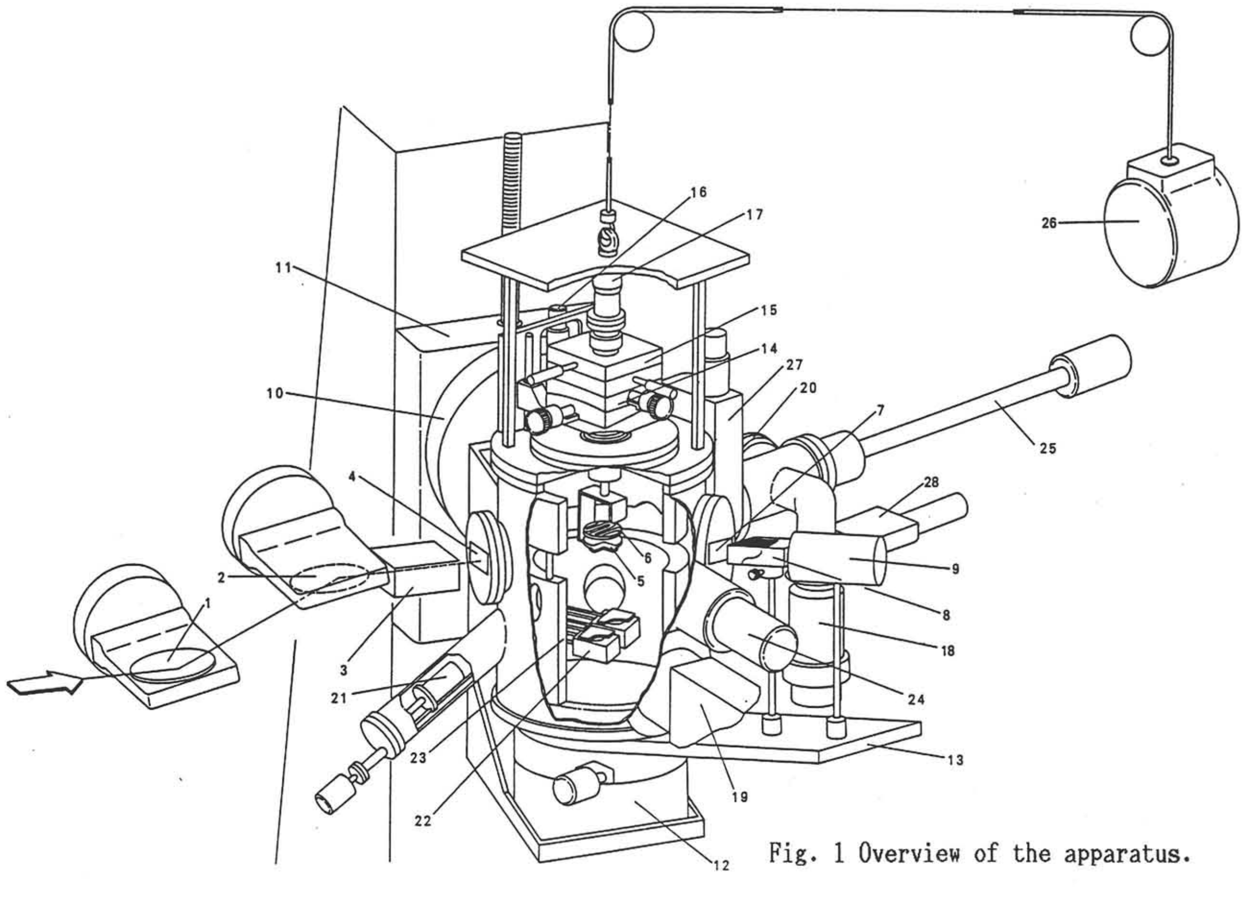

Fig. 1 Overview of the apparatus.

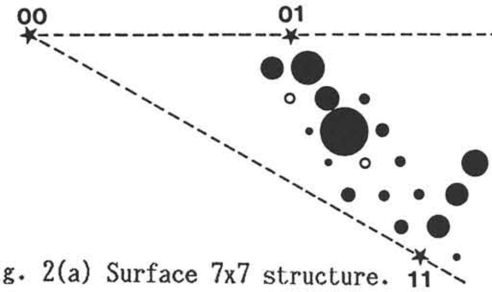

Fig. 2(a) Surface 7x7 structure.

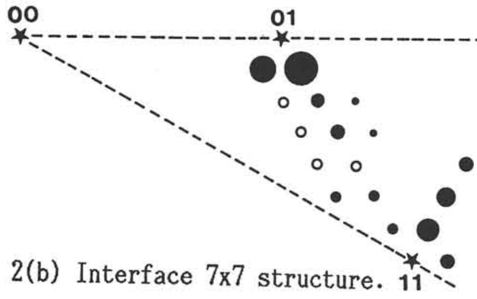

Fig. 2(b) Interface 7x7 structure.

tensities of interface 7x7 structure. Since the intensity of the (3/7 1) peak is weak in comparison with that in the surface 7x7 structure, it is suggested that the deposition of a-Si results in destroying the perodic order of adatoms in the DAS model [5]. The diagram illustrating the observed intensity distribution has a resemblance to that calculated from the stacking-fault structure in the DAS model. This may suggest that the ordering of amorphous layers occurs on the top of the stacking-fault layers and the interface structure results in emphasizing stacking-fault layers.

3. Superstructures of metal/semiconductor interfaces [6]

A metal/semiconductor contact has been extensively studied due to both technological and scientific interest for over thirty years. Above all, the atomic structure at the interface and the mechanism for Schottky-barrier formation are current topics. It was not until a couple of years ago that the atomic structure at a buried interface was directly observed for the metal/semiconductor systems. It was significant that the superstructure was found at the Al/GaAs interface [7]. This result indicated the possibility that the relation between local electronic and structural properties would be clarified, even for conventional polycrystalline-metal/GaAs interfaces, similarly for an single-crystalline-metal/semiconductor interfaces. On the other hand, the anomalous Schottky-barrier height changes were found for metal/GaAs contacts by inserting a chalcogen interlayer and a rare-earth metal interlayer [8]. These observations indicated the importance of understanding the stage at which Schottky-barrier height was definitely determined during the interface evolution for various kinds of interfaces. This paper reports the existence of a super-strucutre at the Yb/GaAs interface observed by grazing incidence X-ray diffraction with use of a synchrotron radiation and the Schottky-barrier height difference for the interfaces with different atomic structures.

The sample structure used in this study consists of a 9 nm thick Al cap layer, a very thin Yb interlayer and (100) Si doped GaAs epitaxial layer. Two kinds of samples were prepared for the present study; one had a 0.3 nm thick Yb interlayer (sample A), while the other had a 2 nm thick Yb interlayer (sample B) and then Al were subsequently deposited at 30 °C in an MBE growth chamber, after a 4x6 surface-superstrucutre was confirmed on the GaAs epitaxial layer surface by RHEED.

Grazing incidence X-ray diffraction measurements revealed that the interface between Yb and GaAs(100) has a 4x1 superstructure and that the two diffraction patterns are obviously different from each other as shown in Fig. 3(a) and (b). Fig. 4(a) and (b) show the partial pair-correlation function (partial Patterson map) calculated from the obseved structure factors for fractional order reflection for sample A and B, respectively. The difference between the two pair-correlation maps appears mainly in the center peak of 4x1 lattice in Fig. 4(b). Because this intensity is very high, the pair correlation

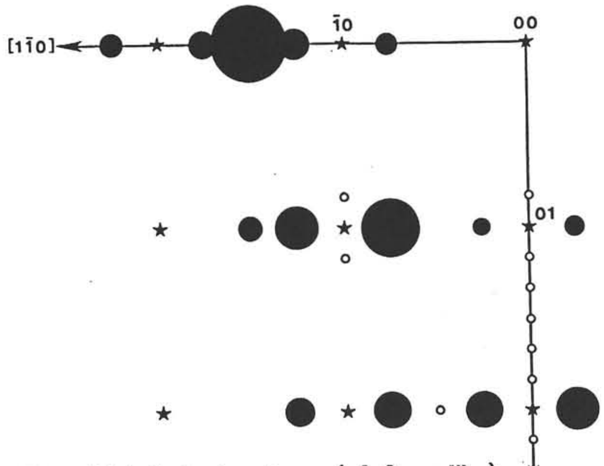

Fig. 3(a) 1x4 structure (0.3 nm Yb).

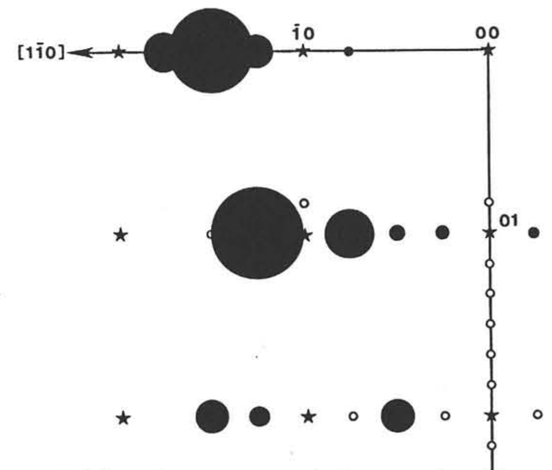

Fig. 3(b) 1x4 structure (2 nm Yb).

comes from the correlation between the Yb atom (with a large atomic structure factor) and any other atoms. Therefore, it can be said that the sample B has a new kind of ordered Yb structure which the sample A does not have. From I-V measurements, Schottky-barrier height of the sample A is 0.75 eV and that of the sample B is 0.84 eV. Ideality factor is 1.06 for the sample A and 1.07 for the sample B. From C-V measurements, Schottky-barrier height of the sample A is 0.76 eV and that of the sample B is 0.82 eV. Note that the Schottky-barrier height value for the sample B becomes larger than that for the sample A by about 80 meV. This observation leads us to the important conclusion that Schottky-barrier height is finally determined upon completion of metallization at a certain specific thickness and that the polycrystalline-metal/semiconductor interface is sufficiently homogeneous

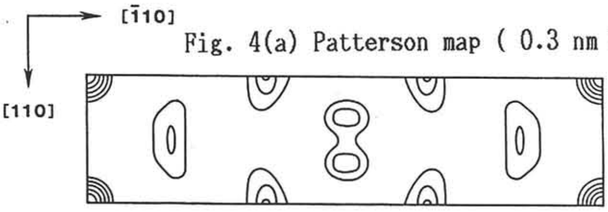

Fig. 4(a) Patterson map (0.3 nm Yb).

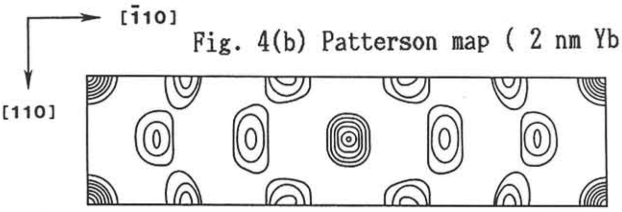

Fig. 4(b) Patterson map (2 nm Yb).

for Schottky-barrier height to reflect the interfacial superstructure difference.

4. Conclusions

It was shown that superstructures exist at several kinds of interfaces by employing the technique of grazing incidence X-ray diffraction with use of a synchrotron radiation. These results give information about the atomic structure at the interface. These interfacial superstructures may enhance our understanding and controlling of electronic properties, such as, Schottky-barrier height.

Acknowledgements

The authors would like to thank Drs. K.Hirose, T.Mizutani for the experimental cooperation at the Yb/GaAs system.

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