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Microstructure and Schottky-barrier height of the Yb/GaAs interface

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Different interfacial structures are found for Yb/GaAs(001) contacts with different Yb thicknesses, namely 3 and 20 Å, by grazing-incidence x-ray diffraction with the use of synchrotron radiation. Different Schottky-barrier height values are also found for these samples. It is concluded that the metal-semiconductor contact, accompanied by reaction and diffusion, is homogeneous in the vicinity of the interface and that the Schottky-barrier height is not finally determined at the initial stage of interface formation for this system.

Metal-semiconductor contact has been extensively studied because of both technological and scientific interest for over thirty years. In particular, the atomic structure at the interface and the mechanism for Schottky-barrier formation are current topics. The atomic structure at a buried interface was directly observed for metal-semiconductor systems only recently.[1-3] The superstructure was found at the Al/GaAs (Ref. 3) interface and also at a-Si/Si$_{1-x}$Ge$_x$ interfaces.[4,5] This result indicated the possibility that the relation between local electronic and structural properties would be clarified, even for conventional polycrystalline-metal–GaAs interfaces, and also for a single-crystalline-metal–semiconductor interface.[6] Although it seems that a few models, such as the unified defect model[7] (UDM) and the metal-induced gap states (MIGS) model,[8,9] can explain a number of the experimental results for Schottky-barrier height (SBH), new observations have appeared which are not explicitly included in these models. Anomalous SBH changes were found for metal-GaAs contacts by inserting a chalcogen interlayer[10] and a rare-earth metal interlayer.[11] For contacts involving transition metals, peculiar SBH dependence on the physical properties, compared to other contacts, was considered to be due to rehybridization between the transition-metal d band and either the Si or the GaAs sp band.[12,13] These observations indicated the importance of understanding the stage at which the SBH was definitely determined during interface evolution for various kinds of interfaces.

This paper shows the existence of different superstructures at Yb/GaAs interfaces observed by x-ray diffraction, by use of synchrotron radiation, and the SBH difference for interfaces with different atomic structures. It is concluded that the metal-semiconductor contact accompanied by reaction and diffusion is homogeneous in the vicinity of the interface and that the Schottky-barrier height is not finally determined at the initial stage of interface formation for this system. Also, these results will be discussed in connection with some SBH models.

The sample structure used in this study consists of a 90-Å thick Al cap layer, a very thin Yb interlayer, and a 0.7-μm thick Si-doped (2×10^{17} cm^{-3}) GaAs epitaxial layer. Two kinds of samples were prepared for the present study: One had a 3-Å thick Yb interlayer (sample A), while the other had a 20-Å thick Yb interlayer (sample B). The epitaxial layer was grown under As-stabilized conditions at 600 °C on (001) Si-doped n^+-type GaAs substrates by the molecular-beam epitaxy (MBE) technique. Yb and then Al were sequentially deposited at 30 °C in an MBE growth chamber, after a 4×6 surface superstructure was confirmed on the GaAs epitaxial layer surface by reflection high-energy electron diffraction. Detailed sample preparation for MBE growth was previously reported.[3] Finally, the sample temperatures were raised to about 170 °C to melt the In solder holding the samples on the sample holders. This temperature is well below that where AlAs formation or enhanced interdiffusion occurs.[14]

The interface atomic structure was studied using a grazing-incidence x-ray-diffraction (GID) technique. The experiment was carried out with synchrotron radiation at beamline 9C, installed at the Photon Factory in Tsukuba, Japan. The 1.5-Å wavelength x ray was impinged on the sample with the 0.3° grazing incidence angle. The detailed experimental geometry was given in a previous report.[5]

In order to measure SBH, diodes 500 μm in diameter were defined after Au-Ti deposition in another deposition chamber. SBH's were carefully determined from both I-V and C-V measurements. SBH's from the saturation current density (J_0) for I-V curves, SBH(I-V), were determined, taking into account the image-force lowering and the tunneling current.[11,15] SBH's from the intercept voltage (V_D) for $(1/C^2)$-V curves, SBH(C-V), were determined, taking into account Fermi energy and the correction-for-depletion approximation.[11,15] Ohmic contacts were made with In solder at the back surface of the substrates.

GID measurements revealed that the interface between Yb and GaAs(001) has a 4×1 superstructure (Fig. 1). Figure 1(a) shows the 4×1 superstructure for sample A with 3-Å thick Yb. Figure 1(b) shows that for sample B with 20-Å thick Yb. The two diffraction patterns are obviously different from each other. We refer to $(1\bar{1}0)$ and (110) indices, as $(\bar{1}0)$ and (01), respectively. The star marks show the fundamental-lattice points [(10), (01), etc.]. The radius of the filled circles were defined as being proportional to the observed structure factor with the correction for the polarization, Lorentz factor, and the variation of the active sample area. At the reciprocal-

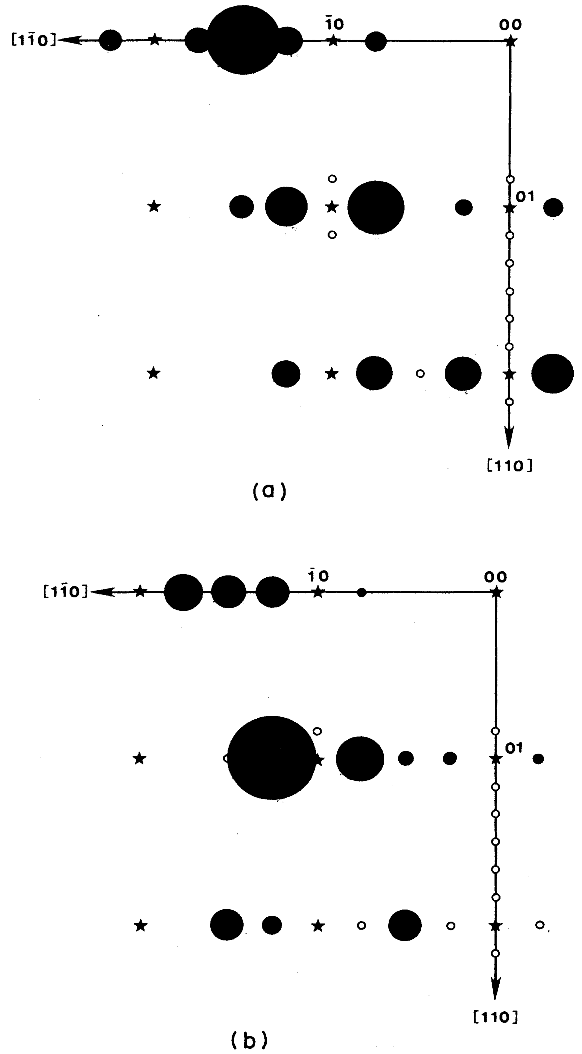

FIG. 1. Observed structure factors from the 4×1 superstructures at the interfaces between Yb and GaAs(001). Before the Yb deposition, 4×6 superstructures were confirmed on the GaAs surfaces. The radius of each filled circle is proportional to the observed structure factor. At the reciprocal-lattice points indicated by open circles, no diffraction peaks were observed. Star marks are the fundamental lattice points. (a) Sample *A* with 3-Å thick Yb, and (b) sample *B* with 20-Å thick Yb.

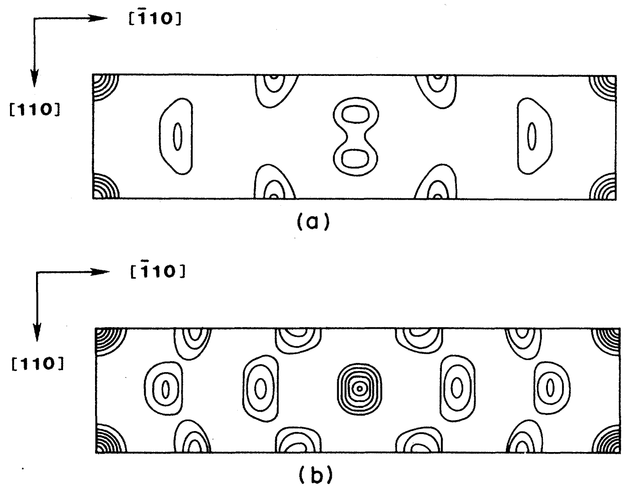

FIG. 2. Partial-pair-correlation function (partial Patterson function) calculated from the observed structure factors for fractional-order reflections in Fig. 1. Positive contour levels above zero are shown. (a) Sample *A* with 3-Å thick Yb, and (b) sample *B* with 20-Å thick Yb.

lattice points indicated by the open circles, no diffraction peaks were observed. Figures 2(a) and 2(b) show the partial pair-correlation function (partial Patterson function)[16] calculated from the observed structure factors for fractional-order reflections in Figs. 1(a) and 1(b), respectively. The difference between the two pair-correlation maps appears mainly in the center peak of the 4×1 lattice in Fig. 2(b). Because this peak intensity is very high, this pair-correlation comes from the correlation between the Yb atom (with a large atomic structure factor) and any other atoms. Therefore, it can be said that sample *B* has a new kind of ordered Yb structure which sample *A* does not have.

Table I summarizes the SBH(I-V), ideality factor (n) determined from I-V measurements and SBH(C-V), carrier concentration (N_D) determined from C-V measurements. Since SBH(I-V) and SBH(C-V) are consistent with each other and since the n values which represent the ideality in I-V characteristics are close to unity (≤ 1.07), these data are sufficiently reliable. SBH's for sample *A* are 0.75–0.76 eV. These are much smaller than those for ideal rare-earth metal/n-GaAs contacts (0.84–0.87 eV) in our previous work[11] as well as those for ideal Al/n-GaAs contacts (0.85–0.86 eV) which we have recently measured under the same condition (in Table I). In other words, the SBH for sample *A* is not an averaged value of those for the two ideal contacts. This means that the measured SBH value is not simply explained by diodes aligned in parallel, consisting of Al/GaAs and Yb/GaAs contacts.[11] This feature seems to be anomalous, because the interface contains only the Al/GaAs contact, if any, except for the Yb/GaAs contact. On the other hand, SBH values for sample *B* are 0.82–0.84 eV, which are close to those for ideal rare-earth-metal/n-GaAs contacts. Note that the SBH value for sample *B* becomes larger than that for sample *A* by about 80 meV.

The present structural study shows that the interfacial superstructures preserved at Yb/GaAs interfaces are quite different from those observed at the Al/GaAs interface.[3] Especially, the 1×6 superstructure observed for the Al/GaAs interface is not found. Therefore, monolayer thick Yb in sample *A* is considered to cover almost all the GaAs surface. The present result excludes the possibility of the presence of large Al domain contacted with GaAs, or Schottky diodes aligned in parallel, consisting of Yb/GaAs and Al/GaAs contacts, for sample *A*. This result for the structural study is in good agreement with the above result on the SBH measurement for sample *A*.

Note that the interfacial structure observed for sample *B* is clearly different from that for sample *A*, although they were the same in diffraction pattern symmetry. That

TABLE I. Electronic properties for Yb/GaAs(001) contacts. Schottky-barrier heights (SBH's) were determined taking into account the image force lowering and the tunneling current for *I-V* measurement. The effective Richardson's constant is 8.6×10^4 A m^{-2}K^{-2}. The experimental error is estimated to be 0.01 eV. The measured SBH for Al/(4×6)GaAs contact is also listed as a reference.

Sample	Yb thickness (Å)	Ideality factor n	SBH I-V (eV)	SBH C-V (eV)	Carrier concentration N_D (cm^{-3})
A	3	1.06	0.75	0.76	2.24×10^{17}
B	20	1.07	0.84	0.82	2.44×10^{17}
Al/(4×6)GaAs	0	1.04	0.86	0.85	1.22×10^{17}

is, sample *B* had a new kind of ordered Yb structure which sample *A* did not have. This is considered to be attributed to interface evolution, including Yb arsenide formation and Ga outdiffusion.[17] Besides, the assumed alloy formation between overlayer Al and Yb is also considered to be responsible for the difference. Thus, the present result tells us that the atomic structure at the Yb/GaAs interface was stable enough not to be completely disrupted, although it was not sufficiently stable to be unchanged when exposed to the reactions and diffusions mentioned above.

It is observed that SBH values differ between Yb/GaAs interfaces with different interfacial superstructures caused by different Yb thicknesses. That is, the SBH increased by 80 meV due to a slight increase in Yb interlayer thickness from 3 to 20 Å with interfacial structure changes. Together with the above discussions on the interfacial structure, this observation leads us to the important conclusion that SBH is not finally determined at the initial stage of interface formation for this system. This conclusion is in contrast to the UDM emphasis on the evidence that the SBH is already fixed within monolayer coverage independent of the adsorbed metal species. On the contrary, this conclusion seems consistent with the MIGS model, which says that the SBH is finally determined at the stage where the metal shows complete metallicity at no more than 20 Å (3–9 Å) for rare-earth metal on GaAs(110).[17,18] However, it will be worthwhile to try to reconcile the observed SBH difference with both of the models, by closer investigation of the actual interface evolution. The SBH change would be explained either by a change in defect state energy distribution during the interface evolution or by a change in the contract metal and/or the chemisorption sites during the interface evolution, within a UDM (Ref. 7) or MIGS model framework,[9] respectively.

In summary, the superstructures and Schottky barrier height values were measured for Yb/GaAs contacts with different Yb thicknesses, namely 3 and 20 Å. Different interfacial structures and SBH values were found for the two kinds of contacts. It was concluded that the ordinary metal-semiconductor contact accompanied with reactions and diffusions was sufficiently homogeneous in the vicinity of the interface and that the SBH was not finally determined at the initial stage of interface formation. The basic concept for the Schottky barrier formation mechanism would be given by a closer study of the stage at which the SBH is finally determined, on the basis of understanding of interfacial structures not only for single-crystalline-metal-semiconductor interfaces but also for various kinds of interfaces.

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[1] E. J. Van Loenen and J. F. Van Der Veen, in *Layered Structures, Epitaxy, and Interfaces,* edited by J. M. Gibson and L. R. Dawson, Materials Research Society Symposia Proceedings, Vol. 37 (Materials Research Society, Pittsburgh, 1985), p. 361.

[2] K. Akimoto, T. Ishikawa, T. Takahashi, and S. Kikuta, Jpn. J. Appl. Phys. **24**, 1425 (1985).

[3] J. Mizuki, K. Akimoto, I. Hirosawa, K. Hirose, T. Mizutani, and J. Matsui, J. Vac. Sci. Technol. B **6**, 31 (1988).

[4] J. M. Gibson, H. J. Gossmann, J. C. Bean, R. T. Tung, and L. C. Feldman, Phys. Rev. Lett. **56**, 355 (1986).

[5] K. Akimoto, J. Mizuki, T. Tatsumi, N. Aizaki, and J. Matsui, Surf. Sci. **183**, L297 (1987).

[6] R. T. Tung, Phys. Rev. Lett. **52**, 461 (1984).

[7] W. E. Spicer, I. Lindau, P. Skeath, and C. Y. Su, J. Vac. Sci. Technol. **17**, 1019 (1980).

[8] J. Tersoff, Phys. Rev. Lett. **52**, 465 (1984).

[9] F. Flores and C. Tejedor, J. Phys. C **20**, 145 (1987).

[10] J. R. Waldrop, Appl. Phys. Lett. **47**, 1301 (1985).

[11] K. Hirose, H. Tsuda, and T. Mizutani, J. Appl. Phys. **64**, 6575 (1988).

[12] K. Hirose, I. Ohdomari, and M. Uda, Phys. Rev. B **37**, 6929 (1988).

[13] A. B. McLean and R. H. Williams, J. Phys. C **21**, 783 (1988).

[14] G. Landgren, S. P. Svensson, and T. G. Andersson, Surf. Sci. **122**, 55 (1982).

[15] E. H. Rhoderick, *Metal-Semiconductor Contacts* (Clarendon, Oxford, 1978).

[16] K. Takayanagi, Y. Tanishiro, S. Takahashi, and M. Takahashi, Surf. Sci. **164**, 367 (1985).

[17] J. Nogami, M. D. Williams, T. Kendelewicz, I. Lindau, and W. E. Spicer, J. Vac. Sci. Technol. A **4**, 808 (1986).

[18] M. Prietsch, M. Domke, C. Laubschat, and G. Kaindl, Phys. Rev. Lett. **60**, 436 (1988).