Surface States for the GaAs(001) Surfaces Observed by Photoemission Yield Spectroscopy

K. Hirose, T. Noguchi*, A. Uchiyama*, and M. Uda*

Fundamental Research Laboratories, NEC Corporation
34 Miyukigaoka, Tsukuba, Ibaraki 305, Japan

Department of Material Science and Engineering, Waseda University
3-4-1 Ohkubo, Shinjuku, Tokyo 160, Japan

The energy distributions of the occupied surface states of GaAs(001) surfaces were measured using photoemission yield spectroscopy. The surfaces are prepared by different kinds of techniques, including molecular beam epitaxy, As decapping, and chemically etching. The surface states are found to change in both distribution and density depending on the surface preparation techniques. A great reduction in the surface states density is revealed for the surface covered with native oxide compared with the other clean surfaces.

1. Introduction

The surface state energy distribution of the GaAs (001) surface dominates the electrical and optical characteristics of devices, and so requires clarification by direct measurement. Photoemission yield spectroscopy (PYS)[1-3] is adequate for observing surface states located very near the band gap region of a GaAs (001) surface whose Fermi level is always "pinned" by surface states. There are two reasons for this: one is that the resolution is limited only by the monochromator used for the measurements. Resolutions down to about 0.01 eV are possible. The other is that the location of the valence band maximum (VBM) in the photoemission yield spectrum can be determined using Ballantyne's theory[4] for the photoemission yield of valence band electrons.

This paper reports the results of a PYS study on the surface states of GaAs (001) surfaces prepared by several kinds of techniques.

2. Experimental

Three kinds of samples were prepared on (001)-oriented GaAs substrates. First, the substrates were degreased, followed by slightly etching in a solution of H_2SO_4, H_2O_2, and H_2O (3.5:1:1) at 60 °C. After rinsing in a HCl solution for 1 min., the substrates were again rinsed in de-ionized water to make thin native oxide. For the first type of sample, a 3000 Å thick undoped GaAs layer was grown by molecular beam epitaxy on an n^+-type substrate at 600 °C under As-stabilized conditions. Then the sample surface was exposed to an As beam flux after growth to make a (2×4) surface superstructure. We refer to this surface as an as-grown (2×4) surface. For the second type of sample, a surface prepared by the above method was successively covered with a metallic As layer at about 0 °C. Then the sample was transferred to an analysis chamber via an ultrahigh vacuum transfer chamber. A (2×4) surface superstructure was prepared in the analysis chamber by removing the As layers at 487 °C. We refer to this surface as a (2×4) surface. For the third type of sample, an as-chemically treated semi-insulating substrate was used. We refer to this surface as a chemically etched surface.

Samples were illuminated by monochromatic light (hν from 3.4 to 6.2 eV) produced by the emission of a deuterium lamp passed through a monochromator. The energy distribution curves (EDCs) were measured by an energy analyzer at 0.01 eV intervals of photon energy. The measured photoelectrons were emitted only from the GaAs layer not from the thin oxide over layer even for the chemically etched surface in this photon energy range, because the oxide induced levels are deep in energy for the valence band of GaAs.[5-7] The total photoemission current was determined by integrating the EDC. The photoemission yield Y(hν) was given by the total photoemission current divided by the photon intensity as measured independently by a calibrated photo diode.

Let the increase in Y(hν) resulting from the increase dhν in photon energy be Y(hν + dhν). Then Y(hν + dhν)-Y(hν) corresponds to the contribution of the states located from hν to hν + dhν below the vacuum level. Making the usual assumption that transition matrix elements and escape probability are constant in the small energy range explored, the derivatives dY(hν)/d(hν) give the effective density of occupied states N(E) within the escape depth of photoelectrons. These derivatives are calculated from the measured photoemission yield spectrum.

Next, the effective density of surface states was obtained by subtracting the effective density of bulk states from the effective density of occupied states. The effective density of bulk states was deduced from equation (1) given by Ballantyne,[4]

$$Yb(h\nu) = \alpha(h\nu - h\nu i)^3/(h\nu)^2 \quad \text{---(1)}$$

where α is a constant and $h\nu i$ is the ionization energy of the GaAs surface. Based on this model, a formula was deduced to represent the effective density of bulk states from the derivative of Eq.(1) with respect to hν. Then the effective density of bulk states with a specific ionization energy for the GaAs surface is given by fitting the derivative of Eq.(1) to the higher-energy part of the measured effective density of occupied states.

3. Results and Discussion

Figure 1(a)-(c) are energy distributions of the effective densities of surface states (broken curves) in the band gap regions and bulk states (solid curves) for the as-grown (2×4), (2×4) and chemically etched surfaces, respectively. Here, the horizontal axes represent energies with respect to the VBM. The energy distributions of surface states are normalized in such a way that the energy distributions of the bulk states are identical for all the samples. This makes it possible to quantitatively compare the surface state energy distributions for all the surfaces.

First, a distinct change is seen in the distribution of surface states for the as-grown (2×4) and (2×4) surfaces. Although both surfaces have the same surface superstructure, one important difference is that the as-grown (2×4) surface has a higher density of surface states located between the Fermi level and the VBM than the (2×4) surface. This indicates that not all observed surface states originate from ordered surface atomic structures. Furthermore, it is thought that the surface states intrinsic to the ordered surface atomic structures exist together with surface states originating from common imperfections on the surfaces, such as domain boundaries or excess As clusters. [8,9]
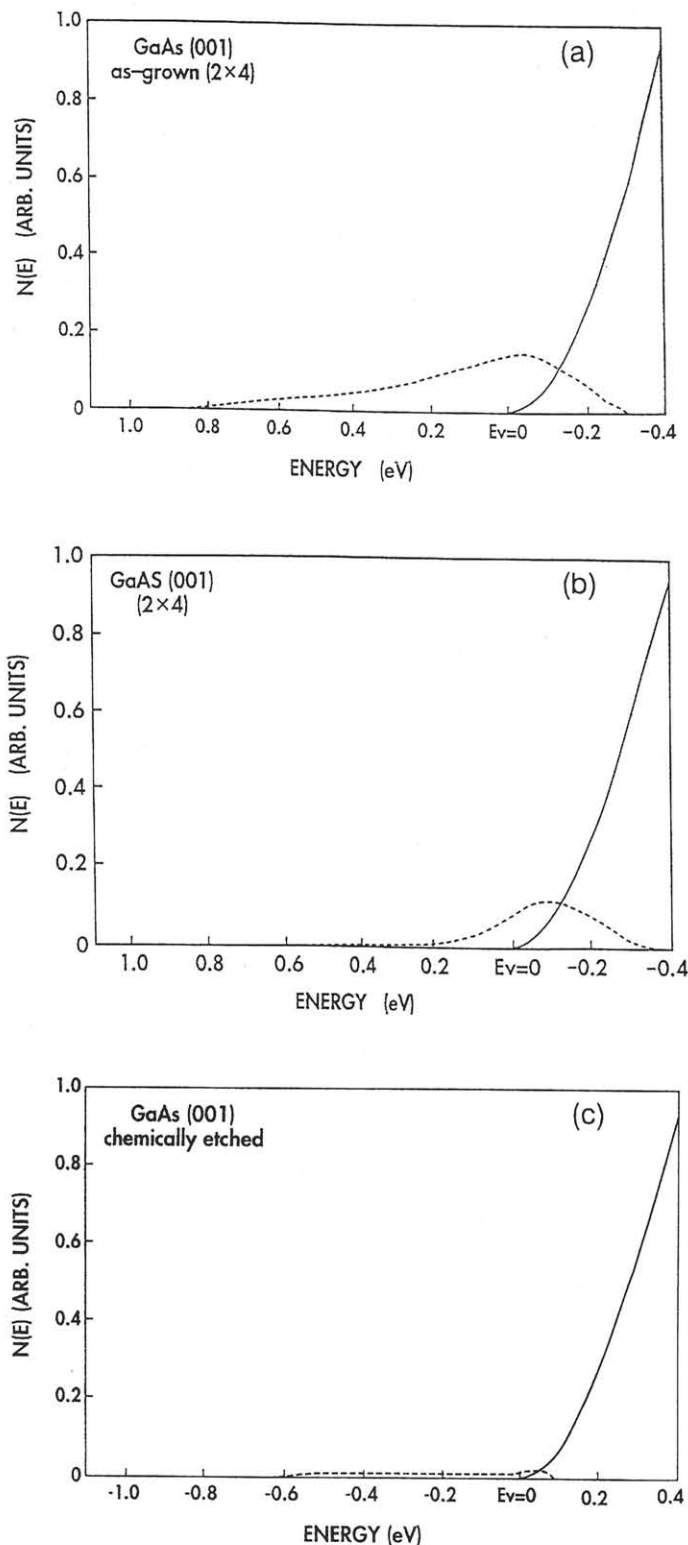

Figure 1 Effective density of surface states (broken curves) in the band gap region and bulk states (solid curves) for (a) as-grown (2×4), (b) (2×4), (c) chemically etched surfaces. Energy is shown relative to the valence band maximum.

Second, a remarkable reduction in the density of surface states is seen for the chemically etched surface compared to other clean surfaces. The reduction by about one order of magnitude was estimated from the relative areas of surface state peaks obtained for clean and chemically etched surfaces. This reduction is in good agreement with the result for oxygen adsorption on a clean GaAs surface.[5]

4. Conclusions

The surface states were found, using photoemission yield spectroscopy, to change in both distribution and density depending on the techniques used in surface preparation. A great reduction in the density of the surface states by about one order of magnitude was revealed for the surface covered with native oxide compared with the density of other clean surfaces.

Acknowledgements

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