Surface restructuring process on a Ag/Ge(001) surface studied by photoelectron spectroscopy

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Introduction

When Ag is deposited on the Ge(001) $c(4\times 2)$ surface at 100 K (LT), Ag aggregates are observed between the adjacent substrate dimer rows (LT surface) by the scanning tunneling microscopy (STM)[1]. The most stable structure of the LT surface was calculated to include Ag ad-dimers between the substrate dimer rows[2]. After the annealing at room temperature (RT), the appearance of the Ag aggregates in STM image significantly changes; the internal protrusions in the aggregate seem to coalesce and rearrange in 4×2 periodicity[1]. Recently, this restructuring process was investigated by angle-resolved photoelectron spectroscopy, and significant changes especially of the Ge dimer backbond state were reported[3]. In the present study, we have examined Ge 3d and Ag 4d core level, and valence band spectroscopy to confirm the electronic states of the LT surface and add new information to the restructuring process.

Results and Discussion

On the clean surface, Ge 3d spectrum consists of 3 surface components[4]. On the LT surface, the components of upper and lower atoms of the dimer disappeared while a new single component appeared as in Fig. 1(a). The Ge dimer back-bond state remained in the valence band spectrum. These observations are consistent with the Ag ad-dimer model in which the substrate Ge dimers are not destroyed. In the model, the charge state of the Ge atom bonded with Ag should be single species. After the RT annealing, the back-bond state was suppressed suggesting significant modification of the dimer structure during the annealing. Ge 3d spectrum slightly changed in higher binding energy region where a small another new component appeared as in Fig. 1(b, c). This suggests a charge transfer from Ge to Ag atoms during the restructuring process. A small energy shift of Ag 4d core level towards the Fermi level (not shown here) is consistent with the charge transfer. Such a rearrangement of the charge distribution was also suggested by an increase of the work function after the annealing.

References

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Fig. 1. Ge 3d core level spectra on (a) LT surface with 1 ML of Ag, (b) after the annealing at room temperature and (c) the difference between them. B, S, U, D are the components originated from the bulk, sub-surface, upper and lower dimer atoms, respectively. N, N' and A are the new components[5].