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Electronic band structure of the √21×√21 phase prepared from the Ag/Si(111)-3×1 surface

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Introduction

Surface superstructures, formed by adsorption of noble metals on Si(111), have been intensively studied. Many types of the √21×√21 structure have been reported, and their models have been examined. We can get these structures by adsorbing alkali or noble metal atoms on √3×√3 structure, formed on Si(111)-7×7 by depositing noble metal atoms, to be 1.1~1.2 ML for their total coverage.[1,2] They are thought to be a strong candidate for the two-dimensional Hume-Rothery-type electron compound, which forms the same long-range ordered phase if a ratio of electron/atom density is equal.[3] Indeed, a number of the valence electrons in the unit cell is all 3 of these similar √21×√21 structure.[4]

ARPES of √21×√21 phase

We found that when we adsorbed Ag on Si(111)-7×7 for 0.33ML to make Ag/Si(111)-3×1 and additionally deposited Au for 0.9ML, we could obtain the √21×√21 phase. We confirmed individual phases by Low Energy Electron Diffraction, LEED. Fig. 1(a) is the LEED pattern of √21×√21 phase. We can see the clear spot corresponding to √21×√21.

Figure 1(b) is gray-scale band diagram obtained from the second derivative of the smoothed spectra of angle-resolved photoelectron spectroscopy (ARPES). An energy-versus-wavenumber plot obtained by reading the peak of the spectra (b) is shown in Fig.2. A parabolic dispersion is clearly visible and it means that there exists a two-dimensional free electron system in the √21×√21 phase. In addition, Fermi energy of this phase is about 1.1 eV from the band bottom and it is higher than Fermi energy of Ag/Si(111)-√3×√3, which is 0.3 eV[5]. This means that additional adatoms have doped electrons to the surface state bands. We can also calculate the effective mass of √21×√21 phase from the fitting. Effective mass m^* is estimated as m^*/m_e=0.29±0.2. m_e is mass of free electron. It is similar value of 0.26, which is effective mass of √21×√21 phase prepared with other method[6]. Fermi wavenumber is estimated as 0.278[$Å^{-1}$] and valence electrons in the unit cell is calculated to be 3.3, which is a reasonable value compared to the previous researches.

In conclusion, we performed the ARPES measurement of the √21×√21 phase made by adding Au for 0.9ML on Ag/Si(111)-3×1. We observed the parabola band dispersion and about 3 valence electrons in the unit cell.

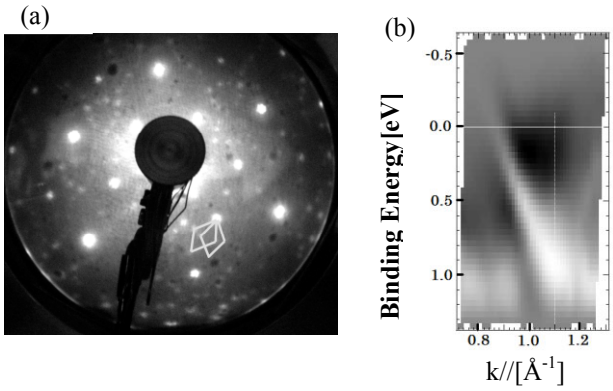

Fig. 1: (a) is LEED pattern of √21×√21 phase. Area surrounded by gray lines in (a) corresponds to √21×√21 unit cell. (b) is second derivative of ARPES spectra.

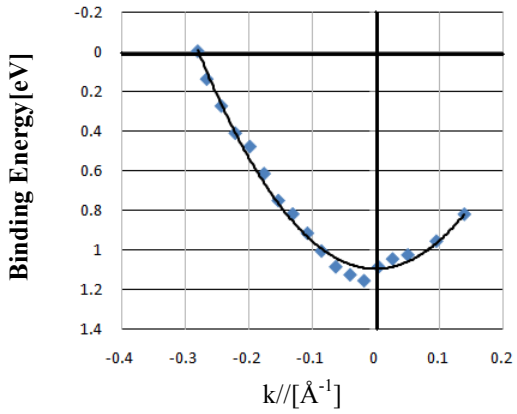

Fig. 2: Energy-versus-wavenumber plot of √21×√21 phase. Parabolic dispersion is visible, and effective mass is calculated to be m^*/m_e=0.29

References

[1] C. Liu *et al.*, Phys. Rev. B **74**, 235420 (2006).
[2] H. Jeong, *et al*., Phys. Rev. B **77**,235425 (2008).
[3]C. Kittel, Introduction to Solid State Physics, Chapter21 (Wiley, 1995).
[4]I.Matsuda *et al* . (to be published)
[5]T.Hirahara *et al.* e-J. Surf. Sci. Nanotech. Vol. 2 (2004) 141-145
[6] I.Matsuda *et al* . Phys. Rev. B **71**,235315 (2005)

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