18A/2001G204

Electronic Structure of the Interface of C_{70}/Si heterojunction

Takanori WAKITA[1], Shozo SUTO[2], Atsuo KASUYA[3], Kazuyuki SAKAMOTO[2], Daiyu KONDO[2], Taichi OKUDA[1], Ayumi HARASAWA[1], Toyohiko KINOSHITA[1]
[1]SRL-ISSP, The University of Tokyo, Kashiwanoha, Kashiwa, Chiba 277-8581, Japan
[2]Department of Physics, Tohoku University,, Sendai , 980-8578, Japan
[3]Center for Interdisciplinary Research, Tohoku University,, Sendai , 980-8578, Japan

Introduction

The adsorption of C_{60} molecules on Si(111)7x7 and Si(100)2x1 surfaces and the interaction at the interfaces have been widely studied during last decade due to the scientific interest and technological importance. A band-offset is one of the key quantities which characterize the electric and optical properties of the fullerene-semiconductor heterojunctions because it reflects the electron distribution at the interface. Nevertheless, there are few reports on the band-offsets of C_{60}/Si heterojunction [1,2], and no report on them of other fullerene/Si heterojunctions, e.g. C_{70}/Si heterojunction. In this report, we have investigated the electronic structures of the interfaces of C_{70}/Si(111)7x7 and C_{70}/Si(100)2x1 heterojunctions by photoemission spectroscopy measurements. The conduction band-offsets are estimated by using shifts of valence bands arising from deposition of K atoms.

Experimental

PES measurements were performed on the beam line 18A at PF in KEK. Commercial *n*-type Si(111) wafer, *n*-type Si(100) wafer and *p*-type Si(100) wafer were used as sample substrates. The Si(111)7x7 and Si(100)2x1 surfaces were prepared by heating the sample up to 1520 K repeatedly. The C_{70} was carefully degassed below 573K for over 24 h prior to evaporation. K atoms were deposited from the well-degassed commercial dispenser at room temperature (RT). All measurements were carried out at RT.

Results and Discussion

Figure 1(a) shows an angle-integrated photoemission spectrum of valence band of C_{70} monolayer film deposited on a Si(111)7x7 surface at RT and it's evolution after deposition of K atoms (for 1min) with a coverage at which the shift of spectra toward higher binding energy side saturates. Figure 1(b) shows the same pair of valence band spectra for C_{70} monolayer film remaining on a Si(111) surface after annealing at 670 K for 5 min. The deposition time of potassium atoms is 3 min. The photon energy is 21.2 eV and the angle of incidence of light is 45 degree. The spectra are measured at normal emission. The same measurements are performed for the samples on both *n*- and *p*-type Si(100)2x1 surfaces. Before K deposition, there is no change in the pinning positions of Fermi levels at the interfaces monitored by the binding energies of Si 2*p* core-levels. The observed shifts in valence band spectra mean that the pinning positions at the interfaces change due to the charge transfer of K 4*s* electrons to lowest

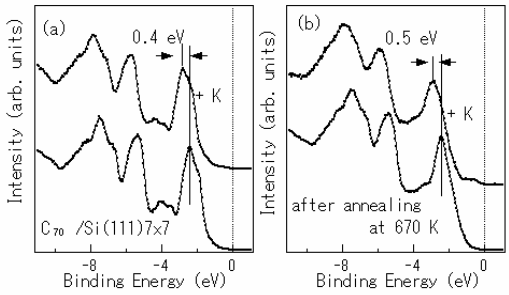

FIG. 1. (a) Angle-integrated photoemission spectrum of valence band of C_{70} monolayer film deposited on a Si(111)7x7 surface at RT and it's evolution after deposition of K atoms. (b) The same pair of valence band spectra for C_{70} monolayer film remaining on a Si(111) surface after annealing at 670 K for 5 min.

unoccupied states of C_{70} monolayer films. From the magnitudes of shifts, we can estimate the conduction band-offset of each sample. The results are summarized in table 1, where the band-offset is defined as $\Delta E_{CM} = E_{CM}(C_{70}) - E_{CM}(Si)$. From this table, it is noticed that for C_{70} monolayer films deposited on Si surfaces at RT, the band-offset depends on the Si surface orientation but not on the kinds of dopants. These results indicate that the surface states have an important role in the determination of band-offsets. After annealing at 670 K, the difference between band-offsets of Si(111) and Si(100) surfaces becomes much smaller. In this stage, the valence band spectra still preserve the features of C_{70} monolayer films but become broader. Thus, it is considered that, after annealing, the interaction between C_{70} molecules and Si surfaces becomes stronger to the extent that no decomposition of C_{70} molecules occurs, and simultaneously, the key factors in the determination of band-offsets change from the surface states to intrinsic physical features of bulk Si and C_{70}.

TABLE 1: Summary of conduction band-offsets of C_{70}/Si heterojunctions. $\Delta E_{CM}(C_{70}/Si) = E_{CM}(C_{70}) - E_{CM}(Si)$.

	Si(111)7x7	Si(100)2x1: *n*-type	Si(100)2x1: *p*-type
RT	- 0.1 eV	- 0.5 eV	-0.5 eV
670 K	0.0 eV	-0.1 eV	-0.1 eV

References

[1] K. M. Chen *et al.*, J. Phys. Condens. Matter. **7**, L201 (1995).
[2] J.-S. Zhu *et al.*, Solid State Commun. **98**, 417 (1996).
* wakita@spring8.or.jp