ARPES で実測された Si(111)ホールサブバンド準位を再現するバンド湾曲モデル

Band Bending Model Reproducing Si(111) Hole Subband Levels Measured by ARPES

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Study of subbands that form in the inversion layer (IL) of MOSFET, in particular its electronic properties, have attracted much attention since the information is important for the device applications. Subband is the formation of quantized 2D energy levels in the IL. It was reported that the IL as in the MOSFET can be obtained by adsorbing metal atoms on a clean semiconductor surface and these atoms induce band bending (BB) [1]. Subband structures form in this IL and are measured directly using angle-resolved photoelectron spectroscopy (ARPES). It has already reported that these measured subband energy levels can be reproduced by Triangle Potential Approximation (TPA) because analytical solution of the Schrödinger equation is available [2]. In the case of Pb/Si(111) IL, the measured energy levels by ARPES were consistent with the calculated levels by TPA [3]. However, it was not in the case of trivalent atoms adsorbed Si(111). Previously, a significant inconsistent results between ARPES and TPA in the case of 1ML Ga/Si (111) surface was reported. They predicted that the BB profile of Ga/Si(111) system is not like TPA [4]. Recently, our 4×1-In adsorbed on Si(111) surface also shows inconsistency with the TPA prediction. The discrepancies were found to occur within 0.2 eV to 0.3 eV [5]. This means that the BB of our system also is a special profile that cannot be approximated by a triangular potential. Therefore, in this study, subbands in the IL with an empirical band bending profile (EBBP) were determined by numerically solving the Schrödinger equation.

It was found that EBBP that best reproduce the experimental results, which has once maximum toward the surface and gradually decrease to the bulk, is Concave Potential Profile (CPP). The energy levels that quantized in the CPP were calculated and we found that the calculated energy eigenvalues from CPP consistent with the measured levels within 0.01 to 0.02 eV as shown in Fig. 1. Besides, from this calculation, the wave function of each energy levels also can be obtained. Furthermore, based on the SIMS and XPS results, the origin of CPP was believed to be the penetration of In atoms at the surface to the subsurface region of Si substrate [5], and the penetrated In atoms possibly act as acceptor at this region which contribute to the concave profile.

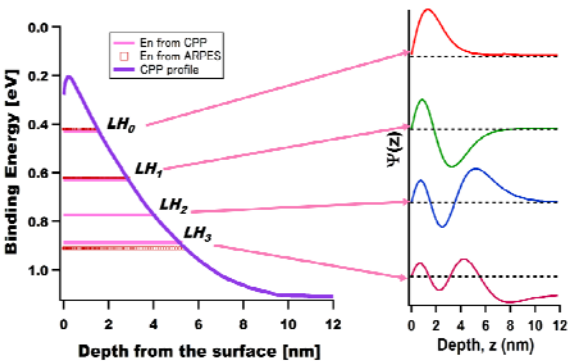

Fig. 1 Quantized energy levels in CPP and the wave function.

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[5] N. Idayu Ayob, *et al.*, *submitted.*