Molecular arrangement of ethylene on Si(001) surface by CAICISS

J.H. SEO, J.Y. PARK, C.N. WHANG, Institute of Physics and Applied Physics, Yonsei University, Seoul, 120-749, Korea, S.S. KIM, Department of Techno-marketing, Mokwon University, Taejeon, 301-729, Korea, D.S. CHOI, Department of Physics, Kangwon National University, Chuncheon, 200-701, Korea, K.H. CHAE, Division of Materials Science and Technology, KIST, Seoul, 130-791, Korea — C_{2}H_{4} molecules have been non-dissociatively chemisorbed on Si(001)-(2\times1) surface at room temperature with an exposure of 100L, and C_{2}H_{4} on Si(001) surface structure has been investigated by coaxial impact collision ion scattering spectroscopy (CAICISS). To determine the adsorption structure of the C_{2}H_{4} molecules definitely, the computer simulation with the 2-D trajectory count method has been performed for the recently proposed most possible two single molecular adsorption configurations (di-σ on-top and di-σ end-bridge). The CAICISS spectra and simulation results show that the di-σ on-top structure is better fit than the di-σ end-bridge structure. It is found that the bond length of Si dimer separation on the Si(001) surface with the adsorption of C_{2}H_{4} is 2.35 ± 0.05 Å. This implies that the bonding of Si dimers stays intact. It is also found that the bonding length of C–Si and C–C is 1.81 ± 0.05 Å and 1.61 ± 0.05 Å respectively.