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A CAICISS study of C_2H_4-chemisorbed Si(001) surface

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One-dimensional ordered structure of ethylene (C_2H_4) molecules on the Si(001) surface is investigated by coaxial impact collision ion scattering spectroscopy (CAICISS) and computer simulations. In the previous paper, the exposed 100L C_2H_4 molecules are adsorbed the di-σ on-top site of the Si(001)-(2×1) surface at room temperature (RT). Subsequently, as increasing amount of C_2H_4 molecules, we have observed the adsorption structure changes of C_2H_4 molecules on the Si(001)-(2×1) surface using low-energy electron diffraction (LEED). When 200L C_2H_4 molecules have been exposed on the Si(001)-(2×1) surface at RT, our suggestion for the structural model is that C_2H_4 molecules on the Si(001)-(2×1) surface remain to occupy unchangeably di-σ on-top sites. In this case the bond lengths of C-C and Si-C are not changed, compared with the previous results, and are 1.61 ± 0.05 Å and 1.81 ± 0.05 Å, respectively. C_2H_4 molecules on the Si(001)-(2×1) surface located in tandem along the dimer-rows. This result is an evidence supporting the mechanism of 1-D nano-structure formation based on the C_2H_4 molecules on Si(001) surface with di-σ on-top site.