Adsorption of Naphthalene on a Si(100)-2x1 Surface

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1. Introduction

Recently adsorption of organic molecules on a Si surface has attracted a lot of interest in relation to possible application to organic-inorganic hybrid devices. Understanding of the adsorption process is indispensable for the control of the properties of the interface and thin film of the devices. In this study naphthalene molecule, one of the fundamental aromatics, was selected and its adsorption process on a Si(100)-2x1 surface was examined using infrared adsorption spectroscopy in multiple internal reflection geometry.

2. Experimental

A Si(100)-2x1 surface was prepared by a combination of a conventional RCA cleaning and a thermal annealing process including thermal flashing above 1550K in a UHV chamber with a base pressure of 1.0×10^{-10}Torr. Naphthalene molecules in the gas phase were introduced into the chamber through a variable leak valve. Their amount of exposure is given in Langmuir (1L=1.0x 10^{-6}Torr·s). Infrared absorption spectra were measured as a function of exposure of naphthalene. The spectrum of the Si(100)-2x1 surface was used as the background reference spectrum. Cleanliness of the Si surface was confirmed by the observation of clear split peaks in the spectrum due to the formation of doubly occupied dimmer (DOD) after atomic hydrogen exposure of 1000L.

3. Results and discussion

Fig.1 shows infrared absorption spectra of naphthalene molecules adsorbed on a Si(100)-2x1 surface at room temperature with simulated spectra for several possible adsorption configurations (Fig.2) in the region of C-H stretching modes. All simulations were carried out in density functional theory method (B3LYP/6-31G(d',p')), and the obtained frequencies were scaled by a factor of 0.945.

At the initial adsorption process (1L), only two peaks at 2943 and 3053cm^{-1} grow up. The spectrum well corresponds to the simulated spectrum for structure1 in both wavenumber and intensity. According to the theoretical calculation, adsorption configuration in structure1 is energetically the most stable. Therefore we conclude that naphthalene molecules adsorb on the Si surface dominantly in structure1 at the initial adsorption process. It is well known that the frequency of C-H stretching (ν_{CH}) of sp^2 carbon appears at 3000-3100cm^{-1}, while that of sp^3 below 3000cm^{-1}. Actually all ν_{CH} peaks of an isolated naphthalene molecule locate above 3000cm^{-1}, reflecting sp^2 character. In the case of the adsorbed naphthalene, the peak at 2943cm^{-1} in the spectrum indicates the formation of the sp^3 carbon. This demonstrates that the plane structure of naphthalene is no more preserved at the adsorption, as shown in Fig. 2(a).

When the amount of exposure increases, other peaks at 2889, 2930, 3013, 3025, and 3043cm^{-1} start to grow up. The result means that naphthalene molecules adsorb on the Si surface not only in structure1 but also sutucture2, 3, and 4 in high coverage condition.

Details of adsorption configurations and their coverage dependence will be presented in the session.

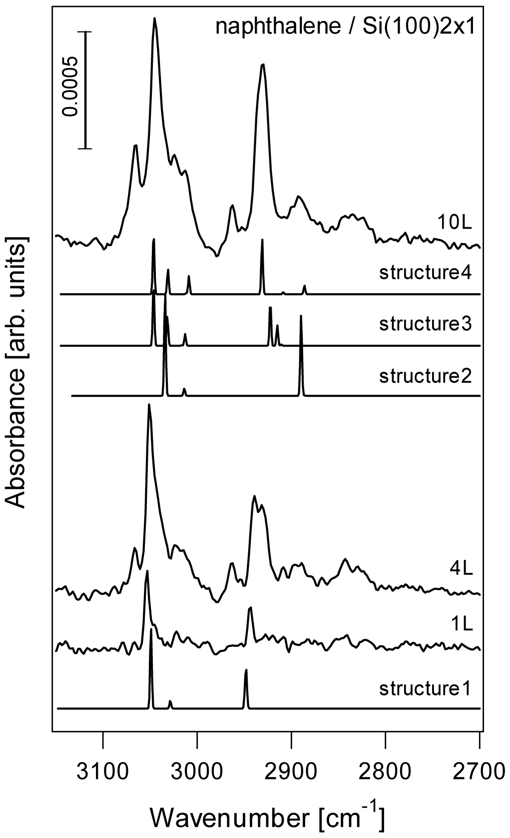
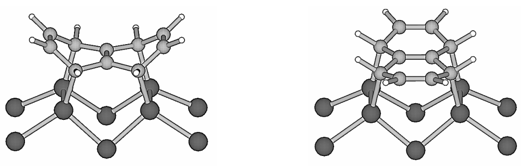
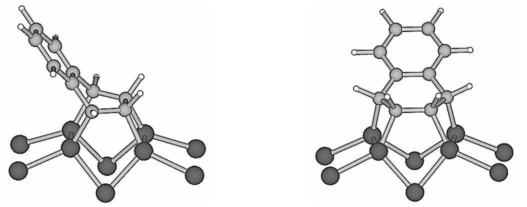


Fig.1 Infrared adsorption spectra of naphthalene molecules adsorbed on a Si(100)-2x1 surface at room temperature and simulated spectra of possible adsorption configurations (see Fig.2)



(a) structure1 (b) structure2



(c) structure3 (d) structure4

Fig2. Possible adsorption configurations of a naphthalene molecule adsorbed on a Si(100)-2x1 surface. Simulations were performed on the system which consists of a naphthalene molecule and a Si cluster of $Si_{15}H_{16}$.