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Preparation and Stability of Silyl Adlayers on 2×1-Reconstructed and Modified Si(100) Surfaces

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Saturation-coverage silyl, $-SiH_3(a)$, overlayers were prepared from Si_2H_6 adsorption on three comparative surfaces: clean unmodified; D-precovered; and atomically roughened Si(100). Together with its precursor-mediated adsorption behavior, the surface reactivity of Si_2H_6 was found to be the highest on the unmodified Si(100)-2×1 surface. This was correlated with its dissociative adsorption mechanism, in which both the $H_3Si-SiH_3$ bond scission and the dual surface $Si-SiH_3(a)$ bond formation require a surface dangling bond 'pair'. The unusually high thermal stability of $-SiH_3(a)$ on the unmodified surface was ascribed to a nearly close-packed $-SiH_3(a)$ coverage of ~0.9 monolayer and the consequent lack of dangling bonds on the silyl-packed surface.

Keywords : Si(100), Disilane(Si_2H_6), Silyl(SiH_3) Adsorption

Ⅰ. Introduction

Driven by their importance in semiconductor device processes, both SiH_4 and Si_2H_6 have been extensively studied for their reactions with Si and Ge surfaces for the past decades [1–2]. Both are known to dissociatively adsorb on those surfaces with negative barriers via precursor–mediated mechanisms at moderate substrate temperatures [3–4]. It has been suggested that dangling bonds are required for their spontaneous dissociative adsorption (chemisorption) at temperatures $<$ 600 K [5–6]. The so–called atomic layer epitaxy (ALE) scheme is based on this self–limited reaction phenomenon, which enables the ultimate control of the layer–by–layer growth in silicon deposition techniques [5].

In general and particularly in heterogeneous catalysis, it is well known that the reactivity of a solid surface increases as the atomic–scale surface roughness increases. This is due to the increased number of unstable, less–coordinated atoms on such surfaces. As one of numerous examples, the dissociative adsorption of SiH_4 occurs preferentially on defect sites on Si(100) and dissociative SiH_4 chemisorption on Si(111)–7×7 is significantly enhanced by surface roughening with inert gas ion bombardments [3]. Hydrogen uptake, as a measure of the total number of dangling bonds per unit surface area, also increases on Si(100), Si(111) and Ge(100) once their stable atomic surface structures are disrupted or roughened [7].

Both SiH_4 and Si_2H_6 dissociatively chemisorb on Si(100)–2×1 via a precursor–mediated channel at a surface temperature (T_s) below 800 K [3–4]. Two competing mechanisms have been proposed for the dissociative Si_2H_6 adsorption on Si(100)–2×1: each physisorbed Si_2H_6 molecule reacts with (1) two

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unrelated surface dangling bonds to give two silyl, $-SiH_3(a)$, adspecies and (2) with paired dangling bonds within a surface dimer to give $SiH_4(g)$ and silylene, $=SiH_2(a)$, adspecies [8]. Suda et al. [5] proposed another mechanism in which $H_3Si-SiH_3$ bond dissociation and the dual surface $Si-SiH_3(a)$ bond formation occur in a concerted fashion.

In this report, data are presented that the dissociative adsorption of Si_2H_6 on Si(100)−2×1 is greatly suppressed when its surface atomic structure is disrupted either by energetic Ar^+ ion bombardments or when its surface dangling bonds are prepassivated with D(a). This unusual reactivity behavior is ascribed to a dominant reaction mechanism in which both the SiH_3-SiH_3 bond dissociation and the formation of two surface $Si-SiH_3$ bonds concur at the dangling bond pair site of each Si dimer [5]. In addition, it is found that the saturation Si_2H_6 exposure at temperatures below 120 K leads to ~0.9 ML of $-SiH_3(a)$, which corresponds to a Θ_H as high as ~2.7 ML (1 monolayer (ML) = 6.78 × 10^{14} H atoms · cm^{-2}, the surface Si atom density). In contrast to the literature reports [1-6,8], the very high thermal stability of $-SiH_3(a)$ on Si(100)−2×1 observed in this work is reconciled with the fact that almost all surface dangling bonds are nearly close-packed by $-SiH_3(a)$. Such a high degree of $-SiH_3(a)$ packing on Si(100)−2×1 was achieved only by the saturation adsorption of Si_2H_6 at a temperature low enough to saturate all surface dangling bond pairs each with a physisorbed Si_2H_6 molecule.

II. Experimental

Experiments were all performed in a turbomolecular-pumped ultra-high vacuum chamber with a base pressure < 1×10^{-10} Torr. Our lightly B-doped, 14-20 Ω · cm resistivity Si(100) samples of a 0.5 × 15 × 20 mm^3 size were coated with 2000 Å of tungsten sandwiched between 200-Å tantalum films to facilitate linear direct-current heating up to 1400 K. The samples were then clamped with a pair of tantalum clips mounted on an electrically insulated and LN_2-cooled OFHC Cu block pair. The substrate temperature was monitored by a chromel-alumel (type K) thermocouple glued into a small hole near the sample edge with Aremco (Ultra^{TM} 516) high-temperature ceramic adhesive.

After a 5-K/s flash heating to 1300 K and 1 K/s cooling, our Si(100) sample was 2×1-reconstructed and clean without native oxide, as checked by Auger electron spectroscopy (AES), low-energy electron diffraction (LEED) and H_2 temperature-programmed desorption (TPD) features. Silane and disilane (both 4% in He; Voltaix) were dosed using a crimped capillary-controlled 3/8-inch diameter tubular doser positioned ~ 1 mm in front of the sample surface. SiH_4 and Si_2H_6 exposures were controlled by varying dosing time at a fixed reservoir pressure of 1.0 Torr behind a pinhole. Atomic D was generated by a hot (~ 1900 K) spiral W filament positioned in front of a 0.25-inch diameter tubular D_2 gas doser facing the sample surface from a distance of ~3 cm.

TPD measurements were made with a shielded, differentially pumped quadrupole mass spectrometer (QMS) through a 3-mm diameter conical aperture positioned ~1 mm away from the sample surface. The small distance suppresses signal contributions from background sources. Multiplexed TPD spectra for various mass-to-charge ratio (m/e) values were taken with a fixed temperature ramp of 3 K/s following each gas exposure at a given surface temperature (T_s).

III. Results and Discussion

Multiplexed SiH_3^+ (m/z = 31) and H_2^+ (m/z = 2) TPD spectra taken off the Si(100)−2×1 surface pre-

exposed to Si_2H_6 at a T_s of 105 K are displayed in Fig. 1. The QMS signals for all other SiH_4 ionization fragments (not shown) tracked the displayed SiH_3^+ desorption intensity at ~600 K with a correct intensity ratio, $Si:SiH^+:SiH_2^+:SiH_3^+:SiH_4^+$ = 60:37:100:80:7, determined *in situ* with the QMS for the back-filled SiH_4 gas, very close to the literature values [9]. Thus, the 600-K SiH_3^+ TPD peak represents the molecular SiH_4(g) desorption. On the other hand, since the SiH_3^+ signal tracked those of all

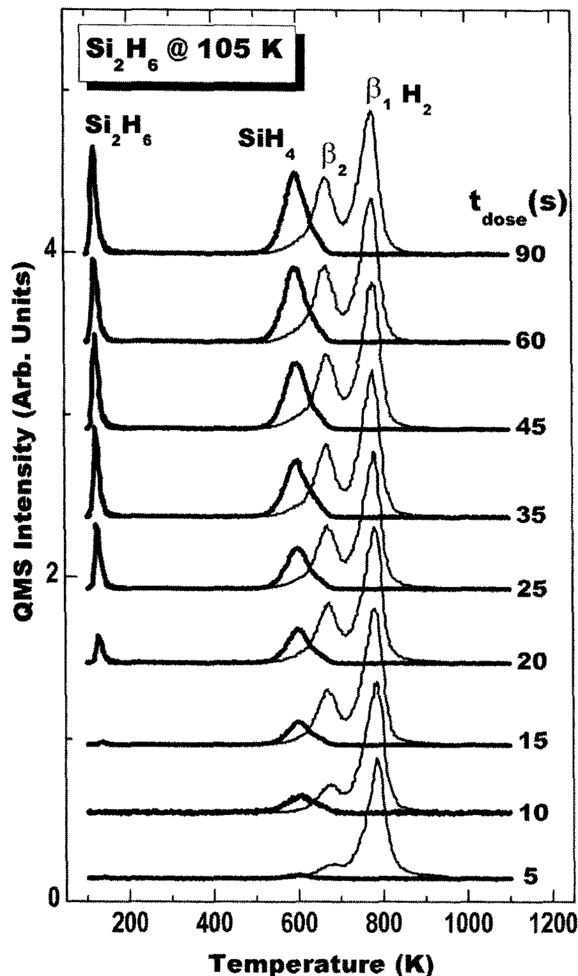

Figure 1. H_2^+ (thin solid curves), and SiH_3^+ (thick solid curves) TPD spectra from Si(100) exposed to Si_2H_6(g) for the indicated times at a reservoir pressure of 1 Torr behind a pinhole-controlled doser at a T_{ads} of 105 K. The desorption peak intensities did not increase any further beyond the 90-sec dose.

other fragments of Si_2H_6 with the correct relative ratio determined *in situ* [10], the extremely narrow SiH_3^+ peak at ~120 K was ascribed to the molecular Si_2H_6 desorption from its physisorbed multilayer(s). The H_2^+ TPD spectra show two distinct features (β_1 and β_2), the well-established associative H_2(g) desorption from the surface-adsorbed mono- and di-hydirde H atoms, respectively.

No further intensity increases of the 120-K SiH_3^+, 600-K SiH_3^+, 660-K β_2 H_2^+, and 780-K β_1 H_2^+ peaks were observed above the 90-s dose, establishing the saturation Si_2H_6 exposure. The maximum β_1-H_2^+ peak intensity (90-s dose) was ~1.2-ML Θ_H, calibrated against that of the monohydride-saturated surface (Θ_H = 1) prepared by an H dose at ~600 K, while that of the 5-s spectrum was ~1.05 ML. The total β_1- and β_2-H_2^+ desorption of the 90-s spectrum was ~1.9 ML. This, together with the 600-K SiH_4 desorption amount of ~0.2 ML SiH_3(a) estimated with the reported SiH_4/H_2 relative mass spectrometric sensitivity [11], gave a total surface H content of ~2.7 ML in the T_s range between 120 K and 600 K. This value corresponds to an initial $-SiH_3$(a) surface coverage of ~0.9 ML, meaning the formation of a nearly close-packed silyl adlayer, i.e., ~90% of all surface dangling bonds are each covered with a $-SiH_3$(a). From the total estimated H coverage of ~2.7 ML and the absence of desorption of any H-containing species between 120 K and 600 K, it is deduced that the surface be mostly devoid of the further dissociated $=SiH_2$(a) and ≡SiH(a) fragments. This unusually high packing degree of $-SiH_3$(a) and the lack of dangling bonds would prohibit further dissociation of $-SiH_3$(a) into $=SiH_2$(a) and H(a) up to as high as 600 K. It can be reasonably speculated that two $-SiH_3$(a) on adjacent dimers collide each other to give SiH_4(g) and $=SiH_2$(a) at 600 K. It should be noted that this reaction pathway of $-SiH_3$(a) would be the unique one, unlike many others reported in the literature [1-6,8], as a result of the highly

$-SiH_3$(a)$-$packed adlayer and the lack or deficiency of dangling bonds and lower hydrides. It is believed that the 120$-$K SiH_3^+ peak represents desorption of Si_2H_6 multilayer molecules weakly physisorbed on top of those strongly physisorbed on each dangling bond pair [12].

Fig. 2 shows the $T_s$$-$dependent Si_2H_6 uptake for a fixed 90$-$s dose. It can be seen that the dissociative Si_2H_6 adsorption increases with decreasing T_s in the entire T_s range studied. This behavior is typical of precursor$-$mediated chemisorption processes, in accord with previous suggestions [3$-$4]. Note that the $\beta_1$$-$$H_2$ peak intensity of the TPD curve for the 600$-$K dosing temperature corresponds to Θ_H of 0.55, far short of passivating the surface dangling bonds. This is attributed to the short lifetime and the consequently reduced concentration of Si_2H_6 trapped in its physisorption well on the surface at the temperature. Note that the 600$-$K SiH_4 desorption is detected only when there are H atoms exceeding 1 ML on the surface, which is the case for all the spectra of T_{ads} 〈 300 K, suggesting the thermal instability of $-SiH_3$(a) below 600 K when there are adjacent dangling bonds. The 600$-$K SiH_3^+ peak intensities of the bottom 6 spectra (T_{ads} = 125 to 600 K) are all lower than that (saturation value) of the top spectrum (T_{ads} = 105 K). This suggests that the dissociation of physisorbed Si_2H_6 into $-SiH_3$(a) and the subsequent $-SiH_3$(a) dissociation into $=SiH_2$(a) and $\equiv$ SiH(a) occur before all surface dangling bond pairs are filled with physisorbed Si_2H_6 molecules when the surface temperature is $\geq$ 125 K. The Si_2H_6 dissociation into $-SiH_3$(a) and the successive $-SiH_3$(a) decomposition into $=SiH_2$(a) and $\equiv$SiH(a) are known to take place readily when surface dangling bonds are available at temperatures as low as 148 K [8], but slowly over several minutes at room temperature [13]. This suggests that our short saturation dosing time of 90 s, together with the very low dosing temperature of 105 K, has ensured the nearly complete packing of all dangling bond pairs each with a physisorbed Si_2H_6 molecule. The rather mobile, weakly physisorbed Si_2H_6 molecules in the multilayer would also fill in the empty dangling bond pair sites. After the 90$-$s saturation Si_2H_6 dose at 105 K, almost all surface dangling bond pairs would thus be covered each with a strongly physisorbed Si_2H_6 molecule [12]. Upon annealing, the remaining weakly physisorbed Si_2H_6 in the multilayer would desorb at 120 K and the strongly physisorbed Si_2H_6 molecule in the precursor state on a dangling bond pair would then dissociate into two $-SiH_3$(a) groups [12,14]. These close$-$packed $-SiH_3$(a) groups are believed to sustain up to 600 K, at which two $-SiH_3$(a) groups would collisionally react to produce disproportionation products, $=SiH_2$(a) and

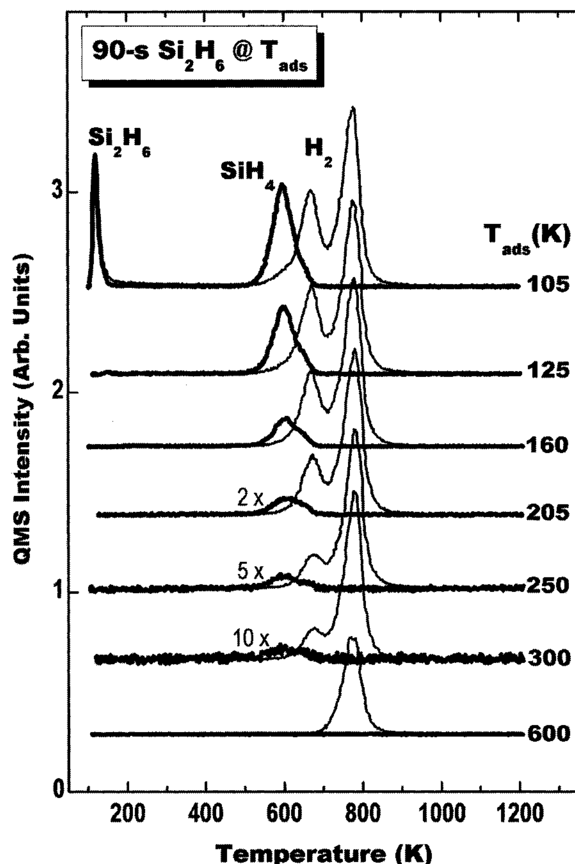

Figure 2. H_2^+ (thin solid curves), and SiH_3^+ (thick solid curves) TPD spectra from Si(100) exposed to Si_2H_6(g) for 90 sec at the indicated surface temperatures (T_{ads}). The scale factors are for the three SiH_3^+ spectra.

SiH_4(g). This reaction scheme is well in agreement with all the aspects of the experimental data of this work.

The H_2^+ and SiH_3^+ TPD spectra obtained with the Si_2H_6 saturation dose at 125 to 600 K in Fig. 2 clearly show total H uptakes smaller than that with the 105-K dose. This suggests that Si_2H_6 dissociates first into two $-SiH_3$(a) upon adsorption and that $-SiH_3$(a) quickly decomposes into $=SiH_2$(a) and $\equiv SiH$(a) at $T_{ads} \geq 125$ K, consuming more surface dangling bonds. The further decomposition $-SiH_3$(a) would occur successively faster at a higher T_{ads}, reducing the number of dangling bond pairs [15]. The strongest 600-K SiH_4(g) desorption from the 105 K-dosed surface in turn supports the high $-SiH_3$(a) coverage (~0.9 ML) or the total H content (~2.7 ML) on the surface prior to the SiH_4(g) desorption at 600 K.

In order to examine the importance of the surface dangling bonds for the dissociative Si_2H_6 adsorption, the Si(100)-2×1 surface was precovered with D prior to the saturation Si_2H_6dose. Fig. 3 and Fig. 4 show H_2^+, HD^+, D_2^+ and $SiH_xD_y^+$ TPD spectra following a 90-s saturation Si_2H_6 dose at 105 K to the Si(100)-2×1 surface precovered with ~ 0.4 and ~ 1.0 ML D, respectively. The 120-K Si_2H_6 desorption (not shown) was observed from these D-precovered Si(100)-2×1 surfaces, implying that the weakly physisorbed Si_2H_6 molecules on the Si_2H_6- and D-precovered Si(100)-2×1 surface have the same similar adsorption energy [12]. The bottom 4 spectra for the various ionized fragments (m/z = 30 - 33) reflect the presence (Fig. 3) and absence (Fig. 4) of molecular SiH_xD_y (x + y = 4) desorption, the final reaction product of dissociation fragment, $-SiH_3$(a). The SiH_xD_y desorption, together with HD and H_2 desorption, is indicative of the Si_2H_6 dissociative adsorption. The results of Fig. 4 clearly indicate that

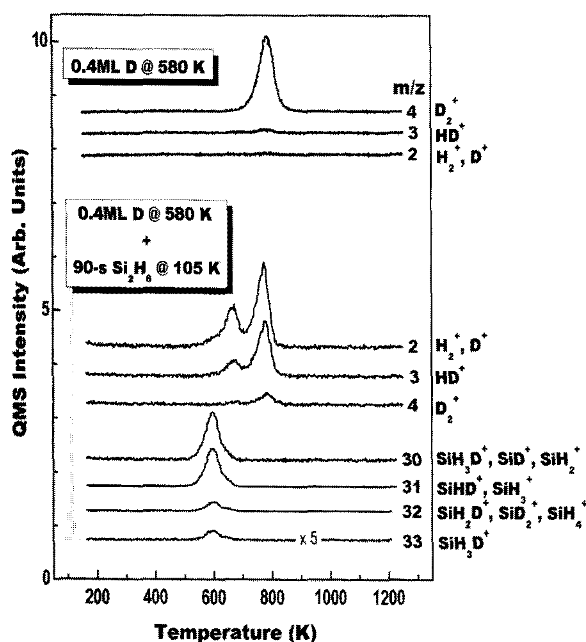

Figure 3. TPD spectra from Si(100) with 0.4-ML D only (top 3 curves) and from Si(100) with a 0.4-ML D precoverage followed by a 90-sec Si_2H_6(g) exposure at 105 K (bottom 7 curves), respectively. The mass-to-charge ratio (m/z) values and the corresponding mass fragments monitored by the multiplexed TPDs are indicated.

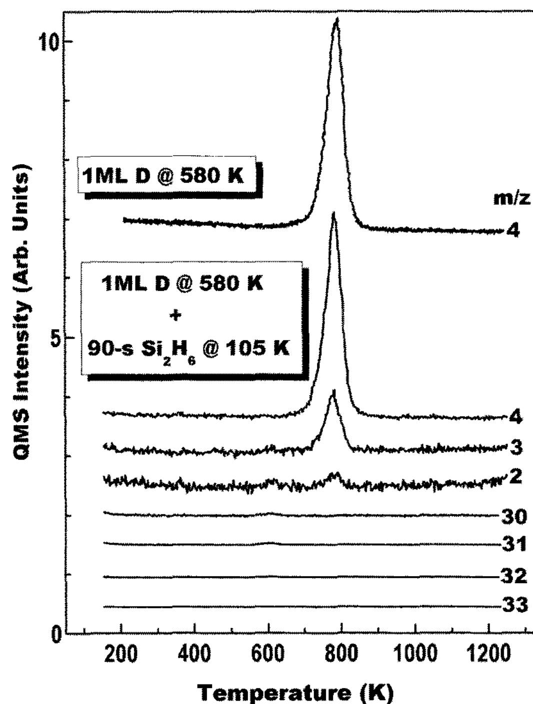

Figure 4. TPD spectra from Si(100) with 1-ML D only (top curve) and from Si(100) with a 1-ML D precoverage followed by a 90-sec Si_2H_6(g) exposure at 105 K (bottom 7 curves), respectively.

the dangling bond passivation by D(a) effectively suppresses the dissociative Si_2H_6 adsorption, confirming the literature reports [3,5-6,8].

In order to assess the importance of the dangling bond dimer structure with respect to the dissociative adsorption of Si_2H_6, the Si(100)-2×1 was bombarded with 1 keV Ar^+ ions at 300 K prior to a 60-s Si_2H_6 dose at 105 K. ion bombardments largely destroy the dimer row structure (dangling bond pairs) and create highly unstable, less-coordinated Si atoms on the surface [16]. H and SiH_4 uptakes increase with atomic-scale roughening of the Si surfaces [3,7], indicative of an increase in the number of dangling bonds on the surface. However, the dissociative Si_2H_6 uptake, monitored by the SiH_3^+ (600 K) and H_2^+ (660 K and 780 K) desorption in TPD, turned out to be significantly smaller on the roughened surface, as shown in Fig. 5. In accord with this, the stronger SiH_3^+ and H_2^+ desorption intensities at ~120 K indicate that more weakly physisorbed Si_2H_6 molecules desorb molecularly from the ion-roughened surface. The nearly complete suppression of both the 600-K SiH_3^+ and β_2-H_2^+ desorption indicates that the surface dangling bond pair, not the dangling bond itself, plays a key or more important role in the dissociative adsorption of Si_2H_6. The total H_2 desorption amount from the ion-bombarded surface was estimated to be ~1 ML, which should be significantly smaller than the number of dangling bonds on the roughened surface. This confirms evidently that the dissociative Si_2H_6 sticking probability is much higher on the surface with paired dangling bonds than the roughened surface even with a higher dangling bond density. These results strongly support the following Si_2H_6 physisorption and the subsequent dissociation pathway on Si(100)-2×1: the preferred configuration of physisorbed Si_2H_6 is such that H_3Si-SiH_3 bond is parallel to the surface Si-Si dimer bond and the concerted H_3Si-SiH_3 bond scission and dual Si-SiH_3(a) bond formation, in good accord with the model proposed by Suda et al. [5].

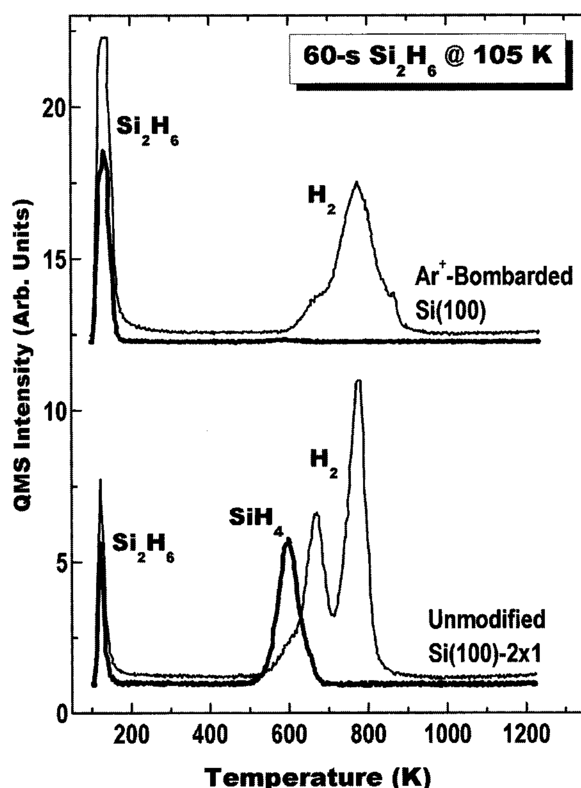

Figure 5. H_2^+ (thin solid curves), and SiH_3^+ (thick solid curves) TPD spectra from a smooth Si(100)-2×1 surface (bottom) and from a atomically roughened Si(100) surface with 1-keV Ar^+-ion bombardments at 300 K (top), both of which were exposed to the same 60-s dose of Si_2H_6(g) at 105 K, respectively.

An uptake comparison for SiH_4 and Si_2H_6 on the Si(100)-2×1 surface is presented in Fig. 6. The TPD spectra for the two saturation exposures, 90-sec. Si_2H_6 and 360-s SiH_4, clearly show that Si_2H_6 adsorption leads to the higher SiH_3(a) and H(a) coverages on Si(100)-2×1. However, this difference was mostly eliminated on the Ar^+-bombarded surface. The fact that the maximum desorption intensity of the SiH_3^+ from the saturation SiH_4 dose (360-s) is much smaller than that from the saturation Si_2H_6 dose (90-s) is in good agreement with the high -SiH_3(a) coverage and Si_2H_6 adsorption mechanism involving the dangling bond pair [5, 17].

The estimated Θ_H of ~2.7 ML, accomplished by the

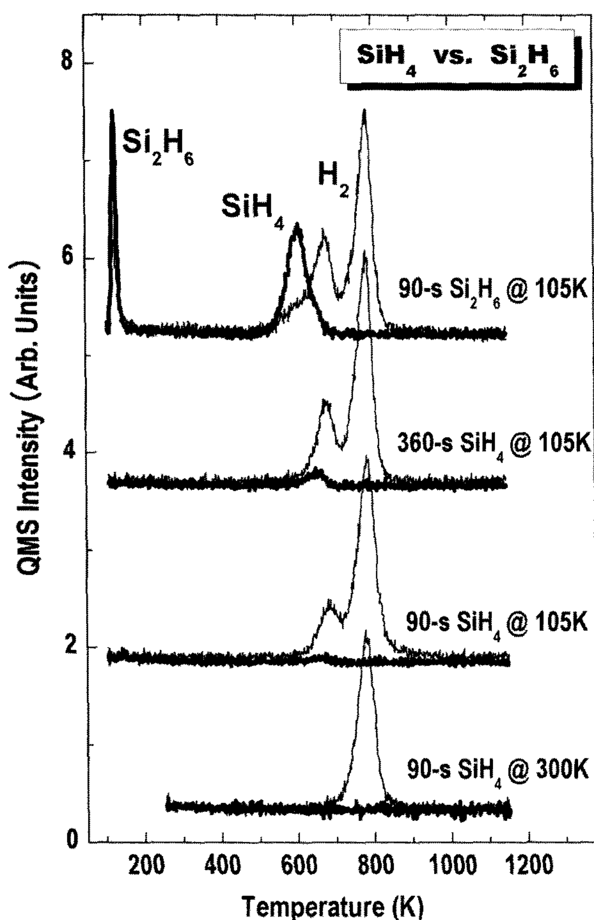

Figure 6. H_2^+ (thin curves) and SiH_3^+ (thick curves) TPD spectra from Si(100) exposed to SiH_4 (bottom 3 curves) and Si_2H_6 (top curve) for the times and at the surface temperatures indicated in the figure.

saturation Si_2H_6 chemisorption, requires that 90% of the surface dangling bonds of Si(100)−2×1 are SiH_3(a)-bonded over a wide T_s range between 120 K and 580 K. The very high packing density and thermal stability of $-SiH_3$(a), despite the expected steric hindrance between $-SiH_3$(a) groups, are interesting. It has been suggested that $-SiH_3$(a) on Si(100)−2×1 can be stable up to ~600 K in the absence of surface dangling bonds [3]. The inhibited $-SiH_3$(a) dissociation is therefore a result of its high coverage of ~0.9 ML, implying a nearly close-packed full monolayer, as depicted schematically in Fig. 7. The $H_3Si-SiH_3$ bond scission of the speculated configuration of physisorbed Si_2H_6 and the dual

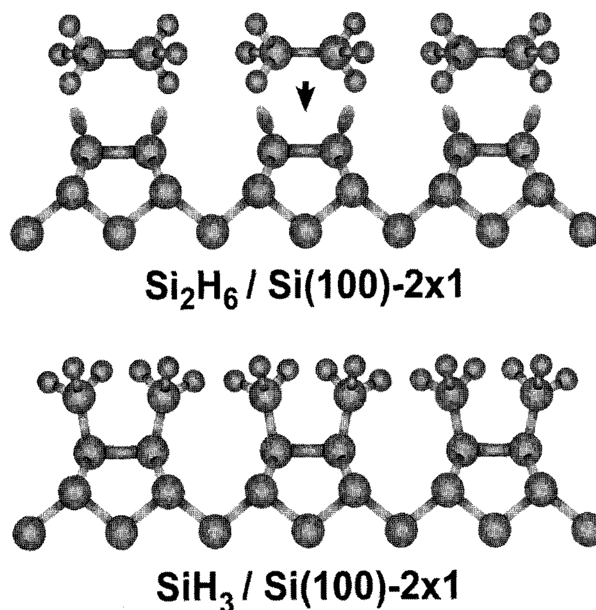

Figure 7. A ball-stick diagram for the physisorbed Si_2H_6 , each on top of a dangling bond pair in a dimer, and chemisorbed $-SiH_3$(a) on Si(100)−2×1. Surface dangling bonds are represented as lobes. The Si-Si bond lengths are approximately 2.40, 2.35 and 2.33 Å for the surface dimer, the bulk lattice and Si_2H_6, respectively [17].

surface $Si-SiH_3$ bond formation can be speculated to occur concertedly. The relevant bond lengths indicated in the caption of Fig. 7 are in good agreement with such a picture.

Ⅳ. Conclusion

Low-temperature (< 120 K) adsorption of Si_2H_6 on Si(100)−2×1 leads to a silyl, $-SiH_3$(a), adlayer of ~0.9 ML. This nearly close-packed $-SiH_3$(a) adlayer is unusually stable up to ~600 K, at which two $-SiH_3$(a) on adjacent dimers within a dimer row collide to give a gaseous SiH_4(g) molecule and a silylene, $=SiH_2$(a), adspeicies [15]. The dangling bond pair on Si(100)−2×1 was found to be a preferred Si_2H_6 physisorption site and a lowest-barrier site for the concerted chemisorption reaction, i.e., the scission of the $H_3Si-SiH_3$ bond and the formation of dual surface

$Si-SiH_3(a)$ bonds.

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Si(100)-2×1 표면과 개질된 Si(100) 표면 상에서 실릴 (Silyl) 흡착층의 형성과 안정성

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깨끗한 Si(100)-2×1, D를 먼저 흡착시킨 Si(100)-2×1, 그리고 이온 빔에 의해 원자 수준으로 거칠어진 Si(100) 등의 세 가지 표면에 각각 Si_2H_6의 흡착시켜 포화 실릴(-SiH_3(a)) 흡착층을 형성시키고 실험적으로 비교 고찰하였다. 전구체 흡착 거동(기작)과 함께 Si_2H_6의 표면 분해(화학)흡착 반응성은 개질을 시켜주지 않은 깨끗한 Si(100)-2×1 표면에서 가장 크게 나타났다. 이 결과는 화학흡착 반응 즉, H_3Si-SiH_3 결합 분해와 두 개의 Si-SiH_3(a) 표면결합 형성이 표면의 Dangling Bond *Pair* 상에서 동시적으로(Concertedly) 일어나는 Si_2H_6의 분해흡착 기작으로 설명될 수 있었다. 또한 Si(100)-2×1 표면에 흡착된 -SiH_3(a)의 매우 높은 열적 안정성은 ~0.9 ML나 되는 표면 덮힘도와 함께 실릴기로 조밀하게 흡착된 표면에 Dangling Bond가 존재하지 않는 것에 의한 것으로 밝혀졌다.

주제어 : 실리콘(100), 다이사일렌(Si_2H_6), 실릴(SiH_3) 흡착

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