Surface Science 186 (1987) L557–L560
North-Holland, Amsterdam


SURFACE SCIENCE LETTERS

# THE ADSORPTION BEHAVIOUR OF $O_2$ ON THE CLEAN Si(110) SURFACE IN THE EARLY STAGE

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Received 17 March 1987; accepted for publication 22 April 1987

This Letter reports on the early stage of adsorption of $O_2$ on the clean Si(110) surface, showing a prominent $5 \times 1$ reconstruction, in ultrahigh vacuum at 300 K. Auger electron spectroscopy (AES) and low energy electron diffraction (LEED) have been used to monitor this solid–gas reaction. Careful measurements of the normalized oxygen Auger signal in the low exposure region reveal, for the first time, a remarkably fast adsorption of $O_2$ up to $\sim 0.15$ monolayer of oxygen, the initial sticking probability being about 1. The LEED measurements suggest that those surface sites which constitute the additional higher order reconstructions, are highly reactive.

The Si(110) surface has received considerably less interest than the (111) and (100) surfaces. A number of questions have remained unanswered concerning, e.g., the geometric and electronic structure of the Si(110) surface and an accurate description of the $O_2$ adsorption kinetics. Most relevant to this last remark is the enormous scatter in the experimentally found initial sticking probability, $S_0$, ranging from $\sim 6 \times 10^{-3}$ [1] via 0.03 [2] to $\sim 0.2$ [3], as determined with Auger electron spectroscopy (AES) [1,3] and differential reflectometry (DR) [2]. Unfortunately, the authors [1–3] did not report on the structure of their clean surface. They all used a different method of preparing a clean surface which, to our opinion, leads to Si(110) surfaces each having a different degree of perfection [4] and reconstruction [5–8].

Furthermore, the exposure curves for $O_2$ on the Si(110) surface, as shown in refs. [1–3], reveal a striking difference in the initial start of the $O_2$ adsorption measurements, i.e., at exposures of 1, 6 and 100 L, respectively, $S_0$ decreasing in that order (1 langmuir (L) = $1 \times 10^{-6}$ Torr s). The exposure curve as measured by Ranke and Xing [3] is interesting since it exhibits two changes in its slope, i.e., at 2 L and at about 30 L, which is an indication of a more complicated reaction kinetics [9,10]. This result suggests that relevant information concerning the initial $O_2$ adsorption stage remains unnoticed if the experiment is started at a more advanced exposure [1,2]. The observed scatter in "$S_0$" may thus be attributed to the difference in the initial start of the $O_2$

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adsorption experiments. The question arises if complementary information about the very early $O_2$ adsorption stage can be gained from an investigation at exposures below 1 L.

This Letter deals with the initial room temperature adsorption of $O_2$ on a clean Si(110) surface, showing a prominent $5 \times 1$ superstructure, and special attention being focused on the adsorption behaviour in the sub-Langmuir region. The work presented in this Letter is part of a more extensive study on the adsorption behaviour of $O_2$ and $N_2O$ on the Si(110)$5 \times 1$ surface at 300 K, investigated by DR, AES and low energy electron diffraction (LEED) [9–11]. In this paper only the AES and LEED measurements performed at low exposures (0–15 L) will be discussed. Our experimental results demonstrate that the initial $O_2$ adsorption stage is remarkably fast.

The experiments were performed in a stainless steel UHV system with facilities for DR, AES–LEED, ion-bombardment and residual gas analysis, recently described in detail [4]. A clean Si(110) surface (10 $\Omega$ cm, boron doped p-type, $10 \times 30 \times 0.2$ mm$^3$, purchased from Siltronix) was obtained by cycles of simultaneous $Ar^+$ bombardment and annealing (600 ° C) (SIBA) and annealing (800 ° C, 60 min). Applying this surface cleaning recipe for the (110) surface, reasonably good patterns showing diffuse spots and streaks in addition to the prominent $5 \times 1$ superstructure were reproducibly obtained [9–11]. In ref. [4] we have argued that the SIBA treatment leads to clean silicon surfaces with probably the best possible degree of perfection. The procedures for gas handling, AES–LEED measurements and the determination of the fractional oxygen coverage in AES, $\theta_{AES}$, as derived from the ratio of the oxygen KLL (510 eV) to the silicon KLL (1619 eV) Auger peak-to-peak heights in the first derivative $(\mathrm{d}N(E)/\mathrm{d}E)$ of the energy distribution, can be found in refs. [4,11].

Fig. 1 shows $\theta_{AES}$ versus small $O_2$ exposure. From the slope of this curve it has been derived [9,10] that the initial sticking probability for an oxygen molecule on the Si(110) surface, $S_0$, is near unity. At around monolayer (ML) coverage the sticking probability has decreased to about $10^{-6}$, slow sorption continuing beyond ML coverage [9,10]. We mean by ML coverage that $4.8 \times 10^{14}$ oxygen molecules have reacted with $9.6 \times 10^{14}$ Si atoms in the surface layer. From fig. 1 can also be derived that "$S_0$" is about 0.1 if the $O_2$ adsorption measurement had been initiated at an exposure of 1 L, which is in reasonable agreement with the results of Ranke and Xing [3]. An initial sticking probability in the range $10^{-2}$–$10^{-3}$ is obtained if the initial exposure would have been 6 L (this work)–100 L [9,10], in accordance with the results of Wierenga et al. [2] and Tougaard et al. [1]. These results strongly suggest that the large scatter in "$S_0$" ([1–3], this work) can be attributed to the difference in the initial start of the $O_2$ adsorption measurement and possibly, to a lesser degree, also to the difference in the reconstruction of the initial clean Si(110) surface. At low exposures (0–2 L), i.e., when $0 \leqq \theta_{AES} \leqq 0.15$

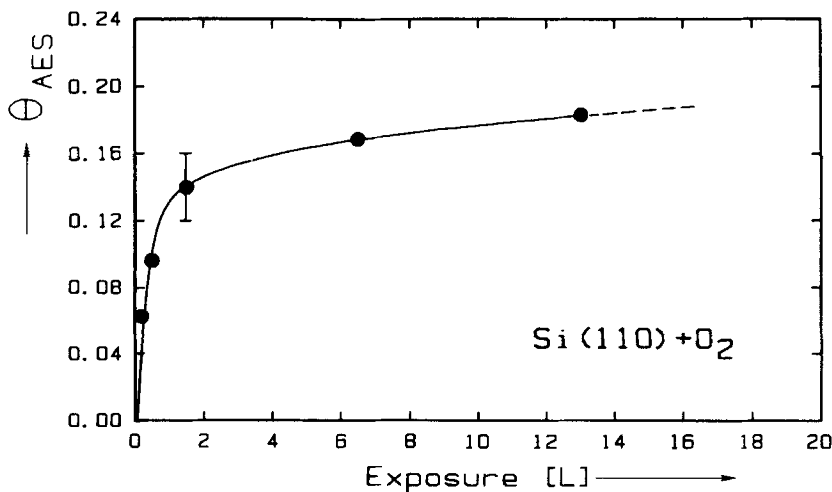


Fig. 1. The fractional oxygen coverage, $\theta_{AES}$, as derived from the normalized oxygen Auger signal [4,11], versus $O_2$ exposure in the initial adsorption stage. Each data point is taken after new exposure on a freshly cleaned surface.

(fig. 1), the diffuse spots and streaks which are observed in addition to the 5 × 1 LEED pattern [9,10] – indicative of higher order reconstruction – rapidly disappear. Or in other words, the quality of the 5 × 1 LEED pattern improves. A possible explanation is that in this region $O_2$ mainly reacts with those surface sites which constitute the additional higher order reconstructions and possibly also with defects on our – SIBA – cleaned Si(110) surface. Additional evidence from DR measurements in favour of this idea can be found in refs. [9,10].

*In conclusion,* the present study demonstrates that careful measurements of the normalized Auger oxygen signal in the sub-Langmuir region reveal additional information about the initial adsorption of $O_2$ at the clean Si(110) surface. It has been shown here for the first time that the initial sticking probability of molecular oxygen on this surface is almost 1. A careful investigation of the low exposure region should always be an integral part of gas adsorption studies on clean silicon surfaces: preliminary results of the room temperature adsorption of $O_2$ on Si(111)7 × 7, studied by the contact potential difference method [12] and NO on Si(100)2 × 1, monitored by AES–LEED and DR [13] both show a distinct adsorption behaviour between 0 and 0.2 L $O_2$ (NO) exposure.

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