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ESDIAD Study of Step Site Bonding on a Vicinal Si(100) Surface upon Cl<sub>2</sub> Adsorption

by

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**Abstract**

Characteristic chlorine bonding sites have been detected on a vicinal Si(100) single crystal surface exposing Si(100) terraces, 7-8 Si atoms in width. These terraces are separated by 2-atom layer height steps. Following annealing to 673 K, three Cl<sup>+</sup> beams are observed by the electron stimulated desorption ion angular distribution (ESDIAD) method. Two of the Cl<sup>+</sup> beams originate from silicon-dimer dangling bond sites on the Si(100) terraces. The third Cl<sup>+</sup> beam is associated with the Si-Cl bond on the step sites, and it emits Cl<sup>+</sup> at a polar angle of  $24 \pm 1^\circ$  with respect to the <100> direction, in the downstairs direction. The direction of Cl<sup>+</sup> emission from the step site is qualitatively consistent with the theoretical model of the step reconstruction proposed by Chadi.

## I. INTRODUCTION

The importance of chemisorption on the steps on Si(100) surfaces in CVD growth processes and in etching chemistry is very well known [1-5]. Despite this, a detailed understanding of adsorbate bonding on defect step sites is still missing. The very small difference in binding energy for adsorbates on terrace sites and on step sites drastically restricts the selection of possible analyzing techniques for discriminating these separate surface species. In general only spectroscopies with very high energy resolution (e.g. polarized infrared spectroscopy [6]), or real space imaging techniques such as scanning tunneling microscopy (STM) [7], or electron stimulated desorption ion angular distribution (ESDIAD) [8] can be used for the discrimination and characterization of species on the step and the terrace sites.

The structure of steps on Si(100) has been the subject of many theoretical and experimental studies [1, 9, 10]. On the nominally "flat" Si(100) surface where 1-atom layer height steps are present, two different arrangements of Si-Si dimer bonds are possible. The first arrangement involves the Si-Si dimer bonds oriented parallel to the step edges, and the other one involves the dimer bonds oriented perpendicular to the step edges. This implies the existence of two different types of 1-atom layer steps depending on the Si-Si dimer orientation on the upper terrace. In contrast to the 1-atom layer steps, the only stable orientation of the surface dimer bonds on the terraces separated by 2-atom layer steps is one in which the dimer bonds are parallel to the edges of these diatomic steps. Two different models of the reconstruction of 2-atom layer steps were proposed theoretically: a  $\pi$ -bonded reconstruction by Aspnes and Ihm [9] and a rebonded structure by Chadi [1]. Recent STM studies by Griffith et al. [10] have favored the Chadi model which is schematically shown in Fig. 1. Additional buckling on the steps was introduced to explain all the observed features [10].

The dissociative adsorption of chlorine on Si(100) surfaces has recently been studied very extensively. The early UV photoemission spectroscopy [11], low-energy electron energy loss spectroscopy [12], and near-edge X-ray absorption fine structure (NEXAFS) [13] studies carried out on the "flat" Si(100) surfaces with a saturation coverage of chlorine were interpreted in terms of Si-Cl bonds inclined from the (100) normal direction. Subsequent SEXAFS and NEXAFS studies [14] were carried out on the vicinal Si(100) surfaces with submonolayer chlorine coverages. The data were interpreted as indicating the presence of Cl atoms bonded to buckled Si-Si dimers on terraces. The orientation of the Si-Cl bond was reported to be within  $10^\circ$  of the  $\langle 100 \rangle$  normal direction. The chlorine bonding at step sites was not considered for the interpretation of the data obtained in these works [14]. Two ESDIAD studies yielding different conclusions have appeared in the literature. In the first, investigated by Bennett et al. [15], only normal  $\text{Cl}^+$  emission was observed on the nominally "flat" Si(100) surface for annealing temperatures in the range of 130 - 670K, and it is explained as a normally oriented Si-Cl bond on an asymmetric silicon dimer. In contrast, on the vicinal Si(100) surface, three  $\text{Cl}^+$  beams were observed at 130K, converting to one beam after annealing to 670K. The existence of single Cl atoms bonded to a symmetric Si-Si dimer site or the presence of dichloride surface species was proposed. The second ESDIAD study combined with HREELS spectroscopy, conducted by Gao et al. [16] on the "flat" Si(100) surface, suggests the existence of metastable bridge bonded Cl for annealing temperatures below 673K and terminally bonded Cl species for temperatures below that of  $\text{SiCl}_2$  desorption ( $\sim 820\text{K}$ ). HREELS energy loss features are in agreement with this assignment. The Si-Cl bond inclination angle from the terrace normal for the terminal species was determined to be  $25 \pm 4^\circ$  after making final state corrections to the experimentally observed  $\text{Cl}^+$  emission angles. The bridge bonded and the

terminally bonded surface chlorine species were also observed by STM after the adsorption of Cl<sub>2</sub> on Si(100)-(2x1) at room temperature by J. Boland [17].

In this work we present an ESDIAD study of Cl<sub>2</sub> adsorption on a vicinal Si(100) surface which is a followup of our "flat" surface studies [16]. This study presents an ESDIAD assignment of Cl bonding on the step site dangling bonds of silicon. The angle of Cl<sup>+</sup> emission from the Si-Cl bond on the 2-atom layer step site is observed to be inclined  $24 \pm 1^\circ$  away from the <100> terrace normal in the downstairs direction. This angle is obtained by the extrapolation of measured Cl<sup>+</sup> emission to zero field without corrections for final state effects (image potential and reneutralization). Computer modeling of the ion trajectories in the ESDIAD analyzer is used for the extrapolation to zero field. The configuration of the Si-Cl bond on the step is compared with two present theoretical models, favoring the rebonded step model by Chadi [1].

## II. EXPERIMENT

Details of the ultrahigh vacuum (UHV) system (base pressure  $3 \times 10^{-11}$  Torr) and the Si(100) sample preparation have been described previously [18]. The UHV system is equipped with a CMA Auger electron spectrometer (AES), an argon-ion sputtering gun, a digital LEED/ESDIAD apparatus, a shielded quadrupole mass spectrometer (QMS) for line-of-sight temperature programmed desorption (TPD) experiments, and an additional QMS coupled with an electron gun for ion mass analysis during electron stimulated desorption (ESD) processes.

The vicinal Si(100) crystal ( $12 \times 12 \times 1.4 \text{ mm}^3$ ,  $10 \text{ } \Omega\text{cm}$ , p-type, boron doped) was cut  $6^\circ$  off the  $\langle 100 \rangle$  direction towards the  $\langle 011 \rangle$  direction. The miscut angle and the step orientation were checked with the Laue back-reflection X-ray diffraction technique. Cleaning of the crystal was performed by combined  $\text{Ar}^+$  sputtering and subsequent annealing at 1200K. After the cleaning procedure the crystal was slowly cooled ( $\sim 3 \text{ Ks}^{-1}$ ) to room temperature. This cooling procedure was employed during all experiments to obtain a well ordered  $(2 \times 1)$  LEED pattern of one domain structure. The concentration of carbon and oxygen impurities was measured by AES before each experiment and was found to be below the detection level ( $< 1$  atomic %) in the depth of sampling. The temperature of the crystal was controlled by a Honeywell programmable temperature controller with the feedback signal from the chromel-constantan (type E) thermocouple which is inserted into a slot in the edge of the Si crystal and isolated from it by a Ta foil envelope [19a].  $\text{Cl}_2$  (research purity: 99.999%) was purchased from Matheson and further purified before experiments by several freeze-pump-thaw cycles. A multicapillary-collimated doser with an absolute calibrated molecular flux and a known angular distribution was used for  $\text{Cl}_2$  dosing [19]. The identity of  $\text{Cl}^+$  ions produced by ESD was determined using the additional QMS with the ionizer turned off. All ESDIAD images were produced at 140K using an electron energy of 120eV. The effect of the structureless background (mainly due to soft X-rays) is minimized by subtraction of the pattern obtained in the configuration where all positive ions are retarded in the ESDIAD analyzer. Small inhomogeneities in the response of the multichannel plate detector were removed by 5 point polynomial smoothing of the ESDIAD patterns [20].

### III. RESULTS AND DISCUSSION

#### A. Chlorine Adsorption and Site Occupancy

The side, top and three-dimensional views of Chadi's model of the reconstruction of the 2-atom layer step on the vicinal Si(100) are shown in Fig. 1. It can be seen that this reconstruction introduces reactive sites on the steps. Since the dangling bonds on the steps do not occur in pairs as on the terraces, it can be expected that chemistry on these sites, interestingly, will represent, in a general way, the transition from the tilted dangling bond pairs on the Si(100) to the normally-oriented isolated dangling bonds on Si(111).

Figure 2 shows the ESDIAD images at 140K, for Cl<sub>2</sub> saturation coverage on the vicinal Si(100) at 140K (Fig. 2a). In addition ESDIAD images after 673K annealing (Fig. 2b) were obtained. In both cases, the crystal was positively biased to 8V. Each image is shown as a three dimensional plot (top part of the figure) and a contour plot (bottom part of the figure). The three dimensional plots have the same vertical scaling with equidistantly stepped contours to show the relative height of the ESDIAD features. The contour plots are presented with six contours equidistantly spaced from zero to maximum intensity. Two basic features can be distinguished in Fig. 2a. A central Cl<sup>+</sup> beam with the maximum of the angular distribution in the <100> terrace normal direction, and a second less pronounced Cl<sup>+</sup> beam originating from the step site which is tilted in the downstairs step direction. A strong increase of the total signal occurs upon annealing to 673K (Fig. 2b) as has been also observed on "flat" Si(100) [16]. The same ESDIAD image can also be obtained upon direct adsorption at 673K. The central beam, pointed in the <100> direction, converts on heating to two equal beams with tilt angles towards the <0 $\bar{1}$ 1> and <01 $\bar{1}$ > directions, which are the directions of the terrace dangling

bonds. The downstairs orientation of the  $\text{Cl}^+$  emission from the step sites does not change upon annealing to 673K. The same thermal conversion of the normal  $\text{Cl}^+$  beam to inclined  $\text{Cl}^+$  beams was also observed in our previous study on the "flat" Si(100) surfaces [16]. The central low temperature feature was interpreted as resulting from a Cl atom, bridge bonded to the symmetrical Si-Si dimer sites. This irreversible thermal conversion to inclined terminally bonded monochloride (higher chlorides were not observed by HREELS [16]) suggests that the terminal configuration is the one with minimum energy. Compared to the "flat" Si(100) surface, we observe on the vicinal silicon surface a new  $\text{Cl}^+$  ESDIAD feature oriented in the downstairs step direction. Looking at the model of the studied surface (see Fig. 1) we can clearly distinguish three possible azimuthal orientations of the surface dangling bonds. Subsequent saturation of these bonds by chlorine will lead to the  $\text{Cl}^+$  emission in the directions that we observe. We exclude the possibility of the appearance of this third beam as a result of the existence of minority domains with the perpendicularly oriented dimers or etching of the surface with loss of silicon surface atoms. In our ESDIAD experiments we do not see any traces of the symmetric counterpart of the step  $\text{Cl}^+$  emission in the upstairs direction. Furthermore, etching is an unimportant process based on molecular beam scattering studies. A negligible etching rate occurs in a thermal  $\text{Cl}_2$  beam for adsorption temperatures which are used in this study [21]. It is seen in Fig. 2 that the  $\text{Cl}^+$  ion intensity from the step sites after 673K annealing is much stronger than from the terrace sites. Since the  $\text{Cl}^+$  yield is strongly dependent on the Cl coverage on Si(100)-(2x1) (the neighboring Cl atoms effectively enhance the reneutralization of the  $\text{Cl}^+$  ions [16]), a possible explanation is that the Cl atoms bonded on the step sites are relatively far from Cl neighbors, have much lower reneutralization probability, and hence a higher  $\text{Cl}^+$  yield.

## B. $\text{Cl}^+$ Emission Angles in ESDIAD

The very high spatial resolution of the ESDIAD apparatus ( $\sim 1^\circ$ ) [22] allows the accurate determination of ion emission directions (characterized by polar and azimuthal angle). The largest polar angle measurable without distortion of the ESDIAD image is limited by the detection solid angle of the microchannel plate. This restriction is experimentally overcome by applying a positive bias to the crystal which causes bending of the ion trajectories towards the macroscopic normal of the crystal, producing compression of the ESDIAD pattern. The zero field emission angle ( $\theta_0$ ) is then obtained by extrapolation of the angle measured for a series of decreasing crystal bias voltages. The extrapolation is performed using computer simulation (program: SIMION) of the ion trajectories in a nearly spherical electrostatic field [16]. The modeling of the field is based on the spatial arrangement of the crystal and the electrostatic optics used in the experiment. The input parameters are the initial ion take-off angle and the ion kinetic energy. Since the macroscopic plane of the crystal, compared to the (100) plane, is tilted along the [011] axis by  $6^\circ$ , care has to be taken in the selection of the reference direction for the  $\text{Cl}^+$  emission angle from the step. In the electrostatic field all ion trajectories are bent towards the normal of the macroscopic plane of the crystal and this direction was used as zero of the polar ion emission in the computer simulations. The  $6^\circ$  inclination angle is then added to obtain the  $\text{Cl}^+$  ion emission polar angles from the step sites relative to the  $\langle 100 \rangle$  direction.

The crystal bias dependence of the measured ion emission angle for the terrace and the step Si-Cl bonds of terminally bonded chlorine is shown in Fig.3. The angles are defined with respect to the  $\langle 100 \rangle$  terrace normal direction. Error bars are obtained from three different experiments for three particular crystal bias voltages (5, 8, 20V). The solid lines represent the result of the computer

simulations and give the extrapolated value of the ion emission angle at zero electrostatic field,  $\theta_0$ . In the case of the terrace site (top part of Fig. 3) the best fit is obtained for the ion departing from the surface with a kinetic energy of 1.1eV, and with a polar angle of  $33^\circ$  relative to the  $\langle 100 \rangle$  terrace normal direction. This kinetic energy is different from the value obtained in our retarding potential ion kinetic energy experiment (most probable energy = 0.35eV; FWHM = 0.6eV) [16]. The discrepancy between the experiment and the best fit of the simulation is probably caused by the unknown difference of the work functions between the crystal and the grid optics [16]. To obtain an estimate of the systematic error of the simulation, we have varied the kinetic energy of the  $\text{Cl}^+$  ion in the range of 0.8-1.7eV. The calculated lower and upper limit for  $\theta_0$  is  $27^\circ$  and  $34^\circ$ , respectively and the cross hatched region indicate the possible range of systematic error in this measurement. The  $\theta_0$  on the "flat" Si(100) was found to be  $27^\circ$  with a range of  $25$ - $31^\circ$  [16]. Thus, within the error of measurement,  $\text{Cl}^-$  emission angles corrected for the electrostatic distortion of the analyzer relative to the  $\langle 100 \rangle$  terrace normal direction agree on the "flat" and vicinal Si(100) surfaces. For the case of a  $\text{Cl}^+$  ion emission from the step site (bottom part of Fig. 3) the best fit corresponds to the  $\text{Cl}^+$  ion leaving the surface with kinetic energy 1.1eV at  $\theta_0 = 24^\circ$ . For the kinetic energy range, 0.8-1.7eV, the polar angle range of  $\text{Cl}^+$  from the step sites is  $23$ - $25^\circ$ , relative to the  $\langle 100 \rangle$  terrace normal direction.

In our previous paper on the "flat" Si(100), the experimental zero field angle ( $\theta_0$ ) was also corrected for the final state reneutralization and image potential effects yielding the Si-Cl bond angle [16]. It was shown that these two effects act in the opposite sense and practically cancel each other giving a relative correction of only  $-2^\circ$ . Since our vicinal surface ( $6^\circ$  off axis angle) consists of terraces only 7-8 atoms wide, it can be expected that the image potential will be influenced by the presence of the steps [23]. Because the quantitative correction is

very complicated in this case, we restrict our discussion only to a qualitative estimate. Using a theoretical study of  $O^+$  desorption from  $W(110)$  by Clinton [24], we are able to determine the sign of the angular correction for both the image effect and the reneutralization effect. For the terrace site  $Cl^+$  emission the situation is close to that for the "flat"  $Si(100)-(2 \times 1)$  surface, and the total correction can be expected to be within the experimental error of the extrapolation. In the case of the step  $Cl^+$  emission, the image potential tends to bend the ion trajectories closer to the terrace normal. The reneutralization also acts in this direction but is much less significant than that on the terrace, since the initial distance between the  $Cl^+$  ions originating from the step site and the lower terrace is much greater. The total correction is then positive, and the true Si-Cl bonding angle will be somewhat higher than the zero field  $Cl^+$  emission angle,  $\theta_0$ , reported here.

### C. Structural Model of Step Sites Based on Chlorine Bonding

The proposed structure of the adsorption sites on the vicinal  $Si(100)$  is presented on Figure 4. This assignment is in qualitative agreement with the theoretical model proposed by Chadi. The Chadi model, where the step dangling bond preserves closely the polar angle orientation of the dangling bond of the terraces (as in Fig. 4), is supported by this work. In contrast, the Aspen and Ihm model would exhibit a step site dangling bond oriented close to the  $\langle 100 \rangle$  terrace normal direction, which is inconsistent with our observation.

## IV. CONCLUSION

We have performed a detailed analysis of chlorine bonding on the 2-atom layer height step site of a vicinal  $Si(100)$  surface. After  $Cl_2$  saturation adsorption

at 140K, we observe the  $\text{Cl}^+$  emission in the  $\langle 100 \rangle$  terrace normal direction, and in the downstairs step direction (inclined from the  $\langle 100 \rangle$  direction towards the  $\langle 011 \rangle$  direction). The  $\langle 100 \rangle$  directed  $\text{Cl}^+$  emission originates from the bridge bonded Cl on the terraces, and the downstairs step  $\text{Cl}^+$  emission from the terminally bonded Cl on the step sites. Upon annealing to 673K, the normal  $\text{Cl}^+$  beam transforms to two equal  $\text{Cl}^+$  beams of the terminally bonded Cl on the terrace silicon dimer sites, inclined in the vertical plane containing the Si-Si dimer bond, as also observed following annealing of a Cl layer on the "flat" Si(100) surface. The polar ion emission angle of the step Si-Cl bond (without correction to final state effects) was found to be  $24 \pm 1^\circ$  with respect to the  $\langle 100 \rangle$  direction and perpendicular to the step edge. This configuration strongly favors the Chadi model of the 2-atom layer step reconstruction. The polar angle of  $\text{Cl}^+$  emission from the terrace Si-Cl bonds was found to be in the range  $27-34^\circ$  in the very good agreement with measurements on two domain Si(100)  $(2 \times 1) + (1 \times 2)$  crystals [16].

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## Figure captions

Fig. 1: Schematic side, top, and 3-D views of the vicinal Si(100) surface with structure proposed by Chadi [1]. Reactive sites are shown in the side and top views as white circles with the specified directions of the dangling bonds shown schematically by a half filled orbital. Four coordinated bulk Si atoms are shown as filled circles. The size of the circles characterizes the height of silicon atoms along the [100] axis. The drawing is not drawn in scale and can not be used to measure the bond lengths and bond angles.

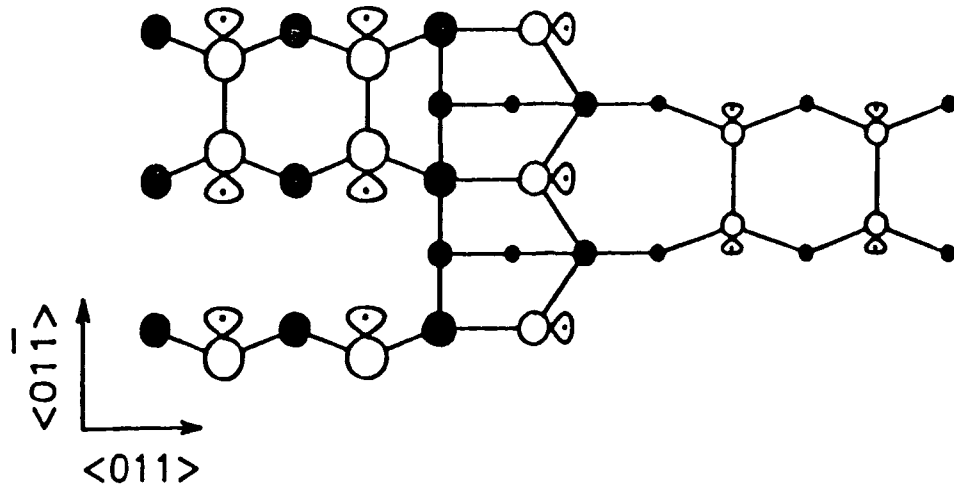
Fig. 2: The thermal development of  $\text{Cl}^+$  ESDIAD patterns for chlorine adsorption on vicinal Si(100) measured at 140K under the following conditions: electron beam energy  $E_e = 120\text{eV}$ ; crystal current  $I_e = 4\text{nA}$ ; crystal bias  $V_b = + 8\text{V}$ . (a) chlorine saturation coverage at 140K; (b) surface containing saturated chlorine layer annealed to 673K.

Fig. 3: The polar angle of the  $\text{Cl}^+$  emission from terminally bonded Cl on the terrace sites and the step sites as a function of the crystal bias. The polar angle is defined with respect to the  $\langle 100 \rangle$  terrace normal direction. The solid lines represent the computer simulation of ion trajectories in the electrostatic field of the ESDIAD analyzer.

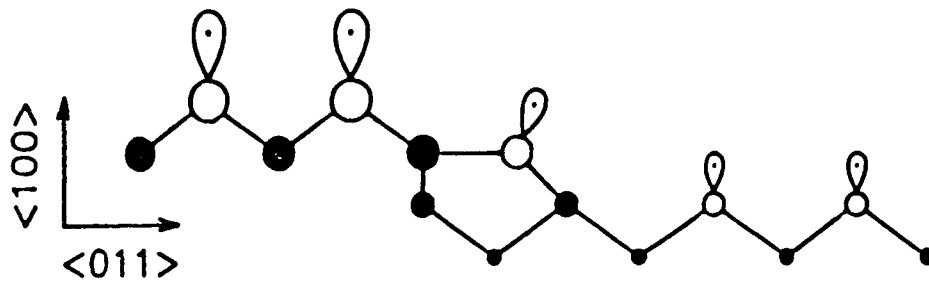
Fig. 4: The zero field polar angle of the  $\text{Cl}^+$  emission ( $\theta_0$ ) for the terrace and the step sites. The value of  $\theta_0$  is not exactly the direction of Si-Cl bond (see discussion in the text).

# Model of Surface Structure of Diatomic Steps on Vicinal Si(100) Surface (after Chadi)

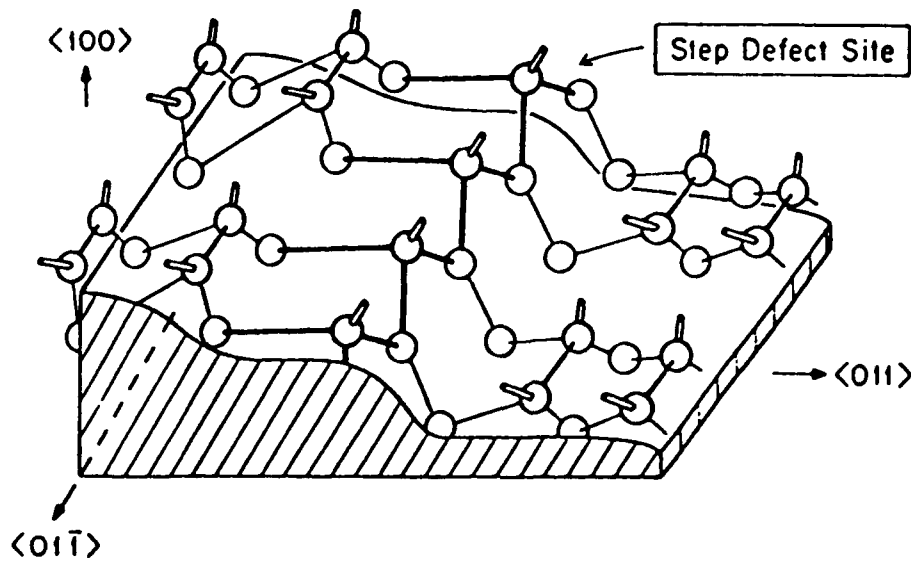
Top View



Side View



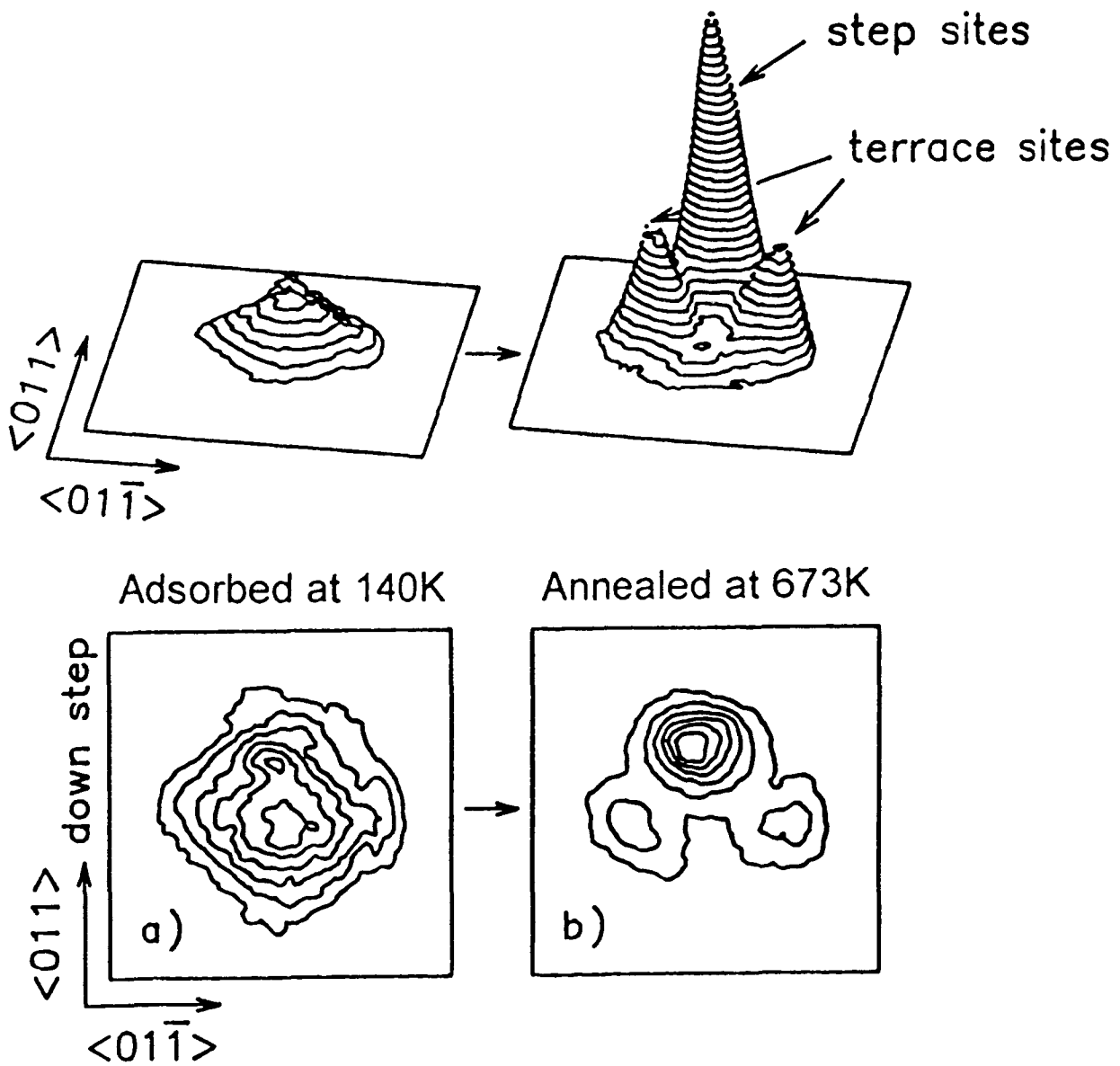
3 Dimensional View



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Figure 1

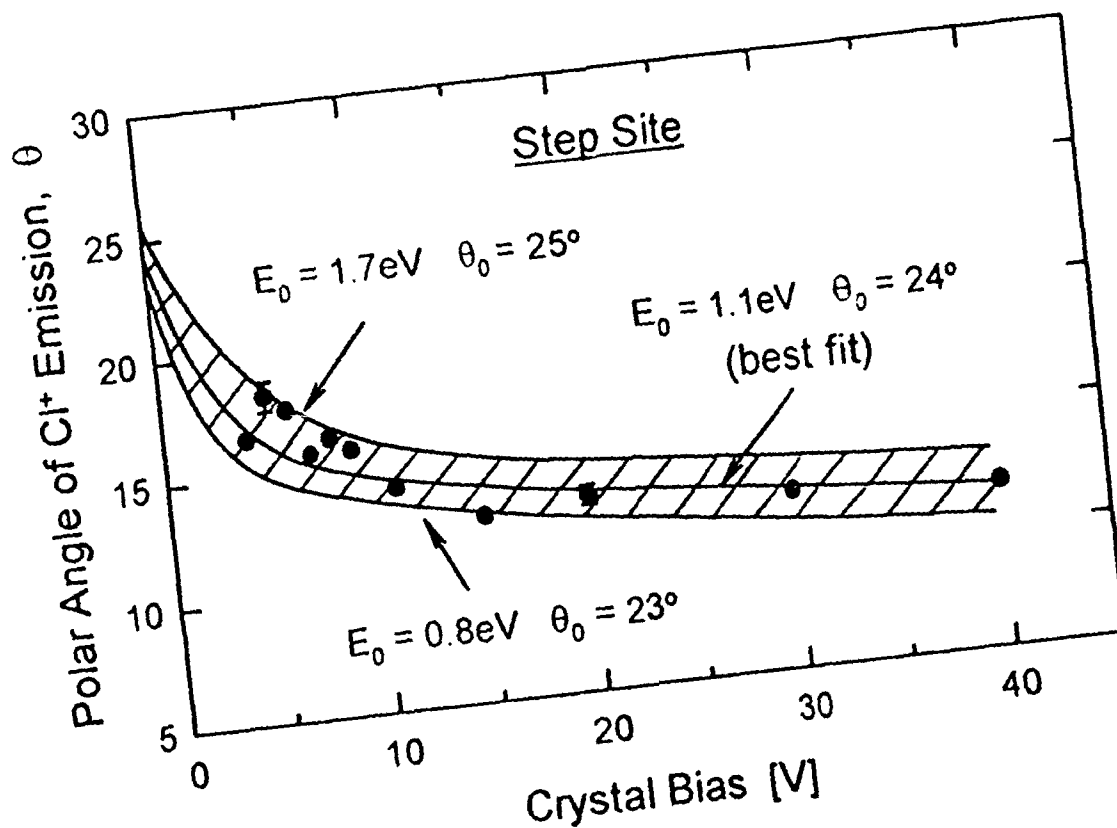
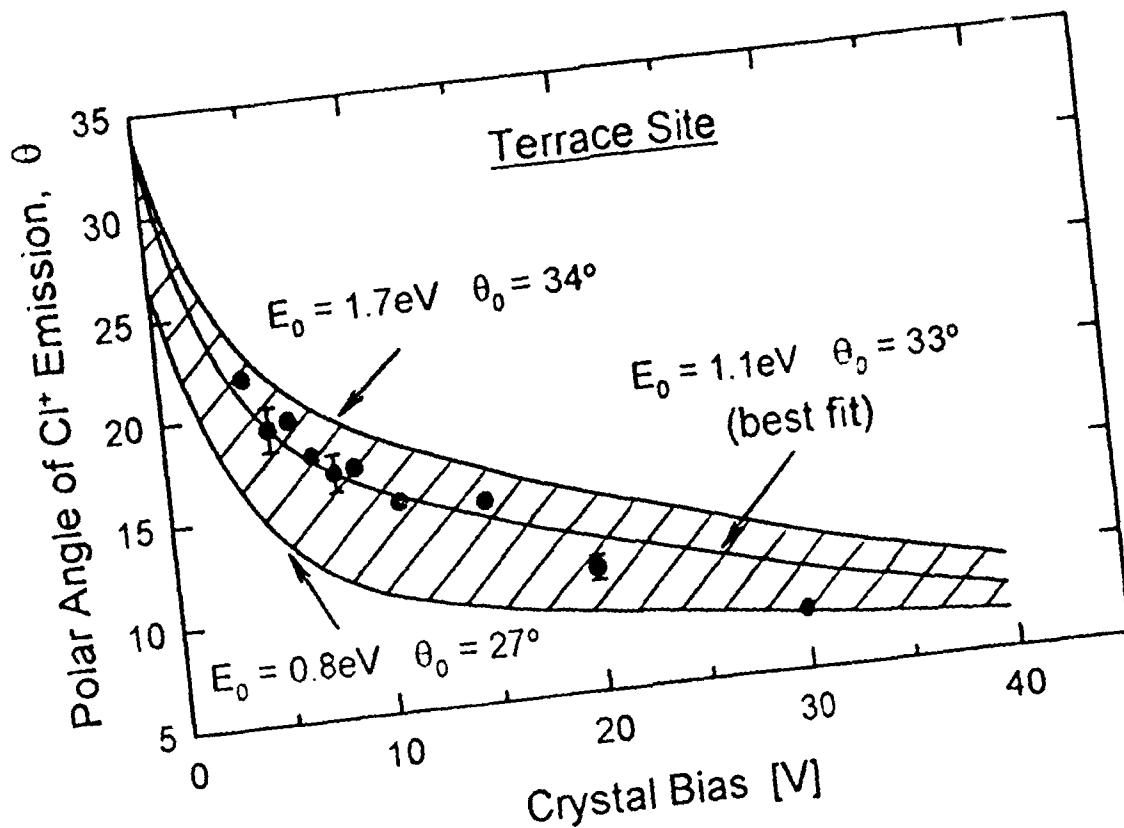
Cl<sup>+</sup> ESDIAD Patterns for Cl Adsorbed  
on Vicinal Si(100)



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Figure 2

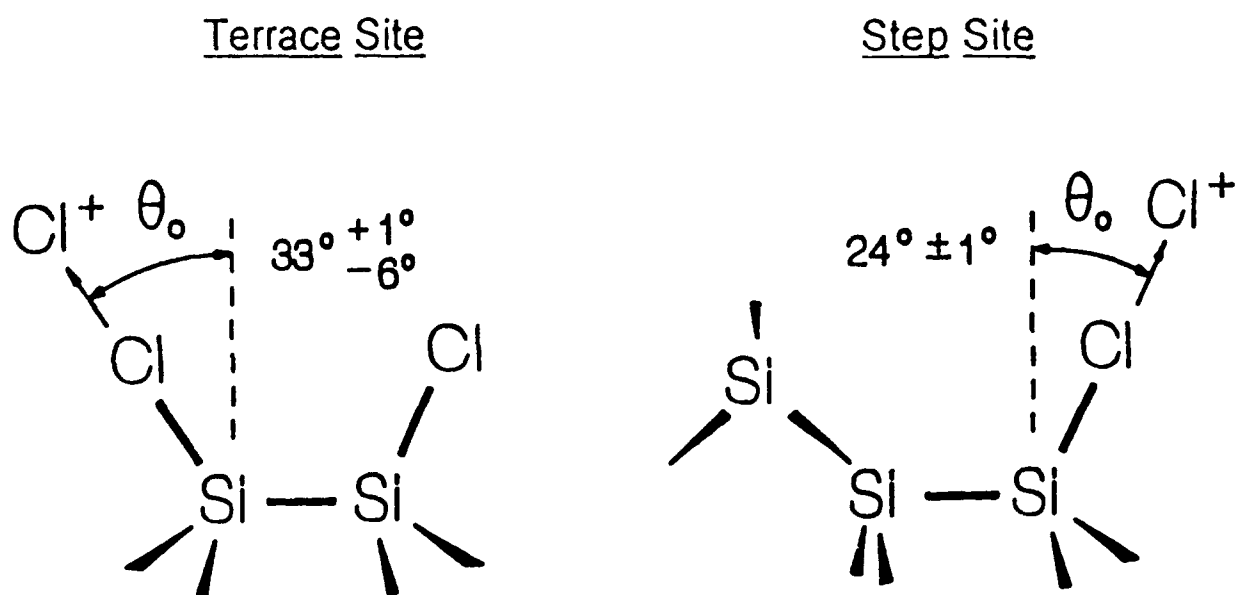
# Effect of Crystal Bias on Polar Angle of $\text{Cl}^+$ Emission (Relative to $\langle 100 \rangle$ Direction)



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Figure 3

# Bonding Configurations and Angles Determined from $\text{Cl}^+$ Emission for Cl on Vicinal Si(100)



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Figure 4

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