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Electronic properties of the *n*-doped hydrogenated silicon (100) surface and dehydrogenated structures at 5 K

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We present a comparative study of the electronic properties of the clean Si(100) and the hydrogenated Si(100):H surfaces performed with a low-temperature (5 K) scanning tunneling microscope. Various surface structures such as single silicon dangling bonds and bare silicon dimers created by local desorption of hydrogen atoms from the Si(100):H surface are also investigated. The experimental scanning tunneling spectroscopy (STS) curves acquired locally on each of these structures are compared with STS measurements performed on the Si(100) and Si(100):H surfaces. First principle density-functional theory calculations of the projected local density of states, taking into account the influence of the dopant atoms (As), enable to assign the observed STS spectra.

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I. INTRODUCTION

The development of molecular electronics requires specific substrates on which, at the same time, molecules can keep their intrinsic properties and good electronic contacts can be realized. For this purpose, the Si(100):H surface appears as a good candidate because of its ability to electronically decouple adsorbed molecules from the silicon substrate.[1,2] Moreover, this surface can be considered as a flexible medium as it can be structured—at will—by locally desorbing hydrogen atoms and thus creating lines,[3,4] spirals,[5] or more complex patterns[6] of silicon dangling bonds. However, despite being investigated at room temperature,[7–9] the electronic properties of the various observed structures on the Si(100):H surface such as single silicon dangling bonds or bare silicon dimers are still badly understood. The role of these dehydrogenated features to create, for example, contacts with single molecules is crucial and motivates the investigation of their local electronic properties.

The scanning tunneling spectroscopy (STS) is a powerful technique to locally investigate the electronic structure and properties of metallic or semiconductor surfaces. For the clean Si(100) surface, previous work, both experimental and theoretical, underlines the influence of the temperature as well as the surface reconstruction on the surface electronic structure.[10–13] The type of doping (*n* or *p*) and the nature of dopant atoms (P or As for the *n* type and B for the *p* type) also play an important role as revealed in the work of Dubois *et al.*[13] One of the main differences between the *n* type and the *p* type (i.e., the energy of the Fermi-level location) essentially results in an energy shift of the surface states of the clean Si(100) surface.[14] Although, the electronic properties of various dehydrogenated species (single silicon dangling bonds, bare silicon dimers, or lines of silicon dangling bonds) observed on the Si(100):H surface have also been the subject of a number of investigations at room temperature,[5,8,9,15,16] there are only few studies which consider the influence of the type of dopant on these local features.[15,17] Yet, the influence of the type of dopant on the Si(100):H surface reconstruction is rarely taken into account experimentally especially at low temperature.[18] From a theoretical point of view, the introduction of a dopant atom in the computation cell is specifically justified since studies of this passivated surface at low temperature require using samples with very high dopant concentrations ($\sim 10^{20}$ cm^{-3}). To our knowledge, the electronic structure of the Si(100):H surface and of dehydrogenated features has never been studied at low temperature and for high concentration of dopants.

Here, we present the first low-temperature (5 K) STS study of (i) the clean Si(100) surface, (ii) the hydrogenated Si(100):H surface, (iii) a single silicon dangling bond, and (iv) a bare silicon dimer on the Si(100):H surface. The low-temperature STS has the advantage of using low tunnel current (<100 pA) combined with stable measurements free from thermal broadening and vibronic coupling effects. In order to fully understand the STS spectra, in particular, the possible charging of the surface states, we have performed the calculations of the projected density of states (PDOS) of the Si(100):H surface and single silicon dangling bond by taking into account the type of dopant present in the silicon substrate (*n* type, As doped).

II. EXPERIMENT AND CALCULATION

Experiments are performed using a low-temperature (5 K) scanning tunneling microscope (LT-STM) (Createc) under ultrahigh-vacuum (UHV) conditions. The Si(100) samples are As doped (*n* type), with a resistivity of 5 mΩ cm. After preparing the clean Si(100)-2×1 surfaces under UHV (base pressure 5×10^{-11} Torr),[19] the sample is kept at 650 K and the hydrogenation is performed as previously reported.[20,21] After hydrogenation, the sample is cooled down and transferred to the STM chamber where all the experiments are performed at 5 K. This procedure allows having a majority of 2×1 reconstruction areas.[21] The $I(V)$ and $dI(V)/dV$ curves are acquired using an external lock-in amplifier (Standford Instruments). The measurements are performed with a voltage modulation of 36 mV at a frequency of 863 Hz and with a constant tip height (we repeated the measurements for various tip heights). Since we work at low temperature, the registered curves are repeatable with a very low noise level. Thus, the acquired STS curves do not need to be averaged and the curves presented in this paper are representative of the various collected ones.

The performed calculations which take the type of dopant into account have been carried out using the first-principles density-functional theory method implemented in the VASP code.[22–24] The geometric optimizations and the electronic properties calculations were performed using the projector augmented wave approach[25] and the Perdew-Wang (PW91) formulation of the generalized gradient approximations for the exchange and correlation terms.[26] The Si(100) surface is modeled by a periodically repeated (6×6) slab containing four Si layers saturated by hydrogen atoms at the bottom. The vacuum region thickness exceeds 15 Å. For the computation made on the Si(100):H surface, the top surface is recovered by a monohydride phase. In the case of the single dangling bond, one hydrogen atom is removed from the top surface. To simulate the *n*-doped surface, one substituted As atom is introduced in the third silicon atom layer. Thus, the total number of atoms in the slab is 252 for the fully hydrogenated surface and 251 for the surface with a single dangling bond. The whole system, apart from the H bottom layer, is allowed to relax until the forces on each ion are lower than 0.01 eV/Å. Due to the large size of the employed supercell Brillouin zone, integrations are performed using a single Γ point approximation.

III. RESULTS AND DISCUSSION

A. Scanning tunneling spectroscopy

For semiconductors, the surface reconstruction strongly modifies the bulk electronic properties. In the case of the Si(100)-2×1, the surface reconstruction leads to the formation of silicon dimers and the creation of specific surface states linked to the presence of σ and σ^*, and π and π^* orbitals.[27] The adsorption of a monolayer of hydrogen atoms on the Si(100) surface induces the breaking of the double Si—Si dimer bond (π and π^* orbitals) and the creation of Si—H bonds (σ and σ^* orbitals), thus keeping the 2×1 reconstruction [Fig. 1(a)]. Consequently, the STS curves of the clean Si(100) surface and the hydrogenated Si(100):H surface as well as the dehydrogenated surface structures [Figs. 1(b) and 1(c)] might contain specific signatures of these different orbitals.

Figure 2 presents the STS curves $\{I(V), dI(V)/dV$, and $[dI(V)/dV]/(I/V)\}$ acquired on the clean Si(100) surface [dark blue curves of Figs. 2(a), 2(c), and 2(e)] and on the hydrogenated Si(100):H surface [black curves of Figs. 2(b), 2(d), and 2(f)]. Note that the STM tip is placed in the middle of the silicon dimer for STS acquisition on the clean Si(100) and the fully hydrogenated surfaces. To identify the various bands that are observed in the curves measured over the Si(100) surface, we compare our curves to the ones that were obtained at room temperature[10,11] and at 77 K.[12,13] According to these studies, for a *n*-type substrate, the energy of the Si═Si dimer π band lies between −0.6 and −1.3 eV below the Fermi level while the energy of the σ band is observed between −1.4 and −2.0 eV.[11] For the unoccupied states, the energy of the Si═Si dimer π^* band lies between +0.2 and +1.1 eV above the Fermi level and the energy of the σ^* band between +1.4 and +1.9 eV. Note that for these bands some slight energy shifts can be observed due to the buckling of the Si dimer [i.e., $c(4\times 2)$ and $p(2\times 2)$] and to the presence of step edges near the location of the STS curves acquisition.[11] We emphasize here that on the clean Si(100) surface, the ensuing σ and σ^* bands are located on the Si—Si dimer[11] and on the Si—Si back bonds (BB) of the dimer. Indeed, as reported in Refs. 12 and 13, the Si—Si dimer back bonds formed between the silicon atoms of the first and the second layers play a significant role in the STS curves measured with a band usually observed around +1 eV above the Fermi level for the *n*-type substrate.

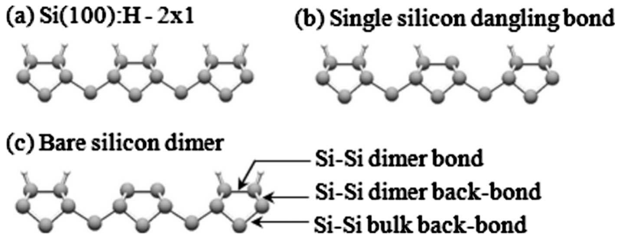

FIG. 1. (a) Cross-sectional view of the Si(100):H-2×1 surface and the dehydrogenated structures: (b) a single silicon dangling bond and (c) a bare silicon dimer. The silicon atoms are in gray and the hydrogen atoms in white. The nomenclature of the σ and σ^* Si—Si bonds is specified in (c).

Considering the above arguments, for the positive voltages, the broadband spreading from +0.2 to +1 eV in the STS curve acquired on the Si(100) at 5 K [dark blue curves of Figs. 2(c) and 2(e)] can be assigned to the π^* bands of the silicon dimers. Since this latter band is not observed in the STS curve of the Si(100):H surface [Figs. 2(d) and 2(f)], the unoccupied π^* character, inherent to the 2×1 reconstruction, is confirmed. In the same way, for negative surface voltages, the signature of the π band can be observed in the STS curve of the Si(100) surface [see the band between −0.6 and −1.1 eV in the curves in Figs. 2(c) and 2(e)] while it is missing in the STS curve of the Si:H surface [Figs. 2(d) and 2(f)]. These attributions for the clean Si(100)-2×1 surface are in agreement with the previous reports in the literature.[11,13]

Contrary to the case of the π and π^* bands, there are similar STS bands that can be observed in both Si(100) and Si(100):H spectra. These bands are centered at ∼−1.4 eV in the occupied states and spread from +1.2 to +2 eV in the unoccupied states. According to Refs. 12 and 13, these bands cannot be mainly ascribed to the single Si—Si dimer bond but rather to the Si—Si back bonds of the Si dimer. This assignment is confirmed when STS measurements [Fig. 2(f)] are performed on a dihydride silicon atom of the 3×1 re-

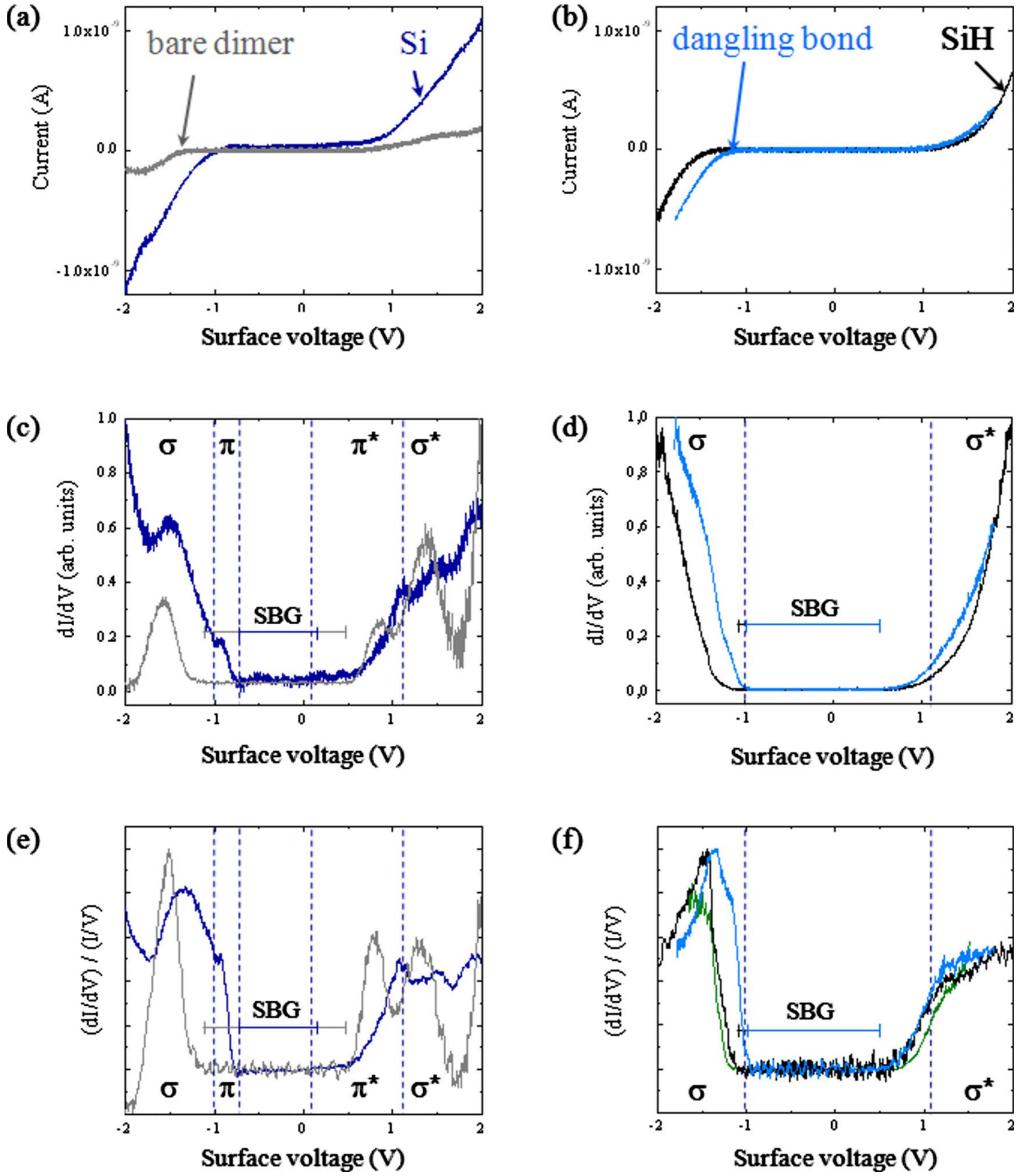

FIG. 2. (Color online) (a) Comparison of the $I(V)$ curves of the clean Si(100) (dark blue curve) and single bare silicon dimer (gray curve), and (b) comparison of the $I(V)$ curves of the hydrogenated Si(100):H (black curve) and single silicon dangling bond (light blue curve). (c) and (d) are same as (a) and (b), respectively, but for the $dI(V)/dV$ curves. (e) and (f) same as (a) and (b), respectively, but normalized $(dI(V)/dV)/(I/V)$ curves. In (f) the normalized STS curve recorded on a dihydride Si atom is added (green curve). Energy zones for the σ, π, π^*, and σ^* bands are indicated as well as the SBG.

construction or of the bow-tie structures.[21] Indeed, on these dihydrogenated structures, the single Si—Si dimer bonds (σ and σ^* bands) do not exist anymore. Thus, the fact that the STS spectra acquired on these dihydride structures show very similar STS bands suggests that they are mainly due to σ and σ^* orbitals from the Si—Si back bonds instead of the Si—Si dimers.[11,13]

Single silicon dangling bonds [Fig. 1(b)] and bare silicon dimers [Fig. 1(c)] can be formed on the Si(100):H-2×1 surface by using the STM tip as a local electron source to desorb single H atoms.[28] The corresponding STS curves are presented in Fig. 2.

The $dI(V)/dV$ and the normalized spectra [gray curves in Figs. 2(c) and 2(e)] acquired at 5 K on the bare dimer present three distinct narrow bands: one at −1.5 eV in the occupied states and two at +0.8 and +1.3 eV in the unoccupied states. These bands are assigned to the σ, π^*, and σ^* bands, respectively. The main difference between the spectra of the clean Si(100) surface and the bare silicon dimer on the Si(100):H surface is the absence of the π band in the latter case. In fact,

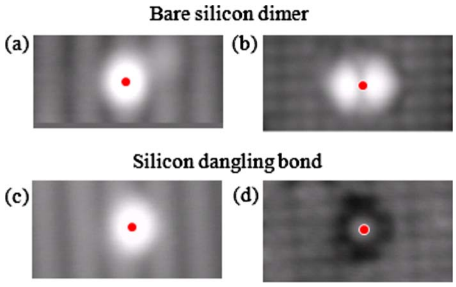

FIG. 3. (Color online) STM topographies ($3.8\times 2.0\ \text{nm}^2$) on the Si:H surface of a bare silicon dimer (a) in the occupied states ($V_S=-1.7$ V and $I=110$ pA) and (b) in the unoccupied states ($V_S=1.8$ V and $I=110$ pA), and of a single silicon dangling bond (c) in the occupied states ($V_S=-1.7$ V and $I=70$ pA) and (d) in the unoccupied states ($V_S=1.7$ V and $I=70$ pA). The red dots indicate the location of the tip during the recording of the STS curves.

the π band can be seen on the clean Si(100) surface because of a strong delocalization along the silicon dimer rows which enables electron transport across the surface even though the π band has an energy located within the bulk band gap.[9,29] In the case of the bare silicon dimer on the Si(100):H surface, the π orbital cannot be seen with the STM since the current cannot flow trough this localized π orbital.

The STS spectra acquired on a single silicon dangling bond formed on the Si(100):H surface are shown in Figs. 2(b), 2(d), and 2(f). As compared to the STS spectrum of the hydrogenated Si(100):H surface, the main difference is the energy shift of the σ band toward higher energies for the single silicon dangling bond. This is most probably due to the upward band bending produced by the negative charging of the silicon dangling bond (see Sec. III C).

B. STM topographies

STM topographies of a single silicon dangling bond [Fig. 1(b)] and a bare silicon dimer [Fig. 1(c)] created on the Si(100):H-2×1 surface are presented in Fig. 3. In the unoccupied states, the bare dimer is seen as two bright lobes separated by a darker line [Fig. 3(b)]. Similar features can be observed at room temperature[8] and 120 K (Ref. 9) with the same apparent symmetry. Such symmetrical feature suggests that either the corresponding bare dimer is not buckled [Fig. 1(c)] or is switching randomly between two stable buckled positions during the STM topography (i.e., the mean position of the dimer is observed). Since our experiments are performed at low temperature (5 K) and with low perturbing scanning parameters (e.g., +1.7 eV and 110 pA), the second hypothesis can be reasonably ruled out.[19] Acquired at +1.7 eV, the unoccupied state STM topography of the bare dimer feature [Fig. 3(b)] must correspond to tunnel current flowing through a mixture of π^* orbital of the double Si—Si dimer bond and σ^* orbital of the Si—Si back bonds of the same dimer. This assignment agrees with previous work performed at room temperature and 120 K.[9,11] The bright protrusion observed in the occupied state STM topography of the bare silicon dimer [Fig. 3(a)] should merely result from tunnel current flowing through the σ band of the Si—Si dimer back bonds[11,13] when STM topography is performed at $V_S=-1.7$ V.

In the STM topography of Fig. 3(c), the single dangling bond appears, for negative surface voltages, as a bright protrusion off center with respect to the dimer row (here on the right side of the dimer row). For positive surface voltages [Fig. 3(d)], the STM topography of the single dangling bond shows a smaller gray protrusion surrounded by a dark halo similarly to what has been observed at room temperature.[15,17] This characteristic unoccupied STM topography is explained by the fact that, on *n*-type substrates, the single dangling bond acquires an extra electron (see Sec. III C), thus inducing a positive charge screening in its surrounding [the dark halo observed in Fig. 3(d)]. In other words, the dangling bond created after the desorption of a single H atom corresponds to one of the Si hybridized sp^3 orbitals which, in the neutral state, contains a single electron. However, on strongly doped *n*-type substrates, a bulk electron can be stabilized in this sp^3 orbital leading to a localized negatively charged state.[15,17]

C. Calculations

To support our experimental results, we performed the calculation of the density of states on a large silicon slab ($1.2\ \text{nm}^3$) allowing us to take into account the presence and

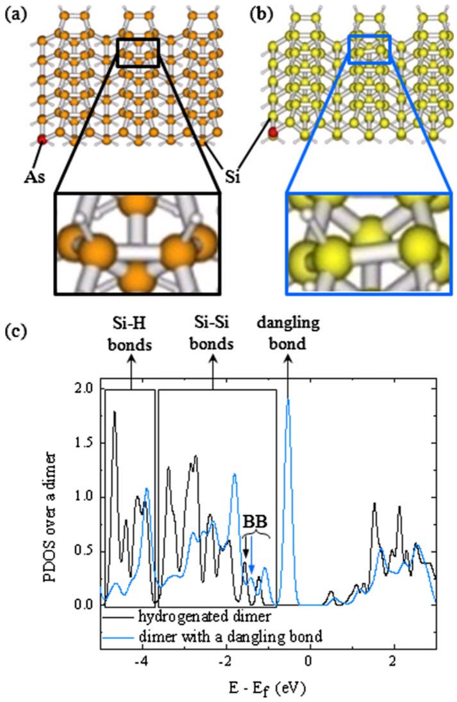

FIG. 4. (Color online) (a) Calculation slab for the fully hydrogenated surface and (b) the same surface with a single silicon dangling bond. Zooms are realized on the silicon dimer considered to project the densities of states. (c) PDOSs on a hydrogenated silicon dimer (black curve), which is composed of two silicon atoms and two hydrogen atoms [black rectangle in (a)] and a silicon dimer with a single dangling bond (light blue curve), which is composed of two silicon atoms and a sole hydrogen atom [light blue rectangle in (b)]. BB corresponds to the Si—Si dimer back bonds.

the nature of the dopant atom. As previously explained (Sec. II), this is realized by replacing a single Si atom of the slab by an arsenic atom [see Figs. 4(a) and 4(b)]. Thus, the relaxation of the slab gives us additional information on the geometry of the silicon dimers. Indeed, for a fully hydrogenated surface [Fig. 4(a)] the Si dimers are found to be symmetrical, similar to previous reports.[30] However, for the case of a silicon dimer with a single silicon dangling bond [Fig. 4(b)], the Si dimer is shown to be tilted at an angle of 7.5° with respect to the surface plane. Indeed, the presence of As dopant atom in the slab induces a charge transfer from the As atom to the silicon dangling bond. In this case, the silicon atom with the charged dangling bond is higher than the Si atom bonded with the H atom. It is interesting to compare this specific dimer geometry with the fully hydrogenated silicon dimer and the individual bare silicon dimer which are both symmetrical.[9] Indeed, the fact that the silicon atoms of the bare dimer are at the same height, identical to the fully hydrogenated dimer, suggests that the bare silicon dimer is neutral. This is also supported by the absence of a dark halo surrounding the two bright features observed in Fig. 3(b).

For the relaxed structures presented in Figs. 4(a) and 4(b), we calculated the PDOS on a single silicon dimer which is either completely hydrogenated [black curve in Fig. 4(c)] or with a single silicon dangling bond [light blue curve in Fig. 4(c)]. In this figure, we can see that the presence of the silicon dangling bond (light blue curve) reveals a specific band centered −0.5 eV below the Fermi level. In addition, compared to the fully hydrogenated dimer, there is a clear energy shift, toward higher energies, of the PDOS bands of the Si—Si BB whose energy lies between −0.5 and −1.9 eV below the Fermi level. This is in good agreement with the experimental STS spectra [Figs. 2(d) and 2(f)] on which the surface band gap (SBG) measured over the silicon dangling bond is slightly reduced in the negative voltage part compared to the Si:H surface. As explained in Sec. III A, this energy shift might originate from the upward band bending due to the negatively charged silicon dangling bond.

We note that the occupied dangling-bond state calculated at −0.5 eV below the Fermi level cannot be seen in the STS spectra of Figs. 2(b), 2(d), and 2(f) while a localized bright feature can be observed on the STM topography of Fig. 3(c). This suggests that the energy shift of the back-bond peaks is favorable to create hybridization with the tail of the dangling-bond band. Thus, when STM topographies are acquired at a surface voltage $V_S < -1.7$ V [Fig. 3(a)] the tunnel electrons, which are mainly flowing through the occupied states of the σ orbitals of the Si—Si back bonds can probe the localized dangling-bond feature because of this coupling. The fact that the dangling bond peak centered at −0.5 eV below the Fermi level cannot be seen in the experimental STS spectra is specific to low temperature. Indeed, previous studies performed at room temperature show STS curves recorded over the dangling bond with two peaks close to the Fermi level: one in the occupied and one in the unoccupied states.[5,31] This difference suggest that, at room temperature, the dangling-bond state is coupled, through vibronic modes, to other conducting surface states.[32,33]

IV. CONCLUSION

This paper reports the first low-temperature (5 K) scanning tunneling spectroscopy of the clean Si(100) and hydrogenated Si(100):H surfaces as well as single silicon dangling bond and bare silicon dimer created on the Si(100):H surface. We also report the first corresponding density of state calculations of the hydrogenated Si(100):H surface and single silicon dangling bond taking into account the doping of the silicon substrate.

Comparison between experimental STS and calculated DOS enables to assign the various observed electronic structures. In particular, the observed Si—Si σ bands are assigned to the Si—Si back bonds rather than to single Si—Si dimer bond. Single bare silicon dimers are found to be symmetric, in agreement with their neutral character. On the contrary, single silicon dangling bonds are found to be asymmetric and negatively charged with a unity charge transferred from the silicon substrate. However, the corresponding silicon dangling-bond state cannot be directly observed in STS measurements due to the electronic decoupling from the conductive surface channels at low temperature.

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[1] A. Bellec, F. Ample, D. Riedel, G. Dujardin, and C. Joachim, Nano Lett. **9**, 144 (2009).

[2] F. Ample and C. Joachim, Surf. Sci. **602**, 1563 (2008).

[3] P. Doumergue, L. Pizzagalli, C. Joachim, A. Altibelli, and A. Baratoff, Phys. Rev. B **59**, 15910 (1999).

[4] T. Hitosugi, S. Heike, T. Onogi, T. Hashizume, S. Watanabe, Z. Q. Li, K. Ohno, Y. Kawazoe, T. Hasegawa, and K. Kitazawa, Phys. Rev. Lett. **82**, 4034 (1999).

[5] T. Hitosugi, T. Hashizume, S. Heike, H. Kajiyama, Y. Wada, S. Watanabe, T. Hasegawa, and K. Kitazawa, Appl. Surf. Sci. **130-132**, 340 (1998).

[6] L. Soukiassian, A. J. Mayne, M. Carbone, and G. Dujardin, Surf. Sci. **528**, 121 (2003).

[7] A. J. Mayne, D. Riedel, G. Comtet, and G. Dujardin, Prog. Surf. Sci. **81**, 1 (2006).

[8] J. J. Boland, Phys. Rev. Lett. **67**, 1539 (1991).

[9] D. Chen and J. J. Boland, Phys. Rev. B **65**, 165336 (2002).

[10] K. Hata, Y. Shibata, and H. Shigekawa, Phys. Rev. B **64**, 235310 (2001).

[11] H. Okada, Y. Fujimoto, K. Endo, K. Hirose, and Y. Mori, Phys. Rev. B **63**, 195324 (2001).

[12] L. Perdigão, D. Deresmes, B. Grandidier, M. Dubois, C. Delerue, G. Allan, and D. Stiévenard, Phys. Rev. Lett. **92**, 216101 (2004).

[13] M. Dubois, L. Perdigao, C. Delerue, G. Allan, B. Grandidier, D. Deresmes, and D. Stiévenard, Phys. Rev. B **71**, 165322 (2005).

[14] H. Luth, *Surfaces and Interfaces of Solid Materials* (Springer, Berlin, 1995).

[15] L. Liu, J. Yu, and J. W. Lyding, *Nanoptterning–From Ultralarge-Scale Integration to Biotechnology*, MRS Symposia Proceedings No. 705 (Materials Research Society, Pittsburgh, 2002), p. Y6.6.1.

[16] K. Bobrov, G. Comtet, G. Dujardin, and L. Hellner, Phys. Rev. Lett. **86**, 2633 (2001).

[17] M. B. Haider, J. L. Pitters, G. A. DiLabio, L. Livadaru, J. Y. Mutus, and R. A. Wolkow, Phys. Rev. Lett. **102**, 046805 (2009).

[18] Y. Suwa, S. Matsuura, M. Fujimori, S. Heike, T. Onogi, H. Kajiyama, T. Hitosugi, K. Kitazawa, T. Uda, and T. Hashizume, Phys. Rev. Lett. **90**, 156101 (2003).

[19] D. Riedel, M. Lastapis, M. G. Martin, and G. Dujardin, Phys. Rev. B **69**, 121301(R) (2004).

[20] J. J. Boland, Adv. Phys. **42**, 129 (1993).

[21] A. Bellec, D. Riedel, G. Dujardin, N. Rompotis, and L. N. Kantorovich, Phys. Rev. B **78**, 165302 (2008).

[22] G. Kresse and J. Hafner, Phys. Rev. B **49**, 14251 (1994).

[23] G. Kresse and J. Furthmuller, Comput. Mater. Sci. **6**, 15 (1996).

[24] G. Kresse and J. Furthmuller, Phys. Rev. B **54**, 11169 (1996).

[25] P. E. Blochl, Phys. Rev. B **50**, 17953 (1994).

[26] Y. Wang and J. P. Perdew, Phys. Rev. B **44**, 13298 (1991).

[27] J. A. Kubby and J. J. Boland, Surf. Sci. Rep. **26**, 61 (1996).

[28] L. Soukiassian, A. J. Mayne, M. Carbone, and G. Dujardin, Phys. Rev. B **68**, 035303 (2003).

[29] K. Sagisaka and D. Fujita, Phys. Rev. B **72**, 235327 (2005).

[30] S. Watanabe, Y. A. Ono, T. Hashizume, and Y. Wada, Phys. Rev. B **54**, R17308 (1996).

[31] J. J. Boland, J. Vac. Sci. Technol. A **10**, 2458 (1992).

[32] M. Berthe, A. Urbieta, L. Perdigão, B. Grandidier, D. Deresmes, C. Delerue, D. Stiévenard, R. Rurali, N. Lorente, L. Magaud, and P. Ordejón, Phys. Rev. Lett. **97**, 206801 (2006).

[33] G. Dujardin, A. J. Mayne, and F. Rose, Phys. Rev. Lett. **89**, 036802 (2002).