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Atomic structure of steps and defects on the clean diamond (100)-2×1 surface studied using ultrahigh vacuum scanning tunneling microscopy

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We report ultrahigh vacuum scanning tunneling microscopy studies of the clean nonhydrogen-terminated diamond (100)-2×1 surface showing single- and double-layer steps that are rebonded. The main defects observed are single, multiple, and row dimer vacancies, and antiphase boundaries. Buckling of dimers is not observed, consistent with symmetric dimers.

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Diamond films grown using chemical vapor deposition (CVD) have a wide range of technological applications due to the unique properties of this material.¹ The atomic structure of steps and defects on the surface plays an important role in the growth of films and nanostructures.² Smooth diamond (100) surfaces are typically produced by exposing the sample to atomic hydrogen at substrate temperatures $\geq 900^\circ\text{C}$, resulting in an inert monohydride-terminated 2×1 dimer reconstructed surface, denoted as diamond (100)-2×1:H.¹ Scanning tunneling microscopy (STM) studies of this surface in air have shown that it consists of single- and double-layer steps that are thought to be nonbonded, dimer vacancies, and local 3×1 reconstructions.^{1,3} The clean nonhydrogen-terminated diamond (100)-2×1 surface is produced by annealing the diamond (100)-2×1:H surface at 1000°C in UHV.¹ The diamond (100)-2×1 surface is reactive, and has been investigated as a substrate for metal films,⁴ buckyballs,⁵ functionalized organic molecules,⁶ and mechanosynthesis of nanostructures.⁷ To our knowledge, the atomic structure of steps and defects on the diamond (100)-2×1 surface has not been reported. In this letter, we report UHV STM studies of the diamond (100)-2×1 surface showing single- and double-layer steps that are rebonded. The main types of defects observed are single, multiple, and row dimer vacancies, and antiphase boundaries. Buckling of dimers is not observed, in agreement with theoretical predictions that dimers are symmetric.

Figure 1 shows schematic representations of single S_A and S_B , and double D_A steps on the (100)-2×1 surface of the diamond lattice.⁸ Open circles denote atoms having dangling bonds and dark circles denote atoms having no dangling bonds. The subscripts A and B denote steps having dimer rows on the top plane perpendicular and parallel to the step, respectively. On the diamond (100)-2×1:H surface, D_B steps are typically not observed.³ As shown in Fig. 1(a), rebonded S_B steps have edge atoms on the bottom plane that are bonded. For such steps, dimer rows on the upper plane end at troughs between dimer rows on the bottom plane, and

the distance from edge dimers on the upper plane to the nearest full dimer row on the bottom plane is $3d$, where d is the lattice constant of the 1×1 surface. For nonbonded S_B steps, dimer rows on the upper plane end at dimer rows on the bottom plane, and the distance from edge dimers to the nearest dimer row on the bottom plane is $2d$, as shown in Fig. 1(b). D_A steps consist of an S_A step on an S_B step, and have edge atoms on the bottom plane that are rebonded or nonbonded in a manner similar to that of S_B steps.² Theoretical⁸ and STM^{2,9} studies of S_B and D_A steps on the Si (100)-2×1 surface have shown that rebonded steps are energetically more favorable than nonbonded steps because they have fewer dangling bonds per step length. In contrast, recent theoretical studies of S_B and D_A steps on the diamond (100)-2×1 surface predict that nonbonded steps are more favorable than rebonded steps because carbon dimers form strong double bonds that effectively reduce the number of dangling bonds.¹⁰

Epitaxial diamond (100) films were grown on 2×2×0.25 mm³ type 2b (100) diamond substrates. The films were grown for 2 h in a UHV compatible hot-tungsten fila-

FIG. 1. Schematic representations of S_B , S_A , and D_A steps.

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FIG. 2. UHV STM image of the clean diamond (100)- 2×1 surface.

ment CVD reactor and were approximately $2\ \mu\text{m}$ thick. The reactor is coupled to a UHV STM chamber at a pressure $<10^{-10}$ Torr via an all-metal through-valve. The CVD growth pressure was 30 Torr with hydrogen and methane flow rates of 200 and 0.5 sccm, respectively. The films were doped with boron during growth using diborane gas at a concentration of 10 ppm relative to hydrogen in order to increase their conductivity for STM studies. The substrate and filament temperatures were 900 and 2200 $^{\circ}\text{C}$, respectively. After growth, the films were exposed to atomic hydrogen for 10 min at 900 $^{\circ}\text{C}$ to produce a smooth surface. This was accomplished by shutting off the methane flow and maintaining all of the other parameters for 10 min. The filament, sample heater and then the hydrogen flow were turned off. The CVD reactor was evacuated to 1×10^{-8} Torr using a turbomolecular pump and the samples were transferred to the UHV STM chamber via a linear translator without contaminating them by exposure to air. The samples were then heated to 1000 $^{\circ}\text{C}$ in UHV to desorb the hydrogen and produce a clean diamond (100)- 2×1 surface. STM imaging was performed for filled states using a sample bias of -1.0 to -1.5 V, and tunneling current of about 1 nA.

Figure 2 shows a UHV STM image of a clean diamond (100)- 2×1 surface prepared as described previously, showing S_B , S_A , and D_A steps. Figure 3(a) is a higher resolution image showing that edge atoms on the bottom plane of an S_B step have a bonding configuration that is different than that of a dimer row, as observed near regions marked "R." Figure 3(b) shows a high-resolution image of the S_B step near the center of Fig. 3(a), and a superimposed schematic of a rebonded S_B step. As shown in Fig. 3(b), the distance from edge dimers on the upper plane to the nearest full dimer row on the bottom plane is $3d$, in agreement with a rebonded step. The STM images of rebonded steps in Fig. 3 are similar to those reported for the Si (100)- 2×1 surface.^{2,9} In Fig. 3, the rebonded rows consist of bright regions that occur at locations corresponding to atoms 1 and 2 in Fig. 1(a). We attribute the bright regions to a bond between atoms 1 and 2. In Fig. 3(b), the dimer row on the top plane, indicated by the unmarked arrow, forms a local nonbonded step. Local nonbonded steps on the Si (100)- 2×1 surface have been ob-

FIG. 3. (a) UHV STM image of the diamond (100)- 2×1 surface showing rebonded S_B steps. (b) High-resolution UHV STM image of the S_B step near the center of (a) and a superimposed schematic of a rebonded S_B step.

served and are thought to be stabilized by vacancies.² Therefore, we attribute the nonbonded step in Fig. 3(b) to vacancy V shown in Fig. 3(a).

Figure 4 shows a UHV STM image of a D_A step on the diamond (100)- 2×1 surface. Edge atoms on the bottom plane have a bonding configuration that is the same as that observed for rebonded S_B steps, indicating a rebonded D_A step. All observed S_B and D_A steps were rebonded. These observations contradict recent theoretical predictions that, on the diamond (100)- 2×1 surface, nonbonded S_B and D_A steps are more favorable than rebonded ones.¹⁰

In addition, Figs. 2 and 3(a) show defects consisting of dimer vacancies, indicated by V, that are single, multiple, and arranged in rows parallel and perpendicular to dimer rows. The density of single and multiple vacancies is about $8\times 10^{12}/\text{cm}^2$, less than in Si.^{2,3} Also observed are a large num-

FIG. 4. UHV STM image of the diamond (100)- 2×1 surface showing a rebonded D_A step.

ber of antiphase boundaries, indicated by P, in which dimer rows are shifted by d . The antiphase boundaries are observed only on type A steps and have a density of about $5 \times 10^{11}/\text{cm}^2$. As shown in Figs. 2 and 3(a), antiphase boundaries occur such that the phase shift is accommodated at a step edge, or vacancy row that is perpendicular to the boundary and has widths of d and $2d$ on either side of the boundary. Antiphase boundaries on the diamond (100)- 2×1 :H surface are accommodated by local 3×1 reconstructions.³ Therefore, we believe antiphase boundaries are formed during exposure to atomic hydrogen and remain after the hydrogen is desorbed. Additional annealing of the sample at 1000 °C in UHV did not change the step distribution or defect density, consistent with the low mobility of atoms due to the high Debye temperature of diamond of 1590 °C.¹

The STM images do not show evidence of buckled dimers. In particular, stabilization of buckled dimers by steps and vacancy defects is not observed. In contrast, such stabilization of buckled dimers has been reported on the Si (100)- 2×1 surface at room temperature.^{2,9} Our observations are consistent with theoretical predictions that dimers on the diamond (100)- 2×1 surface are symmetric, and dimers on the Si (100)- 2×1 surface are asymmetric.¹¹

In summary, we have used UHV STM to study the atomic structure of steps and defects on the clean diamond (100)- 2×1 surface. We observe that S_B and D_A steps are

rebonded, in contradiction with recent theoretical predictions. The main defects observed are single, multiple, and row dimer vacancies, and antiphase boundaries. The step distribution and defect density do not change by annealing at 1000 °C. We do not observe buckling of dimers, consistent with symmetric dimers.

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¹See, for example, *Handbook of Industrial Diamonds and Diamond Films*, edited by M. Prelas, G. Popovici, and L. Bigelow (Marcel Dekker, New York, 1998).

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