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Correlation Switching Between 3x1 and 6x1 Surface Reconstructions on Si(111) with Submonolayer Ag Adsorption

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Title: Correlational switching between 3x1 and 6x1 surface reconstructions on Si(111) with submonolayer Ag adsorption.

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Abstract:

Electron correlations are strongly enhanced in low dimensional systems. Taking correlations as the dominant mechanism, we provide an explanation of the recently observed electrostatically enforced structural phase transition (3x1 to 6x1) on a Si(111) surface with sub-monolayer Ag adsorption.

Key Words: silicon, surface reconstruction, correlations, ultrafast computing

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Main Text:

Submonolayer adsorption of monovalent metal atoms leads to a 3x1 reconstruction of the Si(111) surface [1]. A model which accounts well for most of the experimental data was proposed by Weitering and coworkers [2]. In this model, five-fold Si rings form quasi-one dimensional π-bonded Si chains along the [110] direction, separated by channels which can accommodate up to 1/3 monolayer of atoms. In order to account for the large band gap of this surface, Weitering et al suggested that the π-bonded Si chains undergo a Peierls-like distortion, resulting in alternating single-double bonds along the chain direction, similar to the bond order wave in polyacetylene. Fig.1a shows the outermost layer of the Si(111)3x1-metal surface according to this model.

Recently, Carpinelli and Weitering observed in STM images an intriguing "switch" of the Si(111)-Ag surface from 3x1 into 6x1 reconstruction [1], which was caused, apparently, by the STM tip-surface interaction. In this scenario, the STM tip causes a "flip" of the dimerized chain such that each double bond is shifted by one half period along the chain. The dynamics of the "switch" most likely involves the propagation of a soliton [1]. Fig. 2a shows the Si surface of Fig.1a after such "switch" has occurred in the middle chain. The most intriguing fact is that apparently a *long-range correlation* exists, which aligns the double bonds in neighboring chains. This results in doubling of the surface unit cell in the [100] direction, leading to long-range Si(111)6x1-Ag reconstruction.

In order to explain this fact that the neighboring chains, which are ~10Å apart, "communicate", we attempt an approach to the problem that emphasizes the correlational effects, which are expected to be crucial in this system [3,4]. We consider a classical model that includes only the π electrons that undergo a "switch" between the bonds. These electrons are allowed to collectively jump between two equivalent potential minima located at either side of the bond sites. Coulomb interactions between electrons in different chains are fully taken into account. The effect of the metal atoms depends on the configuration of their valence electrons. For alkali metals, no "active" electrons are assumed to exist at the metal sites since alkali metal atoms are known to donate their valence electrons to the Si bond in the second layer [5]. In contrast, we model the Ag atoms as having an extra electron charge "resonating" at the core. This is typical for transition metal atoms and originates from the centrifugal barrier for nonzero angular momentum in the APW equation for the radial part of the wave function (s-d hybridization)[6]. A simple double well potential can simulate the off-center confinement for such a resonating electron. We assume such double wells at each of the Ag sites.

In order to investigate the stability of the 6x1 phase, we have performed a classical Monte Carlo calculation that simulates an annealing process [7], in which, as the temperature is lowered, electrons have an increasing tendency to move in directions that lower the total energy of the system. For the Si(111)-Alkali case, we find that the 3x1 reconstruction (shown in Fig.1b) has the lowest total energy per electron. The 6x1 reconstruction represents a local minimum in the total energy that is close to, but higher than that of the 3x1 reconstruction. For example, for a 20x20 array of Si electrons, the energy per electron in the 6x1 reconstruction is higher than that in the 3x1 reconstruction by only E=0.01 eV.

For the Si(111)-Ag case, when we assume only a single electron charge associated with each Ag atom, the 6x1 reconstruction (Fig.2b) has slightly lower total energy than the 3x1 reconstruction. For the 20x20 array (now 400 Si electrons and 400 Ag electrons) the 6x1 configuration has energy per electron that is about 0.01 eV lower than that for the 3x1 case. It should be noted that this energy difference increases with increasing charge at the Ag sites.

The 3x1 and 6x1 reconstructions can, in principle, coexist at room temperature, since the small difference in total energy could be accommodated by edge, or impurity pinning. Such a coexistence of these phases has indeed been observed [1]. Also, the energy difference between the two phases is small enough that a "switch" between the phases can be induced by a biased electrode (e.g. by STM tip, as demonstrated in Ref.[1]). In principle, other metal atoms (with $l \neq 0$ for the core resonance) should also lead to 6x1 phase having lower energy.

An interesting application could be envisioned here. The bi-stability of the chains in both 3x1 and 6x1 phases could be utilized, in principle, in ultrafast computing. Imagine a set of surface domains, say 100Å x 100Å, with 3x1 (or 6x1) phases. One could identify by electrostatic means (like in STM) both states of "polarization" of the dimerized chains in each domain. Also, one could "switch" electrostatically (like in STM) the states of each domain, and thereby change the information content of such an atomic-sized memory. Such switching should be very fast (of the order of the phonon speed), operate at room temperature, and the compatibility with the Si technology might allow for a fabrication of "on-chip" electrodes capable of domain switching.

In summary, we have presented a classical model of the 3x1 and 6x1 reconstructions on Si(111)-metal surface. Using a classical Monte Carlo electron annealing simulation we have shown that the 3x1 phase is most stable for the alkali metal atoms. For the Si(111)-Ag, the 6x1 reconstruction has a slightly lower energy than the 3x1 phase. In all cases, however, both phases are found to be closely spaced, stable minima of the total energy, and therefore can coexist at room temperature. These phases can be switched by electrostatic interaction with an electrode (e.g. STM tip), or by near room temperature thermal processing (100 to 200^{0}C). The qualitative agreement of our model with experiment suggests that long-range electron correlations play a dominant role in the 3x1 and 6x1 reconstructions.

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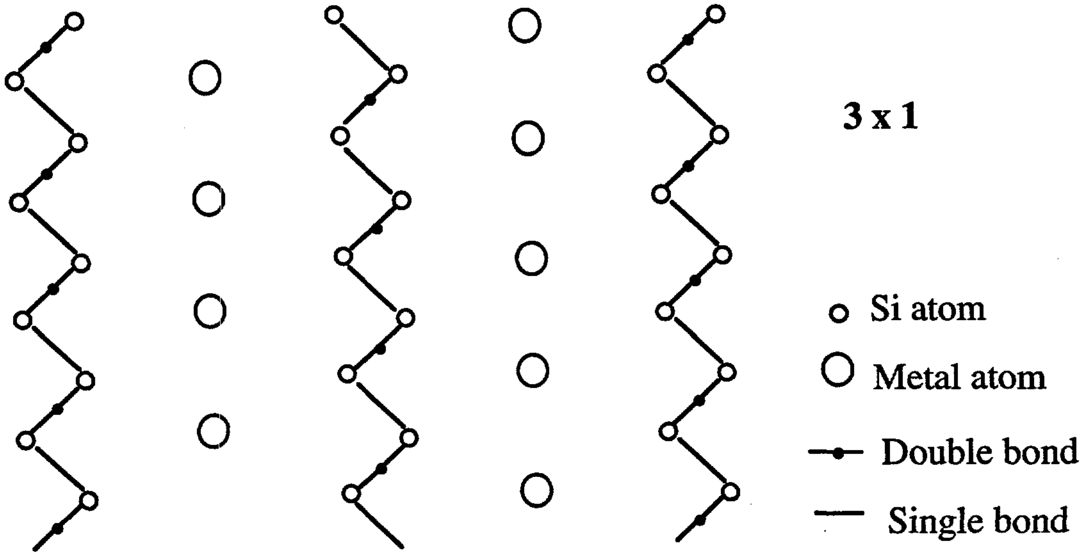
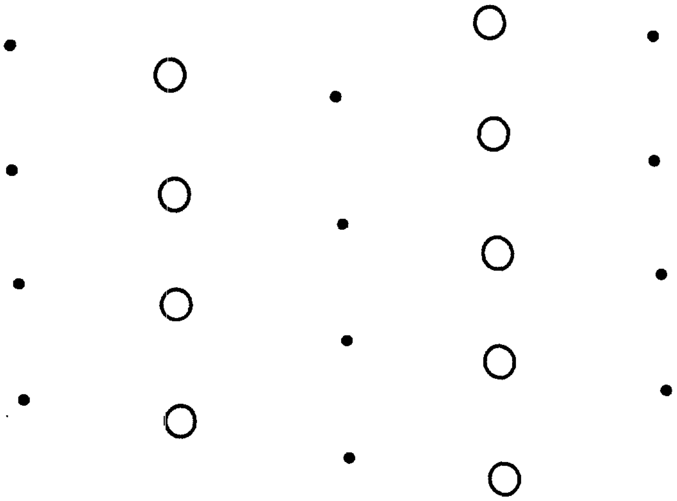
Figure Captions:

Fig.1: Top layer of Si(111) in 3x1 phase of the metal induced reconstruction: a) the model proposed in Ref.[2], b) the corresponding classical model for which the Monte Carlo simulations were performed.

Fig.2: Top layer of Si(111) in 6x1 phase of the metal induced reconstruction: a) the model proposed in Ref.[2], b) the corresponding classical model for which the Monte Carlo simulations were performed.



(a)



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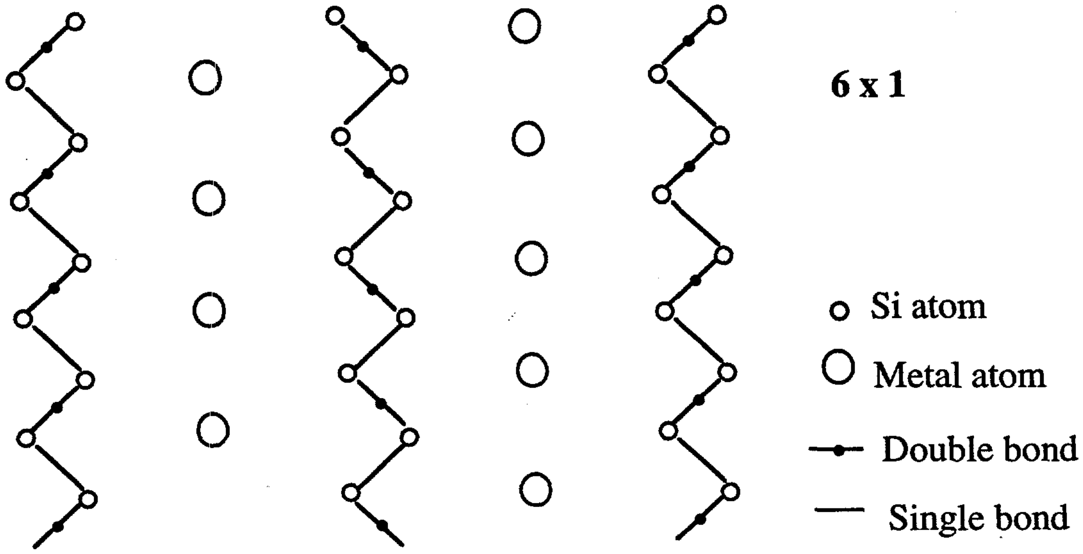

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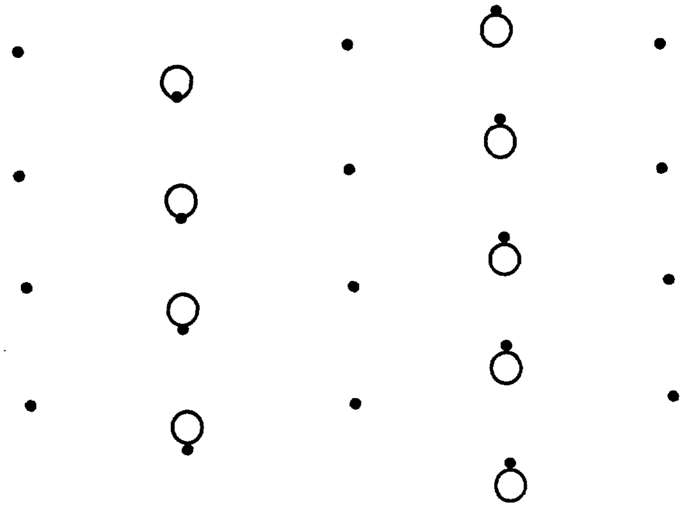

(b)

Acknowledgements

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