First-principles study of adhesion at Cu/SiO$_2$ interfaces

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(April 21, 2003)

The structural, electronic, and adhesive properties of Cu/SiO$_2$ interfaces are investigated using first-principles density-functional theory within the local density approximation. Interfaces between fcc Cu and α-cristobalite(001) surfaces with different surface stoichiometries are considered. Interfacial properties are found to be sensitive to the choice of the termination, and the oxygen density at the substrate surface is the most important factor influencing the strength of adhesion. For oxygen-rich interfaces, the O atoms at the interface substantially rearrange after the deposition of Cu layers, suggesting the formation of Cu-O bonds. Significant hybridization between Cu–d and O–p states is evident in site-projected density of states at the interface. As oxygen is systematically removed from the interface, less rearrangement is observed, implying weaker adhesion. Computed adhesion energies for each of the interfaces are found to reflect these observed structural and bonding trends, leading to the largest adhesion energy in the oxygen rich cases. The adhesion energy is also calculated between Cu and SiO$_2$ substrates terminated with hydroxyl groups, and adhesion of Cu to these substrates is found to be considerably reduced. This work supports the notion that Cu films can adhere well to hydroxyl-free SiO$_2$ substrates should oxygen be present in sufficient amounts at the interface.

PACS: 68.35.-p, 73.20.-r, 68.47.Gh

I. INTRODUCTION

Adhesion of thin metal films to glass substrates have continued to be the subject of intense study for many years because of its importance to the large-area electronics industry. Copper in particular, a noble metal with a high bulk thermal and electrical conductivities, and apparently low electromigration rate, is an excellent candidate for interconnects in integrated circuitry on dielectric substrates, and thus the formation of a strong and highly reliable interface between copper and glass has been an issue of primary importance. Unfortunately, Cu films are often reported to bind rather poorly to oxide-based glass substrates, and films that do adhere at room temperature can show diminished adhesivity after thermal cycling, an effect often attributed to differences of thermal expansion between Cu and the oxide substrate. In many studies, poor bonding is frequently explained by noting that since Cu does not reduce SiO$_2$, a graded oxide layer facilitating the adhesion is unable to form. Chemically, copper possesses a half-empty s shell and a reasonably tightly-bound and filled d-shell, and thus is less reactive than aluminum and many transition metal films, which oxidize well and are observed to adhere more reliably. Thus it is not surprising that adhesion is often improved experimentally by applying transition metal intermediary layers prior to Cu film deposition, or alloying the Cu films with small amounts of Mg or Al.

Adhesion of copper films to oxide glasses is, of course, expected to be highly sensitive to the temperature, oxygen partial pressure, and the condition of the glass surface prior to deposition. A common feature of many studies of Cu films on glass is that they were performed under conditions amenable to surface passivation either before or during deposition of the copper film. For example, Cu films sputtered under high purity conditions in a vacuum do adhere to glass substrates. In particular, Ohmi et al. demonstrated robust adhesion of copper to glass after removing hydroxyl (OH) groups from the interface in situ just prior to deposition. This suggests that dangling bonds at moisture-free glass surfaces would be readily saturated by Cu-O bonds.

Glasses important to industry can be chemically complex, often containing a substantial amount (perhaps ∼ 30%) of aluminum, boron, and other alkaline earth elements. Their primary component, however, is almost always SiO$_2$, which by itself forms one of the simplest glasses, amorphous silica (a-SiO$_2$). In the interest of simplifying the chemistry, we shall restrict our focus to chemically-pure SiO$_2$ glasses for the duration of this study. Amorphous silica has no long range order yet remarkably, on length scales comparable to a Si-O bond, it is nearly perfectly ordered: the bond-length does not vary appreciably from 1.61 Å; each Si atom is tetrahedrally coordinated with O atoms, and the bonds are primarily of a covalent nature. At length scales between 5 Å and 8 Å, minimal variations in O-Si-O and Si-O-Si bond angles result in an appreciable degree of intermediate range orientational disorder. Previous work using molecular dynamics has been performed on both bulk vitreous silica and silica surfaces. Much of it was based on semi-empirical potentials which though able to simulate systems large enough to correctly capture the
II. METHODOLOGY

A. Computational details

Our first-principles density-functional calculations are carried out within the LDA, using the correlation energy of Ceperley and Alder, as implemented within the Vienna ab initio Simulation Program (VASP). We use a plane-wave basis set with a 29 Ry cut-off, and ultrasoft pseudopotentials for Cu and H, projector augmented-wave potentials for O, and a norm-conserving pseudopotential for Si. The Monkhorst-Pack k-point mesh is chosen so that $n_k = 3 \times 3 \times 1$ for the 5 Å × 5 Å × 30 Å supercell which is used in this work. Also, we make use of a Fermi-distribution smearing with the temperature of $k_BT \sim 0.2$ eV to facilitate rapid convergence. These computational conditions provide good convergence of the structure, density of states, and energy differences given here, and are used throughout this work unless otherwise stated.

It should be mentioned that the k-point sampling discussed above is not entirely sufficient for study of the bulk properties of copper. In fact, the total energy of bulk copper obtained with this sampling is converged to about 0.02 eV per Cu atom. However, a sparser mesh turns out to be adequate for this study since energy differences are converged. To demonstrate, we increased our sampling to $n_k = 4 \times 4 \times 1$ for the supercell mentioned above, recalculated total energies and forces, and found that the resulting difference in adhesion energy is less than 4% even in the largest case.

B. Bulk properties of constituent systems

Copper crystallizes in the fcc structure under normal conditions and its lattice constant is 3.615 Å at 291 K. The LDA underestimates this lattice constant as is well known, and we obtain 3.532 Å for the equilibrium value as shown in Table I, in agreement with a previous LDA study. At equilibrium we find $a = 4.975$ Å and $c = 6.907$ Å for the tetragonal cell of bulk α-cristobalite (the $P4_12_12$ structure), in excellent agreement with experiment and previous LDA calculations. Further, the computed Si-O bond length ($\sim 1.606$ Å) is remarkably close to experiment ($\sim 1.603$ Å), and the calculated O-Si-O bond angle is near the tetrahedral ideal value, also in-line with measurement. Conveniently, the choice of α-cristobalite circumvents spurious lattice mismatch when considering the interfaces with Cu overlayers: Compare the lattice constant $a$ of α-cristobalite with $\sqrt{2}a$ of Cu in Table I.
TABLE I. Lattice constants of Cu and α-cristobalite observed in experiment and LDA calculation. Wyckoff positions, two Si-O bond lengths, and four O-Si-O bond angles are also shown for α-cristobalite; the Si Wyckoff position (4a) is shown as (u, u, 0) and the O Wyckoff position (8b) as (x, y, z). The experimental data are taken from Refs. 36 and 38 for copper and α-cristobalite, respectively.

|        | Experiment | This work (LDA) |
|--------|------------|-----------------|
| Cu     |             |                 |
| a (Å)  | 3.615      | 3.532           |
| √2a (Å)| 5.112      | 4.995           |
| α-cristobalite |       |                 |
| a (Å)  | 4.972      | 4.975           |
| c (Å)  | 6.922      | 6.907           |
| u (Si) | 0.3003     | 0.3005          |
| x (O)  | 0.2392     | 0.2389          |
| y (O)  | 0.1044     | 0.1058          |
| z (O)  | 0.1787     | 0.1801          |
| Si-O (Å)| 1.6026 | 1.6056          |
| Si-O (Å)| 1.6034 | 1.6062          |
| O-Si-O (°)| 109.0 | 108.3           |
| O-Si-O (°)| 110.0 | 109.9           |
| O-Si-O (°)| 108.2 | 108.8           |
| O-Si-O (°)| 111.4 | 111.7           |

III. (001) SURFACES OF α—CRISTOBALITE SiO$_2$

As a starting point, we consider an α—cristobalite slab consisting of 5 SiO$_2$ layers, the thickness of which is ≈8.3 Å. Translational symmetry is removed along the c-axis, defining two different (001) surfaces perpendicular to this axis. We embed this α-cristobalite slab, along with about 20 Å of vacuum, within a supercell having dimensions of 5 Å × 5 Å × 30 Å. Oxygen number at the top of our SiO$_2$ slab is then changed to mimic different substrate terminations. Two nonbridging oxygen atoms terminate the bottom of the slab, and two additional H atoms are attached to the oxygens to remove dangling bonds. Forces on the atoms are computed using the Hellmann-Feynman theorem, and the positions of atoms are then updated until the total energy reaches a minimum. The oxygen atoms at the bottom surface, terminated by hydrogens, are fixed at their bulk positions in order to reduce size effects owing to the finite thickness of the SiO$_2$ slab, though the positions of each of the hydrogen atoms are permitted to relax. Previous first-principles calculations of α-quartz surfaces have indicated that about 5 Å away from the interface, the local structural and electronic properties of the slab are bulk-like, and thus the size of our slab is sufficient to approximate both surface and bulk features.

Figure 1 presents views of the relaxed α-cristobalite(001) surfaces. Supercells with slabs having three different surface terminations are considered in this work, which we label as Si-, O-, and OO-terminated. The Si-terminated slab contains five SiO$_2$ units together with two bottom hydrogens; the O-terminated slab is identical to the Si-terminated except that the dangling surface oxygen atom is added; the OO-terminated slab is again a modification of the Si-terminated slab in which two oxygens are added to the surface. Bond lengths and angles are not expected to remain bulk-like at the surface, where the choice of termination can leave non-bridging oxygens with dangling bonds at the surface (e.g., in the OO-terminated cases). Indeed, we find that relaxation significantly changes the Si-O bond lengths within two atomic layers from the surface for all terminations considered, and the nature of these changes is strongly dependent on the termination. In the Si-terminated case, the additional charge carried by the dangling Si bonds forces the Si surface atom above the plane of the surface; as a result the Si-O bonds supporting it from below elongate slightly to 1.64 Å. In the O-terminated case, the surface O atom, bonded to only one other Si, relaxes downward into the surface, and its bond length decreases by more than 5% from 1.6 Å to 1.5 Å. In the OO-terminated case, in some contrast to the Si- and O-terminated slabs, the Si-O bond lengths remain essentially the same as bulk. But the distance between O neighbors on the surface is also 1.6 Å, which is very small compared with typical bulk O second neighbor distances of 2.7 Å. Thus O atoms may evidently saturate dangling bonds through bonding with neighboring O atoms at this surface.

As expected, the total cohesive energies of the supercells decrease substantially with each additional O atom: adding one oxygen atom or two oxygen atoms lowers the cohesive energy by ~7.1 eV or ~11.3 eV per surface Si, respectively. Since the energy required to break the O$_2$ bond is nearly 5 eV per molecule, this energy comparison suggests that the OO-terminated surface may be the most stable of the three terminations, and the O-terminated surface the second. Evidently our first-principles calculations are consistent with the intuition that glass surfaces should be oxygen-rich.

FIG. 1. Relaxed structures of the α-cristobalite(001) surfaces.
IV. Cu/SiO\textsubscript{2} INTERFACES: RESULTS AND DISCUSSION

A. Interfacial structure

We now add five Cu layers to each of the fully-relaxed (001) \(\alpha\)-cristobalite surfaces, obtained as discussed above in Sec. III. The Cu layers are initially positioned on the surface so that a Cu atom in the lowest monolayer lies on the former symmetry axis of the \(\alpha\)-cristobalite slab. The length of the supercell lattice vector normal to the surface (the \(c\)-axis) is fixed to 30 Å as in Sec. III, a value we find to be large enough to accommodate up to five additional Cu layers while keeping the interactions between the surfaces in neighboring supercells minimal. Each monolayer in our supercell contains four Cu atoms, and before relaxation each Cu atom has four intralayer neighbors at a distance of 2.5 Å. Fortunately, the lattice parameter of the \(\sqrt{2}\times\sqrt{2}\) surface of \(\alpha\)-cristobalite is well matched to that of the \(\sqrt{2}\times\sqrt{2}\) surface of copper as shown in Table I (the mismatch is less than 1%). The small lattice mismatch is an artifact of our approximate treatment of amorphous silica as crystalline. In reality, stress induced by lattice-matching is relieved through formation of defects and/or dislocations. (In the case of a truly amorphous substrate, stress may also be overcome through surface reconstruction, a complexity we neglect in the present work.)

The positions of all atoms in the supercell are again relaxed except for the bottom O atoms, and Fig. 2 shows the optimized structures of the interfaces for each termination. The most significant reconstruction at the interface is observed in the OO-terminated case. The O-O bond observed at the free \(\alpha\)-cristobalite surface in Fig. 1 is broken by the deposition of copper, and the O-Si-O angle is changed from 59° to 104° with the Si-O bond lengths kept almost constant. This large rearrangement would indicate bond formation between interfacial O and Cu atoms, suggesting good chemical adhesion between the oxide substrate and the Cu film. Each interfacial O atom has two Cu neighbors, and the Cu-O bond lengths are computed to be \(\sim\) 1.9 Å, strikingly similar to Cu-O distances found in cuprates\textsuperscript{43}, where each copper atom is coordinated by four oxygens and considered to be in a Cu\textsuperscript{2+} state. Similar Si-O and Cu-O bond lengths are observed at the interface between O-terminated surfaces and Cu monolayers, although the Si-O-Cu angles are smaller than in the OO-terminated case by \(\sim\) 15°, as can be seen in Fig. 2. The magnitude of the reconstruction at the O-terminated/Cu interface is less than that at the OO-terminated/Cu interface.

The interface between the Si-terminated substrate and Cu is completely different from either of the oxygen terminated interfaces. In this case, the interfacial Si atom possesses four Cu neighbors, each with bond length \(\sim\) 2.4 Å, and there is negligible atomic rearrangement, implying more metallic-like bonding.

B. Electronic properties

To investigate further the bonding properties of each interface discussed above, we compute the site-projected local density of states (LDOS) for atoms near the interfaces, and compare them with those obtained for bulk-like atoms deeper inside the slabs; the LDOS are shown together for each interface in Fig. 3. In the OO-terminated case, significant hybridization is observed between Cu\textsuperscript{−d} and O\textsuperscript{−p} states just below the Fermi level. A key feature is the slight bump in the O\textsuperscript{−p} LDOS, lying about 1 eV below the Fermi energy, which becomes...
progressively smaller with decreasing O content at the interface, and nearly vanishes in the Si-terminated case. Evidently strong hybridization between Cu—d and O—p states is responsible for the significant reconstruction at the OO-interface. It is worth pointing out here that as the number of O atoms at the interface is decreased, the Si—sp LDOS around the Fermi energy increases, that is the interfacial bonding takes on a more metallic character. This behavior results from the hybridization of Si—sp states with the itinerant Cu—s states around the Fermi energy. In addition, we observe the bandgap computed within the LDA (an underestimate of the true bandgap) opens and gradually approaches its bulk LDA value for LDOS in the middle of the SiO\(_2\) slab, confirmation that our slab exhibits approximate bulk behavior away from the interface.

To examine the degree to which changes in structural and bonding properties are confined to the interface, and to observe the mixing between the electronic states of the SiO\(_2\) substrate and the Cu layers in more detail, we calculate the density difference from the superposition, namely,

\[
\langle \delta n(z) \rangle = \langle n_{IF}(z) \rangle - [\langle n_{SiO_2}(z) \rangle + \langle n_{Cu}(z) \rangle],
\]

where \(\langle n_{IF}(z) \rangle\), \(\langle n_{SiO_2}(z) \rangle\), and \(\langle n_{Cu}(z) \rangle\) are the densities of the Cu/SiO\(_2\) interface, the SiO\(_2\) substrate, and the Cu layers, respectively, averaged over the xy plane (parallel to the interface). To obtain \(\langle n_{SiO_2}(z) \rangle\) \(\langle n_{Cu}(z) \rangle\), we simply remove the Cu layers (SiO\(_2\) substrate) from the fully relaxed interface in the supercell, and then recalculate the electronic structure self-consistently keeping the atoms fixed. The quantity \(\langle \delta n(z) \rangle\) thus indicates the change in electron density resulting from chemical bonding between the Cu layers and the SiO\(_2\) substrate. (To simplify the analysis, we are neglecting additional changes stemming from the atomic rearrangements at the free surfaces of SiO\(_2\) and Cu.) The results of calculations of the \(\langle \delta n(z) \rangle\) appear in Fig. 4. The \(\langle \delta n(z) \rangle\) in the OO-terminated case most prominently deviates from zero around the interface, reflecting significant charge transfer between the two slabs. The charge transfer in the O- and Si-terminated cases is comparatively much smaller. In particular, in the Si-terminated case, the depletion of the density in the vicinity of the lowest Cu layer is not so drastic, suggesting that the localized Cu—d states have less influence on the bonding around the interface.

C. Quantitative analysis of adhesion

To assess the adhesive strength of the interfaces, we have calculated the ideal work of separation, or adhesion energy, per unit area \(W\) from

\[
W \equiv \left( E_{SiO_2} + E_{Cu} - E_{IF} \right) / A,
\]

where \(E_{SiO_2}\), \(E_{Cu}\), and \(E_{IF}\) are the energies of the isolated SiO\(_2\) substrate, Cu layers, and Cu/SiO\(_2\) interface in

![FIG. 3. Local density of states (LDOS) projected by site and angular momentum. The solid lines show the LDOS of atoms at (or near) the interfaces, and the dashed lines show those of atoms in the middle of the slabs (the LDOS of an approximate bulk material). When computing the LDOS, a gaussian smearing method is used with \(\sigma = 0.2\ eV\). The sphere sizes of each atom are taken as 1.11 Å for Si, 0.73 Å for O, and 1.38 Å for Cu.](image-url)

| TABLE II. Adhesion energy (ideal work of separation) \(W\) of the Cu/α-cristobalite(001) interfaces. |
|---------------------------------|--------|
| Si-terminated                  | 1.406  |
| O-terminated                   | 1.555  |
| OO-terminated                  | 3.805  |
the supercell, respectively, and $A$ is the area. Physically, the adhesion energy $W$ is the work per unit area required to separate the interface into the Cu layers and the SiO$_2$ substrate within a microcanonical process, and it can be considered a measure of the strength of the adhesion. For the purposes of comparison, all energies are calculated using supercells of the same size ($5\,\text{Å} \times 5\,\text{Å} \times 30\,\text{Å}$) independent of whether it contains Cu layers, any of the SiO$_2$ substrates, or Cu/SiO$_2$ interfaces. Table II lists the adhesion energy for each case. The adhesion energy in the OO-terminated case turns out to be much larger than those in the O- and Si-terminated cases, and comparable to values previously computed for other metal-dielectric interfaces, such as Co/TiC (Ref. 21) and Nb/Al$_2$O$_3$ (Ref. 22). We note that the computed energies for the OO-terminated case turn out to be much larger than those in the O- and Si-terminated cases, and comparable to values previously computed for other metal-dielectric interfaces, such as Co/TiC (Ref. 21) and Nb/Al$_2$O$_3$ (Ref. 22). We note that the computed energies for the OO-terminated case, $\sim 4\,\text{J/m}^2$, are consistent with values obtained experimentally by Kriese et al. for 100 nm thick films of Cu on SiO$_2$ using an indentation technique. In summary, the magnitudes of adhesion energies computed here for each of the three different interfaces reflect the trends witnessed above in their structural and bonding properties.

1. Local atomic structure

At this point, it is meaningful to investigate further a drawback of using crystalline $\alpha$-cristobalite to model the amorphous substrate. When Cu layers are placed on an amorphous SiO$_2$ substrate, different local atomic configurations are possible at the interfaces because of the non-periodicity of glass. A principal simplification of our model is the imposition of translational symmetry: we are unable to directly assess the difference between the adhesive properties of crystalline substrates and those of amorphous substrates. We are, however, able to investigate the sensitivity of our calculated adhesion energies to changes in local atomic structure. As a first step, we compute the influence of the position of Cu layers, relative to the substrate, on the adhesion energy by translating the Cu layers in the $xy$ plane.

As shown in Fig. 5, the adhesion energy turns out rather insensitive to the initial position of the Cu layers so long as the termination type remains unchanged. This result suggests that the adhesive properties realized in these $\alpha$-cristobalite substrates may well be carried over, to some extent, to those of glass substrates. The insensitivity of adhesion energy to the position of Cu layers does not imply that the detailed structure at the interface is less important for adhesion. In fact, as shown in Fig. 6 for the OO-terminated case, atoms at the interfaces do move significantly relative to the unshifted case. Since the surface atoms have a greater freedom to choose their position than those in bulk, the adhesion energy remains rather constant for various initial positions of Cu layers.

2. Local oxygen surface coverage

Thus far we have investigated the Si-, O-, and OO-terminations independently. Depending on the oxygen partial pressure, however, these terminations are generally expected to coexist on the substrate surface, independent of whether the substrate is crystalline or amorphous. To examine the effects of oxygen surface densi-
ties intermediate between those of the Si-, O-, and OO-terminated cases, we enlarge the supercell by a factor of two along the y-axis (along the horizontal direction of Figs. 1, 2, and 6). For the 1×2-supercells, three new surfaces, in addition to those already considered above, are now possible. These are: a (Si,O)-terminated surface which consists of neighboring Si- and O-terminated surfaces; a (Si,OO)-terminated surface which consists of neighboring Si- and OO-terminated surfaces; and a (O,OO)-terminated surface which consists of neighboring O- and OO-terminated surfaces. [Note that the (Si,OO)-terminated case possesses the same oxygen density as the O-terminated case.] We find that the (Si,OO)-terminated substrate has energy which is higher than that of the O-terminated surface by ∼1.4 eV per Si atom at the surface (per 25 Å²). Therefore, we restrict our focus to investigation of the (Si,O)- and (O,OO)-terminated cases, calculating their relaxed structures and adhesion energies.

Figure 7 depicts the adhesion energy as a function of the oxygen density at the interface. Remarkably, the adhesion energy is not a monotonically-increasing function of oxygen density; at low oxygen density, increasing the number of O atoms a small amount does not necessarily lead to stronger adhesion. However, beyond the oxygen density of 4 nm⁻² where the OO-termination will begin to appear appreciably, the adhesion energy increases, and does so almost linearly. This linear dependence implies that each OO surface unit contributes to the adhesion fairly independently, and thus the locally OO-terminated regions may not necessarily have to form large domains in order to work as an effective “glue”, although it is clear that a critical density of such locally OO-terminated regions is required for strong adhesion.

3. Hydroxylated surfaces

We now address a frequently-cited reason for the weak adhesion at Cu/a-SiO₂ interfaces, namely the existence of hydroxyl groups on the SiO₂ surface. It is well known that hydroxyls are likely to form on the SiO₂ surface under “wet” deposition conditions; to examine the impact of hydroxyls on adhesion from first-principles, we add two hydrogens to the 1×1 OO-terminated surface, and relax all of the atoms. The result is that the cohesive energy of OHOH-terminated substrate, in which a Si atom is terminated by two hydroxyls, is lower than that of OO-terminated substrate by ∼11.2 eV per surface Si atom. This energy difference is much larger than the dissociation energy of H₂ molecule (∼4.5 eV per molecule), suggesting the high stability of the OHOH-terminated substrate. If we now place the Cu layers on top of the hydroxylated surface and relax the interface (Fig. 8), we find that the deposition of Cu layers does not significantly affect the structure at the OHOH-terminated surface, implying little interaction; the hydrogen present at the surface leaves the surface neutral and inert. This tendency is clearly reflected in the calculated adhesion energy, and according to our calculations it is just 0.331 J/m², less than one tenth of the adhesion energy observed in the OO-terminated case.

However, as shown in Table II, the adhesion energies for all other cases studied here (i.e. the OO-, O-, and Si-terminated cases) seem to be of a magnitude which should produce adhesion, especially the oxygen-rich OO-terminated case. It is also noteworthy that the OO-terminated substrate, which has the largest adhesion energy among the three, looks actually the most stable substrate. These facts imply that should dehydroxylation of the substrate surfaces be successfully achieved (e.g. by annealing or particle bombardment of a growing film surface), robust adhesion is entirely possible, at least from...
the point of view of chemical bonding.

V. CONCLUSIONS

We have performed a first-principles study of the adhesive properties of atomically-sharp Cu/SiO\(_2\) interfaces. As a model a-SiO\(_2\) substrate, we used a crystalline polymorph of SiO\(_2\), α-cristobalite, and investigated its Si-, O-, and OO-terminated (001) surfaces in detail. For interfaces between Cu and OO-terminated surfaces, a substantial rearrangement of oxygen positions relative to the free surface is observed, suggesting the formation of strong Cu-O bonds. Analysis of the local density of states at the interface showed that Cu-O interfacial bonds are composed of Cu—d and O—p states. The computed adhesion energy also exhibited a tendency toward much stronger adhesion in the OO-terminated interface than in the O- and Si-terminated interfaces: Substrate surfaces with high oxygen content were found suitable for adhesion.

The adhesion energy is found to be very insensitive to the type of the Cu layers if the termination is unchanged, and this observation suggests that α-cristobalite may serve as a good starting model of a-SiO\(_2\) substrates. The detailed dependence of the adhesion energy on oxygen density at the substrate surface has been investigated, and it shows that the surfaces where the O- and OO-terminations coexist can also lead to relatively strong adhesion.

The possible existence of hydroxyl groups at the substrate surface is thought to be the main cause for the weak adhesion observed in experiment. However, if these hydroxyls are removed beforehand and the oxygen density at the surface is increased (for example, by upping the oxygen partial pressure), Cu layers are predicted to adhere reasonably well to SiO\(_2\). In addition to the possibility of direct comparison to future measurements on crystalline Cu/α-cristobalite(001) interfaces, these results should serve as a starting point for which to study more complicated interfacial geometries, benchmarks for future investigations, and a baseline for experiments attempting to elucidate complicated phenomena affecting adhesion at Cu/glass interfaces.

VI. ACKNOWLEDGMENTS

We thank S. Baker and M. Backhaus for helpful discussions. This work was supported by the National Science Foundation (DMR-9988576), and made use of the Cornell Center for Materials Research Shared Experimental Facilities, supported through the National Science Foundation Materials Research Science and Engineering Centers program (DMR-9632275).

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