

# The role of the atomic structure on the Si/SiO<sub>2</sub> interface strains

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While Si-SiO<sub>2</sub> systems have been under an intensive academic and industrial research since invention of MOSFET in 1960, the underlying physics and chemistry of this interface are still not well understood at the atomic scale level. As the size of electronic devices shrinks into the nanoscale dimension, the importance of understanding the atomic scale structure of Si-SiO<sub>2</sub> interfaces grows. This understanding is very crucial to extend the life of complementary metal-oxide semiconductor (CMOS) technology. In this paper, we present results of a computational study on Si/SiO<sub>2</sub> interface for several modifications of a proposed interface model. The interface model is obtained by removing a (100) layer of Si atoms from the crystalline silicon. Leftover Si atoms on each side of the removed atoms are shifted perpendicularly to the interface to adjust their separation and oxygen atoms are inserted at such positions to preserve usual Si-O bond lengths and angles. The computations were carried out using first-principles density functional theory (DFT) in the local density approximation (LDA). Our calculations revealed the important role of the interface structure on the shear and tensile strains on the interface. The first layer tensile strain was found to increase significantly and linearly with the increase of the O-Si-O bond angle from 102° to 126°. The first layer shear strain was found to decrease slowly and linearly with the increasing the O-Si-O bond angle. On the other hand, the O-O distance along the interface was found to have nearly the opposite effect of the O-Si-O bond angle.

(Received July 3, 2007; accepted October 1, 2007)

*Keywords:* Strain, Si/SiO<sub>2</sub>, Density functional theory

## 1. Introduction

Despite many intense studies [1-9], a quantitative, predictive theory of the effect of local electronic structures on the stability and on barrier heights at the interfaces between semiconductor heterojunctions, is not completely formulated. The real picture of the interface problem lies between two extreme points of view. The first is that: the barrier height (heterojunctions band discontinuity) depends only on the bulk properties of the different semiconductors [10]. This model is called the intrinsic model. The second model which is called the extrinsic model states that: the barrier height depends only on the specific properties of the interfaces. The extrinsic model represents a substantial departure from the intrinsic model, since it considers the defects in the semiconductors as the origin of the interface states that pin the Fermi level [11]. Occupation of these surface states creates a dipole, which does not depend on the properties of the component materials. It is now believed that the intrinsic model gives a better description of the potential barrier at the interfaces [9]. However, the "extrinsic" model provides a description of the interface between two semiconductors in the case an intra-layer has been inserted between the semiconductors. According to the "extrinsic" model, the interlayer may be treated as a continuous defect layer whose presence and properties control the net "extrinsic" dipole.

Regardless of the source of the defect states, if there is charge transfer at the interface, the dipole moment of the interface is calculated by the equation:

$$P = \delta q d ,$$

where  $d$  is the dipole length. The dipole length is the perpendicular distance between the double-charged layers of the interface. The charge  $\delta q$  is the bond charge transfer at the interface. This charge was obtained using a population analysis based on the electrostatic potential (ESP) of molecules.

In a previous study [12], we have carried density functional calculations to investigate the role of the interface structure on the stability of Si/O/Si superlattices and on the electronic properties of the Si(100)/SiO<sub>2</sub> interface. We have shown the feasibility of such structure through the calculations of the shear and tensile stress on the interface as a function of distance between the two Si layers. Although the stress and strain were recently studied on this interface [13], the effect of varying the O-Si-O bond angle and of varying the O-O distance on the shear and tensile strains was not discussed in a detailed manner. Here we present the detailed dependence of the shear and tensile stress and binding energy on the O-Si-O bond angle and on O-O distance at the interface.

## 2. The model and the computational method

Our proposed model of Si(100)/SiO<sub>2</sub> interface is compatible with the subsequent Si epitaxial growth. The model is obtained by removing a (100) layer of Si atoms from the crystalline silicon. Leftover Si atoms on each side of the removed atoms are shifted perpendicularly to the interface to adjust their separation and oxygen atoms are inserted at such positions to preserve usual Si-O bond lengths and angles. The model consists of 26 silicon atoms, 8 oxygen atoms, and 40 hydrogen atoms. Fig. 1

shows this interface model where the solid circles represent oxygen atoms, the small open circles represent hydrogen atoms and the large open circles represent silicon atoms. Also a portion of the interface was magnified to show the O-Si-O bond angle clearly.

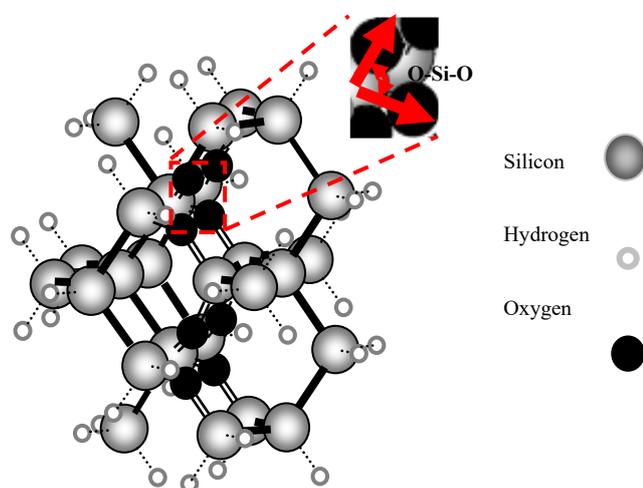


Fig. 1. The Si-O-Si interface model.

Density functional theory (DFT) [14-16] in the local density approximation (LDA) was applied to investigate the proposed interface model [17]. To investigate the effect of the interface structure on the electronic properties of the system, DFT calculations were done on atomistic scale along the interface. Within the local density functional approximation, we have calculated the binding energy per atom which is necessary to estimate the interface model stability. We have also calculated the forces on the interface atoms required to assess the interface strain. Cluster model of the interface has been employed because all the relevant information is atomistically local in nature and the cluster model of the interface is reasonable. In the DFT approximation used in this study, we used Becke 3 parameter functional (B3) hybrid model as the exchange term [18], and the Perdew and Wang (PW91) as the correlational term [19] of the DFT functional.

#### 4. Results and discussion

Five different modifications of the interface model have been considered. The modifications differ in the spacing between the Si atomic layers on each side of the interface. The spacing varies from 1 to 1.6 in the units of  $a/4$ , where  $a$  is the silicon lattice constant ( $a = 5.43 \text{ \AA}$ ). A change in the spacing between the Si layers is accompanied with a change in the distance between the oxygen atoms along the interface and along with a change in the O-Si-O angle at the interface. Fig. 2 shows the binding energy per atom, as function of the O-Si-O bond angle. The binding energy per atom increases slightly as the bond angle increases from 102° to 115° reaching a maximum value of 2.48 eV at O-Si-O bond

angle of 115°. As the O-Si-O bond angle increases further, the binding energy per atom decreases rapidly, reaching its lowest value of 1.73 eV at O-Si-O bond angle of 126°. Fig. 3 shows the interface shear and tensile strain as function of the interface O-Si-O bond angle. As shown in the figure, the interface shear strain values were found to be small and decrease almost linearly with the O-Si-O bond angle from 2 to 1%. The interface tensile strain values, which are large compared to the shear strain values, were found to increase almost linearly with the O-Si-O bond angle from 10 to 21%. The strain was calculated from the forces on the atoms and by using the Si bulk elastic constant. Fig. 4 shows that the Si-O bond charge transfer decreases with increasing the O-Si-O bond angle at the interface reaching a minimum value when the O-Si-O bond angle equals 115°. As the O-Si-O bond angle increases further, the charge transfer increases again.

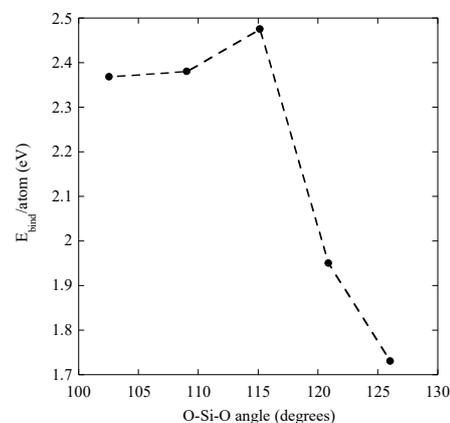


Fig. 2. The binding energy per atom versus the O-Si-O bond angle.

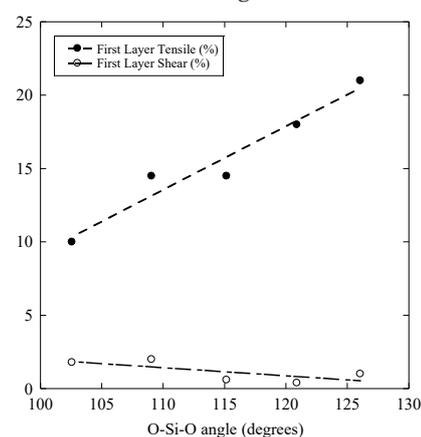


Fig. 3. The equivalent interface shear and tensile strain versus the O-Si-O bond angle.

Knowing that in our model as the O-Si-O bond angle is increased, the distance between the O-O along the interface decreases, we might understand these results as following. When the O-Si-O bond angle is increased, oxygen atoms at the interface become close to each other causing large repulsion which results in increasing the tensile strain almost linearly. As the O-Si-O bond angle gets smaller, the distance between oxygen atoms at the

interface become larger which results in less repulsion at the interface and thus cause less strain. The binding energy of the atoms at the interface was found to increase slightly with the initial increase of the O-Si-O bond angle reaching a maximum value of 2.47 eV when the O-Si-O bond angle equals 115°. As the O-Si-O bond angle is increased above 115°, the binding energy of the atoms at the interface was found to decrease sharply. On the other hand, the Si-O bond charge transfer was found to decrease with the initial increase of the O-Si-O bond angle reaching a minimum when O-Si-O bond angle equals 115° as shown in Fig. 4. As the O-Si-O bond angle is increased further, the Si-O bond charge transfer increases again. The overall low strain values and large binding energy values at O-Si-O bond angle of 115° confirm the feasibility of the Si/O/Si superlattices. Our results mainly confirm the important role of the interface structure on the stability and on the electronic properties of Si(100)/SiO<sub>2</sub> interface. These findings also provide a significant support for the “extrinsic” model of semiconductor interfaces. The reason that the maximum binding energy per atom is obtained for the lowest value of Si-O bond charge transfer at the interface is not well understood and is currently under investigation.

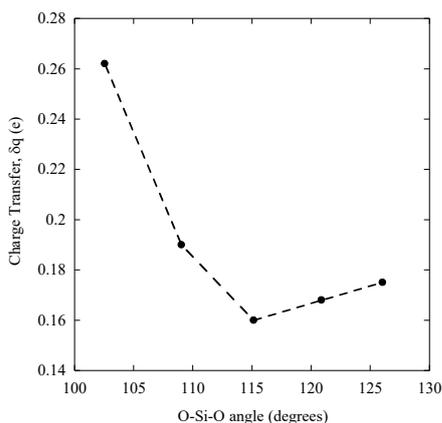


Fig. 4. The Si-O bond charge transfer versus the O-Si-O angle at the interface.

## 5. Conclusion

Our calculations revealed the important role of the O-Si-O bond angle and the O-O distance at the Si/SiO<sub>2</sub> interface on the shear and tensile strains. The first layer tensile strain was found to increase significantly and linearly with the increase of the O-Si-O bond angle. The first layer shear strain was found to decrease slowly and linearly with the increasing the O-Si-O bond angle. On the other hand, the O-O distance along the interface was found to have nearly the opposite effect of the O-Si-O bond angle. Our findings also provided a significant support for the “extrinsic” model of semiconductor interfaces.

## Acknowledgment

This work was financially supported by the Research Affairs at the UAE University under a contract no. 03-02-2-11/05.

## References

- [1] A. D. Katnani, G. Margaritondo, Phys. Rev. B **28**, 1944 (1983).
- [2] P. Perfetti, F. Patella, F. Sette, C. Quaresima, C. Capasso, A. Savoia, G. Margaritondo, Phys. Rev. B **30**, 4533 (1984).
- [3] D. W. Niles, G. Margaritondo, P. Perfetti, C. Quarisma, M. Capozzi, Appl. Phys. Lett. **47**, 1092 (1985).
- [4] D. W. Niles, E. Colavita, G. Margaritondo, P. Perfetti, C. Quarisma, M. Capozzi, J. Vac. Sci. Technol. A **4**, 962 (1986).
- [5] P. Perfetti, Surf. Sci. **168**, 507 (1986).
- [6] J. Tersoff, Surf. Sci. **168**, 275 (1986).
- [7] J. Tersoff, Phys. Rev. Lett. **56**, 2755 (1986).
- [8] L. J. Brillson, Surf. Sci. **300**, 909 (1994).
- [9] W. Monch, Surf. Sci. **300**, 928 (1994).
- [10] J. Tersoff, in “Heterojunction Band Discontinuities, Physics and Device Applications,” (F. Capasso and G. Margaritondo, eds.), p. 3, North-Holland, Amsterdam, 1987.
- [11] W. E. Spicer, I. Lindau, P. Skeath, C. U. Su, P. W. Chye, Phys. Rev. Lett. **44**, 420 (1980).
- [12] I. M. Obaidat, International Journal of Materials Science (IJoMS) **1**(1), 11 (2006).
- [13] Anatoli Korkin, J. C. Greer, Gennadi Bersuker, Valentin V. Karasiev, Rodney J. Bartlett, Phys. Rev. B **73**, 165312 (2006).
- [14] W. Kohn, L. J. Sham, Phys. Rev. **140**, A1133 (1965).
- [15] R. O. Jones, O. Gunnarsson, Rev. Mod. Phys. **61**, 689 (1989).
- [16] J. F. Annet, Computational Materials Science, **4**, 23 (1995).
- [17] Gaussian 98: M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, V. G. Zakrzewski, J. A. Montgomery, Jr., R. E. Stratmann, J. C. Burant, S. Dapprich, J. M. Millam, A. D. Daniels, K. N. Kudin, M. C. Strain, O. Farkas, J. Tomasi, V. Barone, M. Cossi, R. Cammi, B. Mennucci, C. Pomelli, C. Adamo, S. Clifford, J. Ochterski, G. A. Petersson, P. Y. Ayala, Q. Cui, K. Morokuma, D. K. Malick, A. D. Rabuck, K. Raghavachari, J. B. Foresman, J. Cioslowski, J. V. Ortiz, A. G. Baboul, B. B. Stefanov, G. Lui, A. Liashenko, P. Piskorz, I. Komaromi, R. Gomperts, R. L. Martin, D. J. Fox, T. Keith, M. A. Al-Laham, C. Y. Peng, A. Nanayakkara, C. Gonzalez, M. Challacombe, P. M. W. Gill, B. Johnson, W. Chen, M. W. Wong, J. L. Andres, C. Gonzalez, M. Head-Gordon, E. S. Replogle, J. A. People, Gaussian, Inc., Pittsburgh PA, 1998.
- [18] A. D. Becke, J. Chem. Phys. **98**, 5648 (1993).
- [19] J. P. Pedrew, Y. Wang, Phys. Rev. B. **45**, 13244 (1992).

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