Design and Theoretical Study of Silicon Suboxides: Plane Interfaces and Nanowire

Valentin V. Karasiev[1,5], Anatoli Korkin[2],J.C. Greer[3],Gennadi Bersuker[4],Rodney J. Bartlett[5].

[1]*Centro de Quìmica, IVIC, Apartado 21827, Caracas 1020-A, Venezuela.*
[2] *Nano & Giga Solutions, Gilbert, Arizona 85296, USA.*
[3] *Tyndall National Institute, Cork, Ireland.*
[4] *SEMANTECH, Austin, Texas 78741, USA.*
[5]*QTP, University of Florida, Gainesville, Florida, 32611, USA.*

Silicon suboxides, particularly in the form of the plane Si-SiO2 interfaces, play an important role in industrial applications as one of the key elements of today's microelectronic technology. From other hand nanoscale dimensions in thin films, nanowires and quantum dots have growing attention of researchers because of their novel and challenging properties. In this work we present theoretical study of stress energies of Si-SiO2 interfaces with (100), (111), and (110) silicon surfaces [1].
Our study is based on density functional theory (DFT) in the local density approximation (LDA) and generalized gradient approximation (GGA) with localized numerical atomic orbitals and plane wave basis sets. The preliminary results, structure and topology of chemical bonds, of computationally designed Si-in-SiO2 nanowire using the same theoretical methods are also presented. Calculation of stress energy in nanowire shows the same trend relative to the system size as in the Si-SiO2 interfaces.

1. A. Korkin, J.C. Greer, G. Bersuker, V.V. Karasiev, and R.J. Bartlett
Phys. Rev. B, 73, 165312 (2006).

2. A. Korkin, R.J. Bartlett, V. Karasiev, J.C. Greer, T.M. Henderson,
and G. Bersuker, J. Comp.-Aided Mat. Des., 13, 185 (2006).

---

*Corresponding Author.
E-mail Address: vkarasev@qtp.ufl.edu (Valentin V. Karasiev)