

Simple cluster estimations of energetics of silicon interface with aluminum, silicon, titanium, yttrium, zirconium, lanthanum, hafnium and tantalum oxides

Vladimir Golubev *

Sarov Laboratories, Molecular Dynamics Group, 23/16 Varlamovskaya Road, Sarov, Nizhni Novgorod Region, 607189, Russia.

Presently the wide researches are conducted to investigate the properties of materials that can become potential candidates to substitute the SiO₂ as a gate dielectric material for sub-0.1 micron complimentary metal-oxide semiconductor (CMOS) technology. Only few materials can be such candidates, in particular some metal oxides have been pointed out: ZrO₂, HfO₂, Al₂O₃, TiO₂, Y₂O₃, La₂O₃ and Ta₂O₅. All these oxides possess a higher inductivity coefficient as compared to silicon oxide, however their application causes a number of problems concerned with structure and energetics of their interface with silicon. The cluster systems are widely used in ab initio calculations as models to determine some surface and even bulk properties of materials. Simple cluster estimations of energetics of a silicon interface with the mentioned oxides were made. The interface fragments containing only a single bond of a surface silicon atom with a surface oxygen or metal atom of a corresponding oxide metal were modeled. The Si₄H₉-O-Me(OH)_m and Si₄H₉-Me(OH)_m clusters with m = 2 for Al, Y and La, m = 3 for Si, Ti, Zr and Hf and m = 4 for Ta were used. Then the interface fragments containing two bonds of surface silicon atoms were modeled. The Si₉H₁₂-2O-Me₂O(OH)_m clusters with m = 2 for Al, Y and La, m = 4 for Si, Ti, Zr and Hf and m = 6 for Ta were used. Total energy calculations were performed with the density functional theory (DFT) approximation using the Gaussian 98 code. The combined B3LYP functional and several basis sets were used. The LanL2DZ basis set permits to perform calculations for all the concerned systems, the 6-31G(d) basis set - only for the systems containing the Al, Si and Ti atoms. The 6-311+G(d) basis set was used for the main primary system modeling the interface of silicon with silicon oxide for the purpose of precision control in the realized calculations. For more simple one-connected systems the binding energies of the Si-O, Me-O and Si-Me bonds were determined. The zero-point energies were taken into account as for the initial cluster so for the clusters formed after breaking. The mean value of energy on a one generalized bond can be a quite good comparative characteristic for energetics of the interface of silicon with examined oxides. The averaging is made here taking into account the structural formulae of concrete oxides. For example, for silicon oxide the two Si-O and one Si-Si bonds were taken for averaging and for aluminum oxide the three Si-O and two Si-Al bonds were taken. For two-connected systems the binding energies of the Si-O and Me-O bonds were determined similarly. Quite good accordance of the results obtained for the one-connected and two-connected systems was observed. This fact enables to suppose that the obtained energy characteristics are quite adequate.

* Corresponding author. Tel. +7-(831-30)-402-01. FAX +7-(831-30)-448-54.
Email address: gol@socc.ru (Vladimir Golubev).