Monte Carlo-based bond switching method for generation of the SiC/SiO_2 interface

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Efficient approach for generation of amorphous structures without coordination defects can be achieved by using the Monte Carlo method of Wooten, Winer, and Weaire WWW [1]. This method is based on Monte Carlo (MC) approach for generation of random networks by bond switching. New configurations are generated by switching pairs of bonds: two bonds are broken, and new two bonds are created. After randomly selected bond switching, the structure was relaxed using the developed empirical potential for Si-O-C system. The probability of bond switching is determined by Metropolis factor [$\exp(-\Delta E/kT)$, $\Delta E>0$; 1, $\Delta E<0$], where ΔE is the change of system energy as the result of bond switching, T – parameter of modelling.

Energies and structures in local minimum was found by the second-generation reactive empirical bond order potential (REBO2) [2,3] with presented parameters for Si-O-C system. Diffusion atomic oxygen from oxidized bond into not oxidized bond was added to model SiC/SiO_2 interface. The probability of diffusion atomic oxygen is determined by Metropolis factor. Note that bond switching in this case can be applied not only to oxidized bond, but also to not oxidized bond with oxygen in environment.

The interface energy is a key property of an interface and it determines interface stability. Based on the developed potential set for Si-O-C system we investigated interface energies of several SiC/SiO_2 model structures. The interface energy can be calculated by subtracting the bulk energy of the amorphous oxide and crystalline Si and SiC from the total energy. It was found that exist parameter of modelling T in which interface energy approach show that modelling interface SiC/SiO_2 structures more stable then interface of beginning crystal SiC/ β-cristobalite structures.

This algorithm can be applied to model thermodynamic roughening of the SiC/SiO_2 interface obtained in technological processes of oxidation SiC, which cannot be calculated by molecular dynamics because of time of technological processes.

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2. Brenner D.W. et al, 2002, J. Phys.: Condens. Matter, v.14, p.783.
3. Ni B. et al, 2004, J. Phys.: Condens. Matter, v. 16, p. 7261.