

Molecular Dynamics Simulation of High-Temperature Oxidation of 3C-SiC(100): Differences Between Si-face and C-face

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To improve the performance of space vehicles for extremely harsh service environment, the development of the materials and structures for thermal protection systems plays a significant role. Due to the advanced features, composite materials based on carbon, silicon carbide, silica and carbon fibers turn out to be the latest choice for the thermal protection system. However, since the high-temperature and high-pressure working condition, oxidation occurs and can lead to degradation, which is a critical issue that is far from being well-understood. Experimental efforts have limitation of reaching temperature higher than 2000 °C as well as understanding the break and formation of molecular bonding during chemical reaction. On the other hand, numerical simulation based on *ab initio* is too computational expensive to contain sufficient atoms^[1]. To be able to model the breaking and forming bonds at a lower calculation cost, a sophisticated bond-order potential, ReaxFF (reactive force field) method were established by the group of Adri van Duin^[2]. And the parameters have been extended for Si/C/H/O system by David et al.^[1]. They have studied the oxidation process of SiC by O₂ and H₂O under a range of temperatures from 500 to 5000 K without providing information on the remarkable differences between Si- and C-terminate polar face. By utilizing the similar frame, we investigated the effects of polar face on oxidation behavior of 3C-SiC in the present work.

To perform the simulation, a bulk of SiC with (100) surface normal to z-axis was set up, which was terminated by Si-face at top and C-face at bottom. Within the rest of the simulation cell, high concentrations of O₂ molecules were randomly created. Periodic boundary condition was used for such system with size of 17.43 × 17.43 × 52.30 Å and containing 640 SiC atoms and 100 O₂ molecules. Since the high reactivity of both Si-face and C-face led by insufficient coordination number, we first minimized the structure of SiC then equilibrated O₂ molecules at 100 K, by which the initial configuration was obtained. After that, the temperature of the whole system was quickly increased to 2000 K, controlled by a Berendsen thermostat to simulate the NVT ensemble. All the simulations were conducted with the open-source LAMMPS code^[3]. The results have presented notable differences on the oxide structures between Si-face and C-face, which could give a micro-scale illumination on the experimental observations^[4].

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