

N.V. Tokiy, D.L. Savina, V.V. Tokiy

PRESSURE EFFECT ON OXYGEN MIGRATION NEAR THE (100) SILICON SURFACE OF SiC

The study was aimed at ascertainment of physical causes that control defect structure formation and properties of nanocrystalline silicon carbide powders. An atomic model of a cell of silicon carbide surface with defects was built. Software package ABINIT–nanoHUB tool was applied with using density functional theory. The changes in total energy at motion of the oxygen atoms in the surface layers of silicon covering of carbide by the vacancy mechanism with increasing hydrostatic pressure were evaluated.

It was established that:

1. The contribution of the local electron-ion interaction to the total energy of the cell was changed most of all with increasing hydrostatic pressure.
2. The contributions of the local electron-ion interaction and the exchange-correlation energy of the valence electrons reduced the total energy of the cell with increasing hydrostatic pressure. The contributions of the electron-electron Coulomb Hartree energy, the kinetic energy of the valence electrons, Ewald energy and the energy correction of the ion core of all atoms increased it.
3. The controlling mechanism of the influence of hydrostatic pressure on the migration of oxygen was a non-local pseudopotential interaction of valence electrons with the ionic core of all the atoms in a cell.

It was predicted that increase in hydrostatic pressure results in the following:

- 1) change of the direction of oxidation of the surface layer of the silicon carbide to the opposite one, i.e. deoxidation;
- 2) retardation of the oxygen migration at oxidation and deoxidation of the C-layer of silicon carbide surface.

Keywords: silicon carbide, oxygen, ABINIT, nanoHUB, surface, high pressure, density functional theory, total energy

Fig. 1. Cell of silicon carbide with oxygen on Si-surface (100) (*a*) and in the C-layer of Si-surface (100) (*b*): ○ – oxygen atom O, ○ – carbon vacancy V_C , ○ – carbon atom C, ○ – silicon atom Si

Fig. 2. Various contributions to the total energy in SiC: ■ – the kinetic energy E_{kin} , ▼ – the local pseudopotential energy E_{loc} , Δ – the nonlocal pseudopotential energy E_{nonloc} , □ – the Hartree energy E_H , ▲ – the exchange-correlation energy E_{xc} , ▽ – the Ewald energy E_{Ew} , ○ – the correction core energy $E_{corr-core}$, ● – the total energy E_{tot}

Fig. 3. Total energy changes: *a* – at the entrance of oxygen to silicon carbide through Si-surface (100); *b* – at the release of oxygen from the C-layer of silicon carbide through Si-surface (100); *c* – at the downward migration of oxygen from Si-surface of silicon carbide for different pressures: ■ – $V_{cell} = 0.729$, ● – $V_{cell} = 0.857$, ▲ – $V_{cell} = 1$