Motivation

Application of actinide nitrides as a fuel in the fast transmutation reactor offers potentially enhanced performance as compared to conventional actinide oxide fuels [1,2]. These fuels are receiving renewed attention across the world since the commencement of the Generation IV initiative. Unfortunately, one of the problems with actinide nitrides is their interaction with the oxygen which results in effective fuel oxidation and degradation. Therefore, it is significant to know more about chemical properties, reactivity and oxidation mechanism of UN surfaces as well as processes occurring on grain boundaries inside the polycrystalline UN. In this work, we compare results obtained for (110) surface with previous results for (001) surface.

Computational method and model

For simulation of pure and defective UN(001) and (110) substrates with empty and oxygen-occupied vacancies, we employ the DFT plane-wave computational package VASP 4.6 [3], using ultra-soft pseudopotentials combined with the PAW method. We use the Perdew-Wang-91 GGA non-local exchange-correlation functional [3] and the scalar relativistic PAW pseudopotentials representing the core electrons of U (with 6p6R6p6f5s7 valence shell), N (2p2P0) and O (2p2P2) atoms (containing 14, 5 and 6 valence electrons, respectively). The cut-off energy is chosen to be 520 eV. We use the Monkhorst-Pack scheme [4] for 4x4x1 and 8x8x1 k-point meshes in the Brillouin zone (BZ).

Averaged magnetic moments for UN(01) and UN(110) surfaces are larger for (110) surfaces, by ~0.7 eV per U atom for the defect-free UN (001) [5, 6] and UN(110) surfaces. Averaged magnetic moments for UN(110) surfaces are also larger for (110) surfaces, by ~0.7 eV per U atom for the defect-free UN (001) [5, 6] and UN(110) surfaces.

Application of actinide nitrides as a fuel in the fast transmutation reactor offers potentially enhanced performance as compared to conventional actinide oxide fuels [1,2]. These fuels are receiving renewed attention across the world since the commencement of the Generation IV initiative. Unfortunately, one of the problems with actinide nitrides is their interaction with the oxygen which results in effective fuel oxidation and degradation. Therefore, it is significant to know more about chemical properties, reactivity and oxidation mechanism of UN surfaces as well as processes occurring on grain boundaries inside the polycrystalline UN. In this work, we compare results obtained for (110) surface with previous results for (001) surface.