



Structural stability and deformation resistant analysis of borophene and graphene-filled calcium silicate for cement-based materials



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ABSTRACT

The structural stability and anti-deforming capability of borophene and graphene-filled calcium silicate (C_2S) for cement-based materials are studied by employing molecular dynamic simulations. By analyzing and comparing their various potential energies, it is found that the introduction of borophene or graphene into C_2S can effectively improve its structural stability, make the complex nanosheets cling tightly together, and enhance the ability to resist deformation of the configuration at high temperature, especially for borophene-filled calcium silicate (C_2S -B). Structural analyses on the above complexes at a high compression strain (14.06%) and a high temperature (1000 K) indicate that the graphene-filled calcium silicate (C_2S -G) has the best pressure resistance and the C_2S -B has the greatest high temperature tolerance, while C_2S is always the worst. The results indicate that filling graphene and borophene in calcium silicate can significantly improve the structural stability and enhance the resistance to compressive and high temperature.

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1. Introduction

Calcium silicate, a main hydration product of Portland cement, is a promising reinforcing material for cement-based materials. To improve the performance and increase their potential special functions, adding some nano-material to the cement base material has attracted broad research interest in recent years [1–9], and is expected to be a class of novel cement matrix composite. Calcium silicate (Ca_2SiO_4), also referred to as calcium orthosilicate, can be formulated as $2CaO \cdot SiO_2$. Calcium silicate is a compound that can be synthesized with various ratios of calcium oxide and silica [10], such as Ca_3SiO_5 , $3CaO \cdot SiO_2$; Ca_2SiO_4 , $2CaO \cdot SiO_2$; $Ca_3Si_2O_7$, $3CaO \cdot 2SiO_2$; and $CaSiO_3$, $CaO \cdot SiO_2$. Calcium silicate is used in roads, insulation, bricks, roof tiles, and table salt. When used in cements, calcium silicate is called belite (cement chemistry notation: C_2S). Moreover, calcium silicate is a safe alternative to asbestos as a high-temperature insulation material. Calcium silicate boards with high performance can retain their excellent dimensional stability even under damp and humid conditions. These boards can be installed during early stages of the construction program before

wet trades are completed and the building is subjected to weather-tight treatment. Calcium silicate fabricators and installers in passive fire protection are used in installing firestops [7–10].

Borophene is a novel nanostructure with numerous excellent properties. The first experimental evidence of novel boron nanostructures with hexagonal vacancies was provided by Piazza et al. [11]. These structures may be synthesized with appropriate substrates [12]. The new atom-thick boron nanosheets are appropriately termed “borophene” because of their analogy to graphene. Studies have shown that the structure of B_{36} is not only achievable, it is also highly stable [11]. The structure is a perfectly symmetrical disc that is one-atom thick. In this structure, the boron atoms are arranged in a triangular lattice with a perfectly hexagonal hole in the center. A relatively simple spectrum, which suggests a symmetric cluster, is observed under photoelectron spectroscopy. Neutral B_{36} is the smallest boron cluster to possess sixfold symmetry and a perfect hexagonal vacancy that are the potential bases for extended 2D boron nanosheets. Theoretical calculations indicate that the electronic structure of 2D boron nanosheets can be either metallic or semiconducting [13–16]. Owing to the hexagonal holes, the electronic and chemical properties of borophenes can be tuned with various chemical modifications [17,18]. Therefore, borophene constitutes a new class of nanostructures that complement graphene. Borophene has the potential for new applications because

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of its light atomic weight, low mass, super-strong B-B atomic bonds, better economy, and special electronic structure. Moreover, boron resources are highly abundant. Graphene has attracted considerable attention because of its unusual molecular structure and excellent properties [19]. When incorporated as an enhancing component at extremely low loading, graphene can markedly improve the performances of host polymers [20].

In order to further improve the mechanical performance of widely used cement materials, it is necessary to understand their basic structural stability and anti-deformability in any environment. The contribution of a nanosheets filling to reinforced mechanical properties is investigated extensively in the literature [21–24]. To make full use of the structural performance of the nano-composite structures, we have studied the basic configuration and characteristics of monolayer and bilayer carbon nanotubes, graphene and BN nanotubes (nanosheet) [25–33]. We recently investigated the effect of grafted amine groups on the in-plane tensile properties and high temperature structural stability of borophene nanoribbons. We found that grafting amine groups increases Young's moduli, enhances elastic strain range, reduces in-plane elastic anisotropy, and strengthens crack resistance. Grafting amine groups significantly strengthens deformation resistance at high temperatures, reduces thermal expansion anisotropy, and improves structural stability [34]. Recently, we reported on the structural stability and high-temperature distortion resistance of bilayer complexes that are composed of graphene and borophenes [27]. It is found that bilayer borophene, especially for hybrid bilayer nanosheets, can help improve structural stability. The high temperature deformation resistance of bilayer borophene is inferior to bilayer graphene for the same upper and lower layer materials, and the hybrid bilayer nanosheet formed from borophene and graphene, in three-bilayer complexes, has the greatest high temperature tolerance. Structural stability for bilayer borophene is better than for bilayer graphene, but their high temperature tolerances are exact opposites. On the base of these, we conduct further research on the structural stability and anti-deforming capability of borophene- and graphene-filled calcium silicate (C_2S-B and C_2S-G). The nanocomposites on calcium silicate, which possess enormous potential application, are considered to be a class of novel cement matrix composite. In the present study, molecular dynamics simulations with the Universal Force Field (UFF) have been performed to study the impacts of nanosheet-filling on the structural stabilities, to demonstrate the structural stabilities, the uniaxial compressive behavior and high temperature tolerance of calcium silicate. First, a borophene- and graphene-filled calcium silicate model was constructed on the basis of the ideal lattice structure. Meanwhile, we also modeled on pure calcium silicate for comparison. Then, the simulation models were adequately relaxed to attain more favorable configurations. Thereafter, uniaxial compression and higher temperature annealing were performed. Furthermore, we examined the atomic rearrangements and failure patterns of the structures, and compared and analyzed the mechanical responses between filled and unfilled calcium silicate. The results are helpful for the application of high-performance cement-based materials.

2. Calculation model and method

The geometric models of the graphene, borophene and the calcium silicate are first constructed as the atomic space coordinates. The corresponding sizes are 3.8265, 1.4575 nm, 3.7199, 1.4642 nm for the length and width of borophene and graphene nanosheets, and 3.9845, 1.4512 and 1.0833 nm for the length, width and thickness of calcium silicate, respectively. Model construction is shown

in Fig. 1. To ensure thermal stability, each structure underwent 1000 steps (1 ps) of relaxation, 10,000 steps (10 ps) of stabilization at a high temperature of 1000 K, and annealing at a rate of 20 K/ps. Finally, to obtain a stable equilibrium structure, the structure underwent 20,000 steps (20 ps) of equilibrium after annealing to 300 K. Under compression, the simulated structure models of the complexes induced geometric optimization, which enabled the atoms in the structures to rotate and move in relation to one other. Geometric optimization followed a minimization algorithm to minimize strain energy while allowing an equilibrium state to occur. In addition, the periodical boundary conditions are applied to the compressed direction to avoid the potential energy at different positions along the compressed path will exhibit a globally gradually increasing trend when the compressed distance becomes large, which is due to the increasing of surface energy. To better represent the real structure by small nano-structure models, the periodic structural units are built by setting the basic unit of the geometric models in a cuboid crystal lattice ($a = 4.0$ nm, $b = 1.5$ nm, $c = 1.1$ nm). The different settings for lattice parameters affected mainly the interaction between C_2S . Although the effects are probably not very significant, we will still adopt the method of the lattice parameters which are slightly larger than the sizes of the nano-structure models for accurate computing and analysis.

We employed the Universal Force Field (UFF) method [35,36] to optimize the geometric structures of borophene and calcium silicate under different in-plane compressive strains. Furthermore, we calculated the different types of energies of these structures. The force field method is a highly accurate empirical technique used to optimize structures and involves minimal computational burden. The UFF is parameterized for the full periodic table and is utilized to investigate the structures of main group, transitional inorganic metals, organic, and organometallic compounds. The force field parameters of interest are hybridization set, effective nuclear charges, and connectivity. The potential energy is expressed as the sum of bonded and non-bonded interactions, as follows:

$$E_T = E_b + E_a + E_t + E_i + E_v + E_e \quad (1)$$

where E_b , E_a , E_t and, E_i are functions that belong to bonded interactions and represent bond stretching, angle bending, dihedral angle torsion and inversion term, respectively. Van der Waals E_v and electrostatic interaction E_e are nonbonded interactions. Bond stretching, angle bending, and torsion and inversion are expressed as a harmonic term, a three-term Fourier cosine expansion, and cosine-Fourier expansion terms, respectively. The van der Waals interaction and the electrostatic term are described by the 6–12 Lennard–Jones potential and coulomb interaction, respectively. A parameter generator in the UFF can calculate force field parameters based on atomic properties. Thus, the composing parameters for various types of force field can be generated as requested. For further details, including relevant equations, see Refs. [35–37].

3. Results and discussion

3.1. Structural stability analysis

To compare the structural stability of C_2S , C_2S-G and C_2S-B in Fig. 1, the C_2S is regarded as components of the upper and lower bilayer nanosheets (denoted further as C/C in this section). The C_2S-G (or C_2S-B) can be considered as a trilayer complex formed by a monolayer graphene (or borophene) sandwiched in the C/C (denoted further as C/G/C or C/B/C in this section). The binding energies E_b , interaction energy E_i and the van der Waals energies

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