Annals of Nuclear Energy 63 (2014) 100–106

Contents lists available at ScienceDirect

Annals of Nuclear Energy

journal homepage: www.elsevier.com/locate/anucene

A molecular dynamics study about graphite and boron coated graphite at reactor temperatures

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ARTICLE INFO

Article history:
Received 7 March 2013
Received in revised form 21 July 2013
Accepted 25 July 2013
Available online 17 August 2013

Keywords:
Graphite
Boron coating
Nuclear reactor
Moderator
Reflector
Molecular dynamics

ABSTRACT

Nuclear graphite is exclusively produced as a moderator and reflector material in nuclear industry. It has low density, high strength, low thermal expansion, high thermal conductivity, high hardness and good thermal resistance. We simulated graphite structure in a box using LAMMPS (Large-scale Atomic/Molecular Massively Parallel Simulator) to obtain heat flux, atomic displacements, pressures and total energy values for 300 K (room temperature), 1273 K (gas-cooled reactor operating temperature) and graphite temperatures in the reactor (from 573 K to 1123 K). Also boron coated graphite (BCG) was investigated by the same method and to estimate the same parameters.

1. Introduction

Nuclear graphite has several special features such as low neutron absorption rate, high thermal conductivity and high-temperature strength and stability. It is high purity synthetic graphite. Also the density of nuclear graphite (1.74–1.85) is lower than graphite (2.09–2.23). It slows down neutrons which are produced during the fission process. It is generally used in nuclear reactors as moderator, reflector and structural material. Its thermal properties are an important issue for the nuclear reactor designer.

Recently in literature there are many studies about nuclear graphite material. Some of these studies, thermal parameters of nuclear graphite and properties of nuclear graphite under different irradiation conditions in the foreground. Contescu et al. investigated relationship between nuclear graphite microstructure and its oxidation resistance. In this study, it was reported that nuclear graphite may be a candidate for use in the very high temperature gas-cooled reactors (Contescu et al., 2012). Zhmurikov et al. studied the thermophysical properties of three different graphite composites from 300 K to 1675 K. Heat capacities and thermal conductivity values of samples were given (Zhmurikov et al., 2012). Yang et al. implemented H^+ ion irradiation on nuclear graphite samples. They determined surface deformations and reported XRD and Raman spectroscopic results about their experiments (Yang et al., 2012a,b). In terms of next generation nuclear reactor plans microstructural properties of nuclear graphite was evaluated (Karthik et al., 2012). In another paper, interactions between nuclear graphite and molten fluoride salts at 773 K were investigated by synchrotron X-ray diffraction and carbon K-edge X-ray absorption near-edge structure (Yang et al., 2012a,b). To determine stress analysis and lifetime prediction of nuclear graphite, several creep models for irradiation responses to it were investigated. As a result of this study, the Kennedy model considered compared to other models for the HTR process (Fang et al., 2012). Statistical analysis via three distributions of experimental results about nuclear graphite strength tests were made by researchers (Hindley et al., 2012). A study was performed about the successful recycle of irradiated graphite to fabricate new nuclear graphite (Burchell and Pappano, 2012). Molecular dynamics simulations at high temperatures (up to 1800 K) was made and this paper focused on especially threshold displacement energy of graphite by MSD (mean square displacements) calculations (Hehr et al., 2007). In the reactor applications coating of materials with boron and boron compounds such as B_4C is widespread. Boron coated graphite for fusion reactor applications was produced. In this study, boron coating was suggested a suitable candidate for the first wall and limiter coatings in toroidal magnetically confined fusion reactors (Pierson and Mullendore, 1979). B_4C coating has been suggested fusion devices of next generation ITER and DEMO (Buzhinskij and Semenets, 1999; Buzhinskij and Otroshchenko, 2011). For the first wall of W7-X thick B_4C coating was developed (Kötterl et al., 2001). Four types of B_4C/Mo based composite coating for fusion applications was performed (Lin et al., 2013).

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http://dx.doi.org/10.1016/j.anucene.2013.07.036

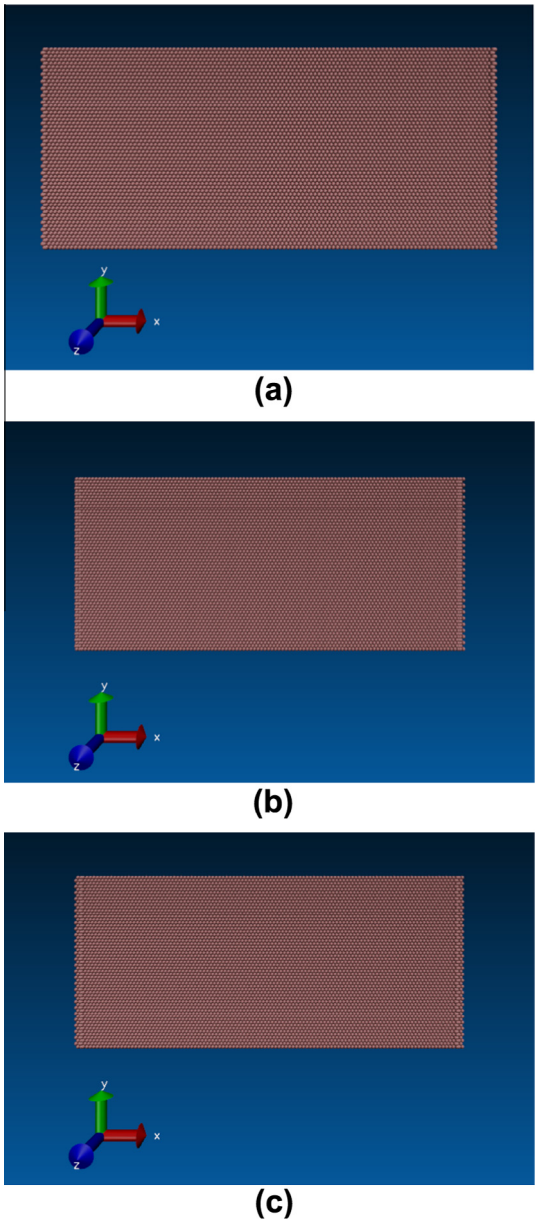

Fig. 1. Atomic arrangements of graphite (a) 300 K, (b) 1273 K, and (c) 573–1123 K.

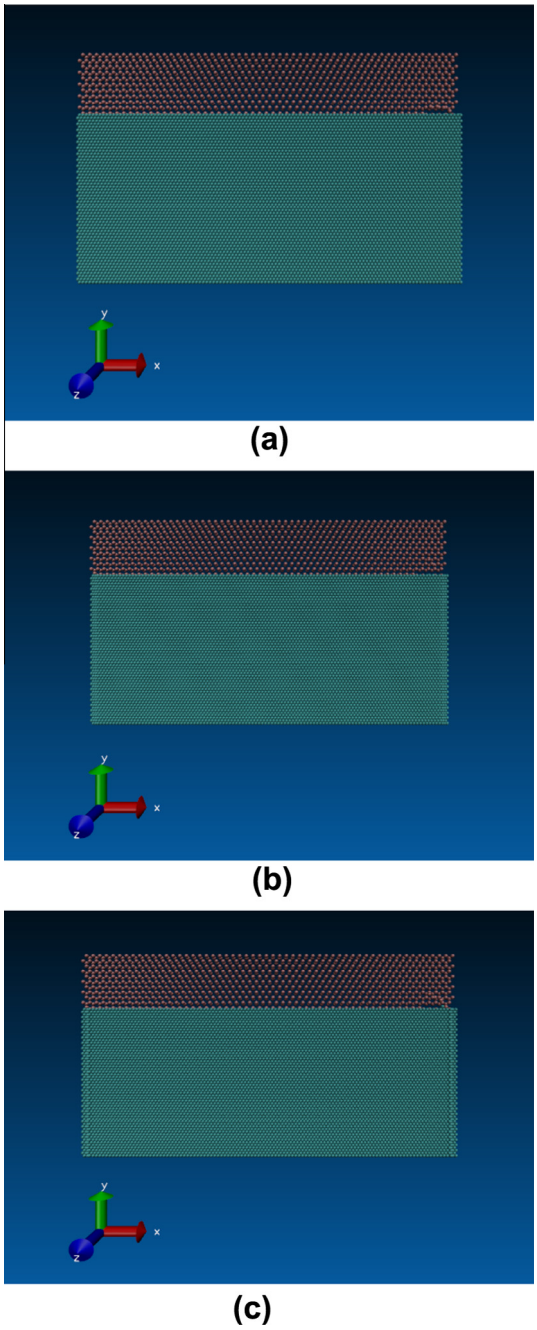

Fig. 2. Atomic arrangements of BCG (a) 300 K, (b) 1273 K, and (c) 573–1123 K.

In this paper we performed LAMMPS molecular dynamic simulations about thermal properties of graphite and BCG under room temperature, gas-cooled reactor operating temperature (1273 K) (Samolyuk et al., 2011) and nuclear graphite temperatures in the reactor. In these temperatures atomic arrangements, energy values, heat fluxes, pressures and atomic displacements were given.

2. Molecular dynamics simulations

Molecular dynamics is a method for computer simulation of complex systems including atoms, bonds, angles, dihedrals, etc., modeled at the atomic level. Numeric solutions by MD are based on the Newton's equations of motion mentioned below as Eqs. (1) and (2).

$$F_i = m_i \cdot a_i = m_i \cdot dV_i/dt = md^2r_i/dt^2 \quad (1)$$

$$F_i = -GRAD_iE \quad (2)$$

Generally molecular dynamics simulations consist of four steps as (1) system setup, (2) equilibration, (3) simulation run and (4) output and data analysis.

In the 1990s, a large-scale parallel classical MD code LAMMPS started to develop by Sandia National Laboratory (Plimpton, 1995). It is an open source code and it is updated regularly. It can run on a single processor or as parallel. An input script should be written by the user to run LAMMPS. In the input script there are molecular properties such as lattice parameters and atomic masses of desired material. Also selecting potentials to be used is a very important issue in LAMMPS. To define atomic coordinates for each atom type, several commands can be used or a data file can be written.

The MD simulations were performed in LAMMPS using a time step of 0.005 fs. We wrote an input script including graphite