



Phase transformation research of fusion reactor first wall material tungsten



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HIGHLIGHTS

- Surface melting velocities and melting point are gotten in surface melting process.
- Uniform melting processes are analyzed using RDF, SSF and average atomic energy.
- The highest limiting superheat shows tungsten is the best plasma-facing material.
- New material combinations will be required based on the tungsten in fusion reactor.

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ABSTRACT

Tungsten is remarkable for its robustness; especially it has the highest melting point of all the non-alloyed metals. Tungsten and tungsten alloys have been widely used in aerospace, weapon, nuclear industries and fusion reactor. Tungsten is expected to become fusion reactor first wall material for this reason. In this paper, phase transformation processes of fusion reactor first wall material tungsten have been investigated via molecular dynamics simulation based on the modified embedded atom model. Surface melting velocities at different temperatures are calculated as $V(T) = -5.082 + 0.00136T$ and thermodynamic melting point is determined by fitting front advance velocities. Structure changes, thermal expansion coefficient, radial distribution function, static structure factor and average atomic energy for uniform melting processes are studied to simulate plasma thermal shock heating to superheat state of tungsten in fusion reactor. The superheat limit of tungsten crystals can be gotten according to simulation results. The superheat limit for tungsten crystal melting is about 27.2%. Tungsten is the best plasma-facing material because of its highest melt point and highest limiting superheating of all the non-alloyed metals.

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1. Introduction

The shortage of fossil energy and environmental pollution are two main barriers for the development of human beings. Among all alternative energy researches, fusion energy has been emphasized by scientists and international organizations to take the place of gradually scarce traditional energy. Thermal shock damage and plasma irradiation effects in the fusion device would largely shorten the lifetime of first wall and change material properties, thus plasma-facing materials is one of great scientific challenges for development and design of magnetic confinement fusion reactor. Tungsten, also known as wolfram is remarkable for its robustness,

especially the fact that it has the highest melting point of all the non-alloyed metals and the second highest of all the elements after carbon. Therefore, tungsten is expected to become fusion reactor first wall material. Tungsten is the most potential material for first wall and a tungsten-coating fusion device has been proposed in 2004 [1].

Plasma-facing material, namely directing interaction with plasma material, due to the high-power and high-energy electron bombardment, escaping the impurity particles deposition and plasma fuel particle bombardment when high heat load plasma bursting, so the material performance requirements are very harsh. Tungsten and its alloy material has the advantages of high melting point, low steam pressure, low tritium retention and low sputter etching rate, so they are widely regarded as plasma-facing materials. At present, the main manufacturing technology is tungsten/copper composite coating [2,3], vanadium alloy V–4Cr–4Ti coating

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[4], tritium permeation layer TiC, SiC [5], neutron shielding and absorbing materials B4C [6] on the structural steel by plasma spraying method.

Tungsten has some good features [7], such as high melting point, high thermal conductivity, strong corrosion resistance and low thermal expansion coefficient. Tungsten in the impact of the intense heat may produce changes in physical properties, which will affect the safety and stable operation of fusion reactors. Thus, thermal and transport properties of tungsten coating and film is one of the important and fundamental topics in fusion reactor device design field. As an important fusion device component, microscopic study and micro database for tungsten are very limited. Through phase transformation research, we can get some important micro databases and melt parameters as a reference in fusion device's design, construction, and operation.

Owing to early using of incandescent lamp, experimental study on tungsten metal has obtained some basic thermal properties [8,9], for instance, melting point and thermal conductivities. However, testing exact physical properties for coatings, phase transformation is a great challenge for the experimental and theoretical study so far. Fortunately, with the development of computing capabilities, molecular dynamics (MD) simulation has been utilized to simulate the thermal and transport processes under heat shock or pressure fluctuations. Because of size effects and time limitation, the nano-scale films have exhibited significantly different thermal behaviors from their bulk structures [10]. Molecular simulation for nano-system would be helpful to deeply understand the thermal properties and transport process mechanism. Many studies [11–15] have focused on micro scale flow, basic thermal and transport properties and described thermal expansion coefficient, melting processes, thermal conductivity and diffusion coefficient for tungsten and other materials. There are still some difficulties to simulate heat transport processes for metal by using classical molecular dynamics method because of electronic contribution. So far, tungsten and tungsten alloys have been widely used in aerospace, weapon, nuclear industries and fusion reactor, where many extreme conditions have been demanded. Accordingly, it is essential to make a deep research on the phase transformation processes of tungsten.

2. Molecular dynamic simulation

2.1. Force field model

The embedded-atom method (EAM) based on density-functional theory was developed for some face-centered cubic (FCC) and body-centered cubic (BCC) metals, then Baskes et al. modified the EAM to include directional bonding that is necessary to explain the behavior of non-FCC materials, and extended it to a large number of elements [16]. In this paper, modified embedded-atom method (MEAM) potential [17] has been used here to describe the interactions between tungsten atoms, which have been applied into studying the crystalline structure and physical properties of metals. The potential energy equations of the system can be given as follows

$$U = \sum_i \left\{ F_i(\bar{\rho}_i) + \frac{1}{2} \sum_{i \neq j} \phi_{ij}(r_{ij}) \right\} \quad (1)$$

where $\phi_{ij}(r_{ij})$ is the pair potential between atom i and atom j , $F_i(\bar{\rho}_i)$ is the embedding energy function, and $\bar{\rho}_i$ is the environmental electron density at the position of atom i . $F_i(\bar{\rho}_i)$ is expressed as

$$F_i(\bar{\rho}_i) = A_i E_i^0 \bar{\rho}_i \ln \bar{\rho}_i \quad (2)$$

where A_i is adjustment factor, E_i^0 is the cohesive energy. $\phi_{ij}(r_{ij})$ is expressed as

$$\phi_{ij}(r_{ij}) = \bar{\phi}_{ij}(r_{ij}) S_{ij} \quad (3)$$

$$\bar{\phi}_{ij}(r_{ij}) = \frac{1}{Z_{ij0}} [2E_i^u(r_{ij}) - F_i \hat{\rho}_i(r_{ij}) - F_j \hat{\rho}_j(r_{ij})] \quad (4)$$

$$E_i^u(r_{ij}) = -E_{ij}^0 (1 + a_{ij}^*(r_{ij})) e^{-a_{ij}^*(r_{ij})} \quad (5)$$

$$a_{ij}^* = \alpha_{ij} \left(\frac{r_{ij}}{r_{ij0}^0} - 1 \right) \quad (6)$$

where E_{ij}^0 , r_{ij0}^0 , α_{ij}^0 are related parameters with atom i and j , Z_{ij0} is decided by atoms mutual structure in simulation system. $\hat{\rho}_j(r_{ij})$ is the environmental electron density effect on the r_{ij} . S_{ij} is the scanning function decided by the cut-off radius.

2.2. Computational details

Two systems are used to simulate heat transfer processes. A $20a \times 20a \times 50a$ (a corresponds with lattice constants at different temperatures) simulation box in $[1\ 0\ 0]$, $[0\ 1\ 0]$ and $[0\ 0\ 1]$ directions are used in system I, which is utilized for surface melting simulation. In the simulation, the surface melting is that quasi-liquid films can be shown as the increase of free atomic motion distance on solid surfaces. The solid melts homogeneously from the outside to the inside. In the case, the solid always melts from the outside inwards, never from the inside. The uniform melting is that the whole solid's volume gradually increases with increasing temperature, and then it entirely grows to be the liquid state. In the case, the solid would not melt from the outside because of periodic boundary conditions in every direction. The two-dimensional periodic boundary conditions are used in $x\ [1\ 0\ 0]$ and $y\ [0\ 1\ 0]$ directions, along which the lengths of the specimen are infinite. Free boundary conditions in which the boundary atoms would leave from simulation box are used instead of periodic boundary conditions which are applied to generate a pair of symmetrically free surfaces in $z\ [0\ 0\ 1]$ direction. The simulation box is divided into a number of layers in z -direction, and then thermodynamic parameters at different temperatures will be calculated layer by layer.

The second system is designed for uniform melting simulation. We build a perfect BCC tungsten crystal box and the dimensions of the simulation box are $10a \times 10a \times 10a$ in $[1\ 0\ 0]$, $[0\ 1\ 0]$ and $[0\ 0\ 1]$ directions, respectively. Periodic boundary conditions are executed all these three directions. The symbol a , initial lattice constant, is 0.31652 nm at 298 K. In the simulation, we have first carried out a constant temperature and pressure (NPT) simulation based on the simulation box for a perfect BCC tungsten crystal to obtain the lattice constant and the thermal expansion coefficient α_T at a given temperature range. Uniform melting point can also be estimated by a step-change of volume of tungsten crystal box. Then a canonical ensemble (NVT), using corresponding lattice constant, is applied to calculations of physical properties. Time step is 1 fs, and temperature increases 100 K every 10,000 steps. The system should be equilibrated at predetermined temperature for 5×10^5 time steps, which are sufficient and necessary to get reliable results.

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