Nuclear Inst, and Methods in Physics Research B 432 (2018) 24–28

Contents lists available at ScienceDirect

Nuclear Inst. and Methods in Physics Research B

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

Theoretical study of the performance of refractory materials for extreme conditions applications

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ARTICLE INFO

Keywords:
Molecular dynamics
Radiation damage
Debris
Nanoimpact

ABSTRACT

Refractory metals are widely used in nuclear engineering and aerospace industry, due to their high resistance to extreme conditions, such as high temperatures, and wear. When used in this context, these materials are subjected to a flux of high-energy radiations that change their microscopic structure by means of the generation of a high number of defects. The production of defects can reach a dramatic amount, thus affecting the macroscopic properties of the material. It is crucial to understand the microscopic changes that occur in these materials, in order to enhance their performances and endurance. Damage production and displacement cascade take place in a very short time scale and are impossible to be studied directly with experimental techniques. Molecular Dynamics, operating in the nanometre scale and covering a time-scale that spans from tenths of femtoseconds up to nanoseconds, can provide a deep insight into the micro-structure of the materials in the first moments after the impact. Our study focuses on the analysis, at the atomic level, of the response of niobium as a reference refractory metal against the impact of a high-energy debris. The goal of this work is to prepare a computational set-up to give a preliminary insight on the behaviour of refractory metals and state their efficiency as shielding components in aerospace and nuclear industry. In the present work, we report preliminary results of damage response in niobium as shielding material, showing low energy dependence on dislocation density for debries energies over the 10 keV. Moreover, we present basis of our methodology and the interest of extending this study to further comparison with other refractory metals, like tungsten, tantalum, of industrial interest.

1. Introduction

Refractory metals and their alloys have a widespread use in the main industrial applications that involve extreme conditions, such as nuclear engineering and aerospace industry, due to their high melting point that gives them an elevated resistance to heat, and their tolerance to wear. Such metals can be found as components of nuclear reactors and spacecraft; these materials undergo a continuous flux of radiations, which can interact with the materials. As a result, a considerable number of defects is generated. The kinetic energy of the colliding particles transfers, in part, to the atoms of the material and then propagates into the structure, causing the removal of some atoms from their equilibrium positions: these atoms, still keeping a great amount of kinetic energy after the impact, collide with their neighbours in the crystal structure. This provokes a displacement cascade, and the number of defects generated by this mechanism can reach a huge amount and affect the macroscopic properties of the materials. In this way, long-term exposition to high-energy radiation environments can lead to a change in the mechanical properties of the material, with consequent deterioration and worsening of their performances and, eventually, a shortening of their lifetimes. Even if it is possible to study the damage produced on the material structure after the irradiation, by means of analysing the micro- and macroscopic changes in exposed materials [1–3], damage production and displacement cascade are very rapid (they take place in a timescale of picoseconds) and it is impossible to monitor them in real time using experimental techniques. In this context, Molecular Dynamics (MD) is a very good tool since it works in short timescales (from tenths of femtoseconds up to nanoseconds) and provides a deeper understanding of the microscopic changes that occur in the materials, thus allowing to study the amount of defects production and to predict the behaviour consequent to expositions to high-energy radiations. In this way, it is possible to properly model the

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https://doi.org/10.1016/j.nimb.2018.07.010
Received 30 October 2017; Received in revised form 10 July 2018; Accepted 11 July 2018

structures, and to obtain materials with improved lifetimes and performances. Several theoretical studies have been performed to analyse radiation damage in a nuclear reactor environment [4–9], by simulating the transfer of a huge amount of radiation energy to an atom of the crystal structure of the material (known as Primary Knock-on Atom, PKA), and the consequent displacement cascade. However, to our knowledge, no studies have been reported yet to address massive damage cascades at the atomic scale originated by high-energy debris. High-energy debris are a phenomenon that can occur both in inertial nuclear fusion [10] and in aerospace environments, and can lead to similar modifications in the inner structure of the materials. It consists on the impact, on their surface, of scattered pieces of a broken material. They are known as debris. The dimensions of the debris cover a very wide range - from nano to macro - and its energy may vary. When the energy of the debris is sufficiently high, it can provoke the removal of the atoms of the lattice from their equilibrium positions, and a displacement cascade, as in the case of PKA, is observed. The study of the impact of debris on the surface of materials is still unexplored. The purpose of our study is to apply Molecular Dynamics to analyse the impact of a debris on the surface of a model refractory metal like niobium, with the aim to provide a future comparison between the behaviour of different refractory metals, to state which one performs better as a shield in materials used under extreme conditions that involve radiation environment. In this work, we will present our current results, regarding the analysis of niobium.

2. Simulation methods

The study is carried out performing Molecular Dynamics simulations with the open source software LAMMPS [11], which allows parallel computing thus enhancing the speed of the calculations. A ternary embedded atom method (EAM) potential is used for all the systems investigated, with ZBL corrections [12] that allow to treat distances smaller than 0.5 Å. This EAM potential has been developed in the framework of EU-FP7-RADINTERFACES project and was employed to model the interactions Cu–Nb, Cu-He and Nb-He in a Cu/Nb interface by means of atomistic MD simulations using the LAMMPS code in its GPU implementation [13,14]. Parallel simulations are run on machines equipped with Intel Core Processors 3.60 GHz, using Graphical Processing Units (GPUs). The simulations are run at 0 K in a NVE ensemble using periodic boundary conditions in x and y directions while shrink boundary conditions in the impact direction (z). The size of the cell simulation is fixed to 115x115x90 lattice units, with 2381024 particles, to avoid possible interactions of a particle with itself. Different energies of the debris are set up as parameters, while keeping the debris size fixed to 4.0 Å: 5, 10, 15, 20 and 25 keV. Debris were built by clustering 524 relaxed Nb atoms. For statistical reasons, three set of simulations are run for every energy value, in each one debris rate has a great z-component while x- and y- rates are kept much smaller than z- component, but not equal to zero (to avoid channelling propagation). The timestep of simulation is varied between a value of 10^{-6} picoseconds and $5x10^{-5}$ picoseconds, to keep the total energy always constant. Total simulation time is of 65 ps. Simulations results are post-processed using the open source software OVITO [15]. To describe the behaviour of materials under extreme conditions in nuclear and aerospace environments we have set up a methodology to analyse the following properties:

- number of interstitial and vacancies - extracted using the Wigner–Seitz (WS) Analysis. The interstitials and vacancies are generated after transferring kinetic energy from the impacting debris to the atoms in the lattice, that in this way escape their equilibrium positions;
- evolution of dislocation density with time - studied using the Dislocation Extraction Algorithm (DXA) [16,17]. Dislocation density is defined as the total line length of a dislocation divided by the volume of the cell. It is useful to monitor the amount of dislocations, which are one of the causes of deterioration of the materials and degeneration of their mechanical properties;
- number of particles ejected from the surface. This measurement quantifies the damage in terms of erosion of the material. Furthermore, the ejected particles could remain in the nuclear chamber or in the aerospace environment after the impact and, as a consequence, turn themselves into a potential bullet;
- evolution of the average kinetic energy of some selected particles in the surface. We monitor how the high kinetic energy of the debris is dissipated through the atoms in the material;
- average propagation speed of the shock wave. The increase in kinetic energy of the material results in the diffusion of a shock wave through the structure. The shock wave propagation speed is supposed to be different depending on the material. It is a useful tool to classify it regarding its resistance towards the impact.

3. Results and discussion

In this section, we report preliminary results on niobium as a reference to prepare the 'test bed' for further comparison and selection of materials under high-energy debris irradiation. We show the results of the analysis of the impact of a high-energy debris on a *bcc*-niobium structure. The dynamic of the impact can be generally divided into three parts: immediately after the impact, and consequently to the transfer of kinetic energy from the colliding particles to the atoms in the lattice, defects generation takes place. Then, it follows a step characterized by the recombination of interstitial and vacancies; finally, a steady state, without further changes in defects amount, is reached. The length of each part and the number of defects produced are related to debris energy. As expected, the higher the energy of the debris, the higher the number of defects at the end of the simulation, and the longer is needed for the system to equilibrate after the impact. A graphical description of the dynamic after the impact is shown in Fig. 1.

3.1. Defects and dislocations

The first part of our analysis is focused on the evolution of point defects and dislocations with time. In Fig. 2 we show the number of interstitial/vacancies at the end of the simulations as a function of debris energy. As expected, the number of generated defects depends on the energy of the impact. There are two contributions to defects production: one is the transfer of the kinetic energy from the particle to the atoms of the lattice, to move them from their equilibrium position; the other is the implantation of new atoms from the impacting debris in the structure. Fig. 3 depicts dislocation density as a function of debris energy, computed as an average over the last 16 timesteps of the simulation. Interestingly, results show a decrease in dislocation density, which has been ascribed to the interaction between different dislocations when the density starts to grow due to the high-energy transferred to the atomic network. Indeed, the perturbation propagates through atom planes and, the higher energy transferred to the atoms by the impact, makes two dislocation lines interact.

3.2. Number of particles ejected from the surface

In the following subsection, we focus on the some of the features of the surface of the materials affected by the impact of the debris. In Table 1, we collect the number of particles that have been ejected from the surface at the end of the simulation. We counted all the particles whose distance from the surface is bigger than a threshold value. A very small percentage of particles is ejected, even for higher-energy impacts. The erosion of the surface by the debris can be observed. This phenomenon results in the creation of a void, shown in Fig. 4. The extent of the void can be another useful measurement to classify the material towards resistance in radiation environments and to estimate the