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Characterization of neutron induced damage effect in several types of metallic multilayer nanocomposites based on Monte Carlo simulation

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ABSTRACT

Metallic multilayer nanocomposites are known to have excellent interface self-healing performance when it comes to repairing irradiation damages, thus showing promise as structural materials for advanced nuclear power systems. The present study investigated the neutron irradiation displacement damage rate, spectra of the primary knocked-on atoms (PKAs) produced in the cascade collision, and the H/He ratio in four kinds of metallic multilayer nanocomposites (Cu/Nb, Ag/V, Fe/W, and Ti/Ta) versus neutrons' energy. Results suggest that the three neutron induced damage effects in all multilayer systems increased with the increasing of incident neutrons' energy. For fission reactor environment (1 MeV), multilayer's displacement damage rate is 5–10 $\times$ 10^{22} dpa/(n/cm^2) and the mean PKAs energy is about 16 keV, without any noteworthy H/He produced. Fe/W multilayer seems very suitable among these four systems. For fusion reactor environment (14 MeV), the dominant damage effect varies in different multilayer systems. Fe/W multilayer has the lowest displacement damage under the same neutron flux but its gaseous transmutation production is the highest. Considering the displacement damage and transmutation, the irradiation resistance of Ag/V and Ti/Ta systems seems much greater than those of the other two.

1. Introduction

Metallic multilayer nanocomposites have received significant attention in recent years for their excellent self-healing properties in trapping and releasing defects [1–6]. The microstructure of multilayers with small individual layer thickness of nanometer order size is proved to be much more stable than bulk materials after ion implantation [7]. Molecular dynamics (MD) simulations demonstrate that interfaces between the neighboring heterogeneous layers of the multilayer nanocomposites act as efficient sinks for the interstitial atoms and can immediately emit them to nearby vacancies. Through the "absorb and re-emit" mechanism, the velocities of defect recombination in multilayers become more rapid [8]. Recently, Misra et al. developed a novel approach to process such nanocomposites in bulk form by fabricating a 4 mm-thick Cu/Nb multilayer nanocomposite with crystallographically stable interfaces via accumulative roll bonding technique [9,10]. As a result of this remarkable breakthrough in nanocomposite manufacturing techniques, bulk nanocomposites have become promising candidates as structural materials for advanced nuclear power systems.

Since most investigation focus on the interface self-healing performance of multilayer nanocomposites, however, its radiation induced damage effects in reactor radiation environment are seldom concerned. Just as the traditional block materials, metallic multilayers' radiation damage effect varies depend on the material system and the radiation condition. For instance, nickel alloy has a strong anti-displacement damage feature but its gaseous transmutation production problem in fusion reactor environment is serious. Hence, knowledge of the radiation-induced displacement damage rate, energy transfer between the incident neutron and primary knock on atoms (PKAs), and the gaseous transmutation production under neutron irradiation with different energy is of primary importance in achieving the goal of designing radiation-tolerant materials. The current paper presents the neutron irradiation damage effects on four kinds of metallic multilayer nanocomposites (Cu/Nb, Ag/V, Fe/W, Ti/Ta), which have been tested using the Monte Carlo method toolkit MCNP and Geant4. These four kinds of multilayers have good interface self-healing properties [11–14].

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2. Methodology

2.1. Molding of metallic multilayers

In our work, we set the multilayer nanocomposites as a 200 μm × 200 μm × 100 μm box. The box is composed of 10,000 single layers (10 nm thick) and the material in each layer varies alternately between two metallic elements, such as Cu/Nb, Ag/V, Fe/W and Ti/Ta. The mono-energetic neutron source is set to locate on the central axis of the model and its incidence direction is parallel to the depth direction of the multilayer. Because we set the material outside the multilayer as vacuum, neutrons don't lose any energy until they are implanted into the multilayer (Fig. 1).

2.2. Calculation method of displacement damage (dpa) using MCNP

Displacement per atom (dpa) is often used to evaluate materials' displacement damage. It can be calculated from the following equations:

$$\mathrm{dpa} = \left(\int \sigma_{\mathrm{dis}}(E) \cdot \varphi(E) dE\right) \cdot t \quad (1)$$

$$\sigma_{\mathrm{dis}}(E) = \frac{\beta}{2E_{\mathrm{d}}} \sigma_{\mathrm{damage}}(E) \quad (2)$$

where $\sigma_{\mathrm{dis}}(E)$ is the atomic displacement cross section for neutron at an energy E, $\varphi(E)$ is the incident neutron flux, and t is the irradiation time. $\sigma_{\mathrm{dis}}(E)$ can be calculated from the damage energy cross section $\sigma_{\mathrm{damage}}(E)$. The factor β is a normalized constant (displacement efficiency) with the value of 0.8. E_{d} is a constant, which refers to the displacement threshold energy. Values of E_{d} in different metal materials used in the simulation are listed in Table 1 [15].

In this work, we performed the dpa calculations using the Monte Carlo neutron-transport code MCNP [16]. Unlike the first principle and the molecular dynamics calculation, the effect of materials' crystallinity is not taken into account in the simulation.

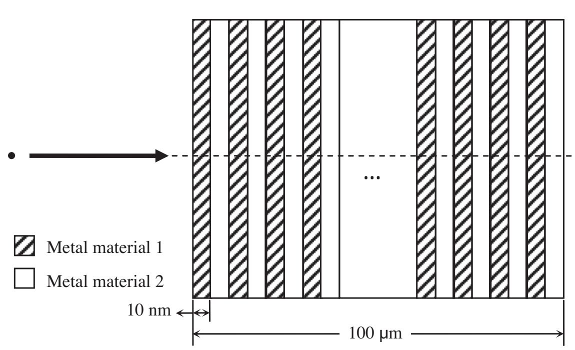

Fig. 1. Geometry of the metallic multilayer nanocomposites model in the Monte Carlo simulations.

Table 1
Displacement threshold energies of elemental metals.

Metal	E_{d}/eV
Cu	18.3
Nb	28.2
Ag	26.0
V	28.0
Fe	17.4
W	44.0
Ti	20.8
Ta	26.7

The neutron flux $\varphi(E)$ was scored by F4 card. $\sigma_{\mathrm{damage}}(E)$ is the cross section of 444 reaction channel.

2.3. PKA and gaseous transmutation production score using Geant4

Geant4 package is another Monte Carlo toolkit for simulating the transport of particles through matter [17]. In implementing customized complex scoring, we had to handle the information of each step around the particle track, which was unavailable through MCNP. In the Geant4 simulation, we used the physics list QGSP_BERT_HP to define the physical process without any modifications. As reflected in its naming scheme, QGSP_BERT_HP is based on Bertini cascade models and also includes high-precision methods for transporting neutrons with energies below 20 MeV [18]. All particles (neutron, ion, gamma ray, electron, etc.) used in the simulation and their processes are included in it. 1×10^7 events were performed to ensure the accuracy of the calculation results.

3. Results and discussion

3.1. Neutron's energy influence on dpa

Most Gen IV fission reactor and fusion reactor neutrons' energy is in the range of 0.1–14 MeV. At this scale, not only do the neutron flux and irradiation time determine materials' radiation damage, the neutrons' energy also affects it markedly. From the perspective of neutron interaction probability in materials, the interaction cross section of neutron reduces with increasing neutron's energy,

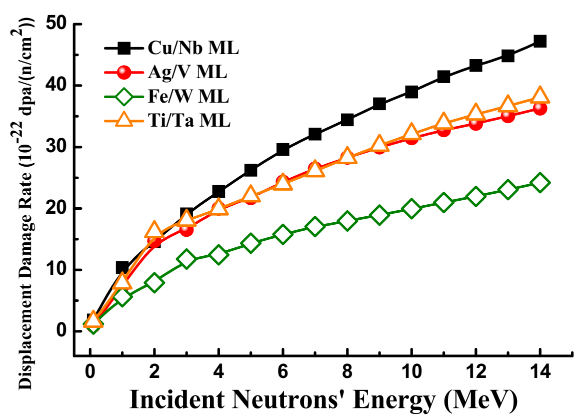

Fig. 2. Neutron induced displacement damage rate in four multilayer systems versus incident neutron's energy.

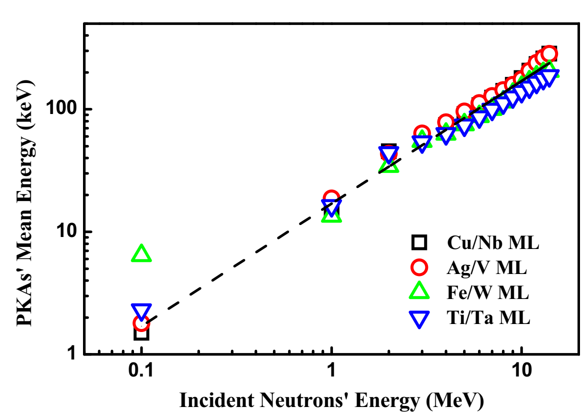

Fig. 3. The mean PKA energies produced by incident neutrons with different energies.