

## Simulation of accumulation of radiation damage and He atoms in Al-B<sub>4</sub>C neutron absorber

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### 1. Introduction

Significantly oxidized surface of surveillance coupons of an Al-B<sub>4</sub>C neutron absorber used in spent nuclear fuel (SNF) pool for up to 8 years and 3 months was recently reported [1]. This severe degradation of the absorber was truly unexpected since the 40 years of service life was guaranteed based on separated accelerated corrosion tests and gamma irradiation tests [2]. This premature degradation of the absorber was immediately attributed to radiation-accelerated corrosion since numerous radiation-induced bubbles were observed from the TEM analysis, which was suspected to be filled with hydrogen and helium from the electron energy loss spectroscopy (EELS) [1]. They suggested that the MeV level energetic ions emitted from <sup>10</sup>B(n,α)<sup>7</sup>Li reactions may have accumulated enough radiation damage with gaseous helium atoms near the B<sub>4</sub>C particles in the absorber [1].

Several heavy-ion irradiation experiments have been conducted for Al-B<sub>4</sub>C MMC to experimentally estimate the accumulated radiation damage in the absorber, which is desperately needed to evaluate the safety consequence of the irradiation-assisted corrosion behavior of the absorber in the long term [3]. However, tested radiation doses for those ion-beam experiments have not yet been determined or crosschecked with any computational simulation because there has not been any safety and performance code developed for neutron absorbers.

As a preliminary effort to develop such a code, several existing codes relevant to the purpose TRITON, ORIGEN, CSAS6, and SDTrimSP are coupled to simulate the radiation damage in the absorber and a multi-scale simulation is carried out to suggest quantitatively the vacancy concentration and helium atom density. The computational strategy and the coupled codes are described in Section 2. Calculated results, basically displacement per atom (dpa) and gaseous atom concentration within B<sub>4</sub>C particle and the surrounding aluminum alloy matrix, are summarized in Section 3.

### 2. Simulation description

#### 2.1. Workflow

Figure 1 illustrates the schematic flow chart of the simulation. Following variables and parameters are sequentially calculated: 1) nuclide inventory, 2) neutron emission rate, 3) neutron flux distribution in the absorber, 4) the reaction rate of <sup>10</sup>B(n,α)<sup>7</sup>Li reactions in a B<sub>4</sub>C particle, and 5) vacancy and helium atom densities.

Radiation damage and helium ion distribution in a B<sub>4</sub>C particle and the aluminum matrix are stochastically calculated by SDTrimSP, a Monte-Carlo program based on binary collision approximation [4]. The SDTrimSP code was originally designed for a one-dimensional cartesian coordinate system under a single point irradiation, therefore, we modified the code to be applicable for spherical mesh considering the shape of the B<sub>4</sub>C particle and the surrounding aluminum alloy matrix. Module for multiple point ion emission is developed to consider the simultaneous ion emission through intraparticle regions.

Neutron flux in the absorber should be evaluated to calculate the rate of <sup>10</sup>B(n,α)<sup>7</sup>Li reactions of a particle prior to SDTrimSP calculation. CSAS6 of SCALE code system is used to calculate the neutron flux in neutron absorber [5]. In addition, the calculation of neutron flux at the intraparticle region is necessary to consider the ions from the central region, which mostly interact with lattice atoms of B<sub>4</sub>C particle. The radiation damage in this region can be excluded in respect of the absorber integrity, whereas gaseous atom accumulation of intraparticle regions changes the stopping power of matter. Thus, the module for neutron flux calculation in the B<sub>4</sub>C particle region has been developed.

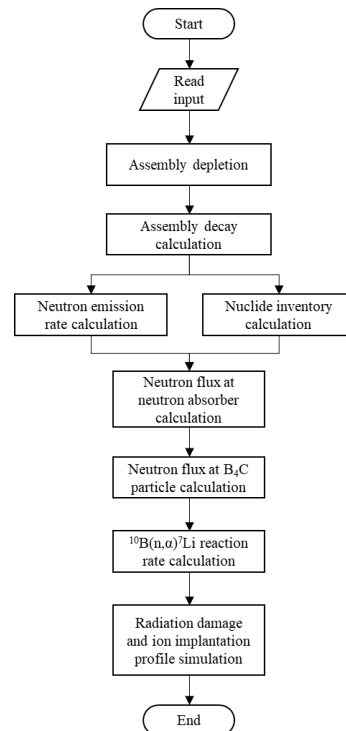


Figure 1. Flow chart of the simulation

Evaluation of nuclide inventory is highly required value for the neutron flux calculation. Irradiated fuel materials containing fission products and transuranium nuclides have to be filled in simulated spent assembly. For this purpose, depletion of fuel assemblies and pin by pin decay calculation are conducted at each time-step.

CSAS6 calculates the stochastic result, which can be converted to neutron flux with the neutron emission rate of the simulated system. In this simulation, the neutron emission rate of assembly is calculated based on the number of nuclides in the spent fuel assembly.

### 3. Results

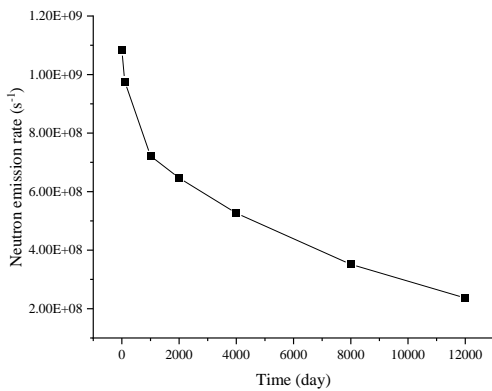


Figure 2. Neutron emission rate of spent nuclear fuel assembly which is irradiated to 52,714 MW/MTU

The fuel assembly, which has 16x16 configuration, is irradiated to 52,714 MWd/MTU for 1,620 days in the simulation. Figure 2 shows the neutron emission rate of the spent assembly with decay time. The emission rate has been exponentially decreased the decay of <sup>242</sup>Cm and <sup>244</sup>Cm, which are the governing spontaneous fission and (α,n) reaction sources.

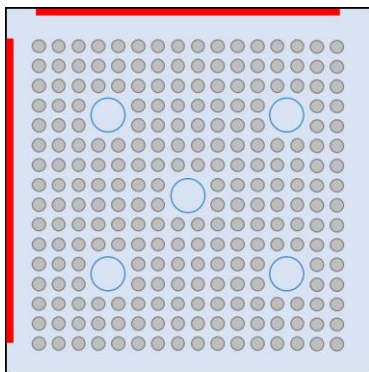


Figure 3. Transverse image of the spent nuclear fuel pool

The transverse image simulated spent fuel pool is illustrated in Figure 3. The spent assembly is placed in the center and surrounded by stainless rack, black line in the figure, and neutron absorbers, which are colored in red, are attached to left- and up-side. Periodic boundary condition is imposed on all lateral boundaries.

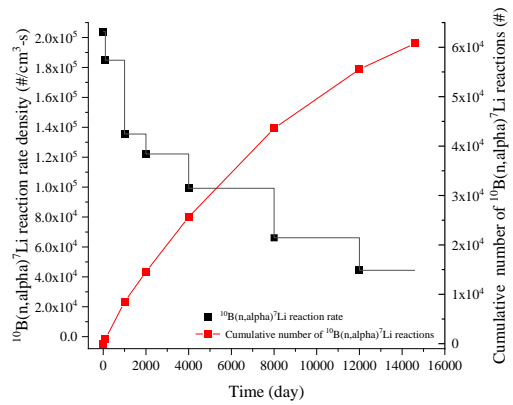


Figure 4. <sup>10</sup>B(n,α)<sup>7</sup>Li reaction rate density of each time-step and cumulative number of reactions

The highest neutron flux is calculated at the surface of the middle region of the neutron absorber. <sup>10</sup>B(n,α)<sup>7</sup>Li reaction rate density and the cumulative number of <sup>10</sup>B(n,α)<sup>7</sup>Li reactions of a 5 μm radius B<sub>4</sub>C particle are plotted in Figure 4. The reaction density at the start of a time-step is used for the time-step for the conservative result. After 14,600 days irradiation, the cumulative number of <sup>10</sup>B(n,α)<sup>7</sup>Li reactions of the particle is 6.08×10<sup>4</sup>.

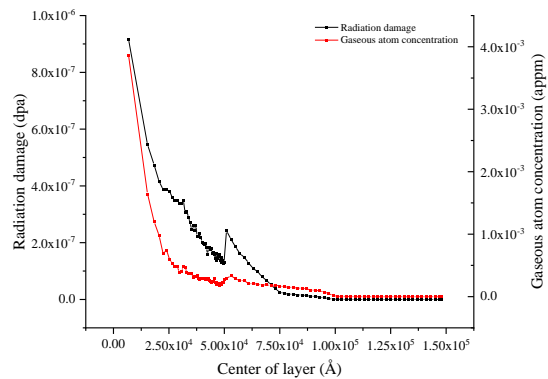


Figure 5. Radiation damage (in dpa) and gaseous atom concentration (in appm) of 5 μm radius B<sub>4</sub>C particle.

Figure 5 shows radiation damage predicted by modified Kinchin-Pease model [6] and gaseous atom concentration within the B<sub>4</sub>C particle and the aluminum alloy matrix. Both results spike at the particle-matrix interface since the number density of lattice atom nonlinearly decreases in the matrix layer. In the particle center region, the results are relatively high because of the isotropic angular distribution of ion emission at the periphery region. At innermost mesh of aluminum alloy matrix, radiation damage is 2.42×10<sup>-7</sup> dpa and helium atom concentration is 2.91×10<sup>-4</sup> appm.

#### **4. Conclusions**

As a preliminary effort to develop a safety and performance code for Al-B<sub>4</sub>C MMC neutron absorber used in spent nuclear fuel pool, we modified SDTrimSP code, originally a one-dimensional simulation code for ion and lattice atom interaction, to be applicable for the geometry and irradiation characteristics of the neutron absorber. The modified SDTrimSP code was then coupled with several codes, TRITON, ORIGEN, and CSAS6 of SCALE, to simulate the radiation damage and helium atom accumulation due to <sup>10</sup>B(n,α)<sup>7</sup>Li reactions. Using the integrated code, a multi-scale simulation was carried out to suggest quantitatively the vacancy concentration and helium atom density in the neutron absorber. This result may improve the understanding on the irradiation-accelerated corrosion of the neutron absorber and help further development of the performance code for the absorber.

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