# Understanding of radiation effect on sink in aluminum base structure materials

Sang Il Choi, and Ji Hyun Kim\*

Ulsan National Institute of Science and Technology (UNIST) 100 Banyeon-ri, Eonyang-eup, Ulju-gun, Ulsan, Republic of Korea 689-798 \*Corresponding author: kimjh@unist.ac.kr

#### 1. Introduction

Aluminum and its alloy are most favorable materials in the research reactor society as structure materials because it's unique characteristic such as high thermal conductivity, neutron economy and corrosion resistant properties [1]. From the many experimental work, it was verified that aluminum is safety materials as structure materials for the reactor life time. Although its excellent properties, radiation induced degradations are most important concern of the safety concept. In case of aluminum, a slightly different approach is needed for the evaluation of radiation damage. Unlikely other structure materials such as zirconium alloy and iron based alloy, aluminum generate not only matrix defect but also much transmutation.

Quantitative analysis of radiation damage of aluminum have been done in two research method. First research method is calculation of radiation damage quantity in the matrix. In this research, quantity of transmutation and matrix damage are evaluated by KMC simulation from ENDF database of IAEA [2]. Most recently, radiation damage such as defect and transmutation are calculated in the MNSR reactor environment [3]. The second research method is evaluation of sink morphology change by irradiation, which research method focus on accumulating behavior of radiation defects. Matrix defect and transmutation are clustering or dissolved by thermal diffusion and energy statue. These clustering defect such as dislocation loop, void and bubble directly affect mechanical properties.

In this research area, it is hard to using deterministic method because it should describe envious and various reaction module in detail. However, in case of probabilistic method, it could be explained without detail reaction module. Most recently, there was KMC modeling about vacancy and helium cluster [4]. From this cluster modeling, transmutation is quantitatively analyzed. After that cluster effect on swelling are explained. Unfortunately, silicon, which is another transmutation of aluminum, effect are neglected. Also primary cluster, which is generated by cascade, effect are neglected.

For the fundamental understanding of radiation effect on aluminum alloy, it is needed that more various parameter such as alloy element and primary cluster effect should be researched. However, until now there was not general modeling which include alloy element and primary cluster effect on aluminum.

However, there was not specified KMC platform for the quantitative analysis of irradiation effect on aluminum alloy. Therefore, this research object is establishment of research framework and rationale for the fundamental understanding of sink structure behavior in aluminum matrix by using KMC modeling.

## 2. Reaction framework

In order to establish KMC simulation, basic assumption of the framework should be defined properly. In case of calculation of radiation damage quantity in the matrix, it was assume that defect and transmutation are generated by only neutron fluence of specific reactor (other radio activity source are ignored such as proton and electron). Degree of aluminum purity was assumed 100% for the simplification. The experiment result of cross section and fluence was used ENDF database [2] and equation of the calculation are follow general defect generation equation. In case of evaluation of sink morphology change, much more complex assumption are used for each sink case.

## 2.1 Generation of defect and transmutation equation

Equations for the calculation of defect and transmutation are represented as below:

$$R_{d} = N \int_{\breve{E}}^{\breve{E}} \Phi(E_{i}) \sigma_{D}(E_{i}) dE_{i}$$
(1)
  
*Where*  $N$  = the lattice atom density,

 $\Phi(E_i)$  = the energy-dependent particle flux  $\sigma_D(Ei)$  = the energy-dependent displacement cross section.

$$\sigma_D(E_i) = \int_t^\iota \sigma_D(E_i, T) \nu(T) dT$$
(2)

Where  $\sigma_D(E_i,T) = the probability that a particle of$ energy Ei will impart a recoil energy T to astruck lattice atom<math>v(T) = the number of displaced atoms

$$v = k(E - S_e)/2E_d \tag{3}$$

Where E = the total energy of the PKA,  $S_e =$  the energy lost in the cascade by electron excitation  $E_d =$  damage energy. (4)

$$T_{d} = N \int_{\vec{E}}^{\vec{E}} \Phi(E_{i}) \sigma_{T}(E_{i}) dE_{i}$$
Where  $N =$  the lattice atom density,  
 $\Phi(E_{i}) =$  the energy-dependent particle flux  
 $\sigma_{T}(E_{i}) =$  the absorption cross section.

Ê

Equation from (1) to (3) is about matrix defect. The defect quantity is proportion with neutron fluence and displacement cross section. PKA induced matrix defect are calculated by NRT modeling. Equation (4) is about transmutation. Transmutation could be calculated by same method of matrix defect. However, absorption cross section does not proportion with PKA energy.

#### 2.2 Various extended defect in the aluminum matrix

Before the defect reaction mechanisms are establishment, extended defect characteristic should be defined. In the aluminum, extended defect are composed only dislocation loop and void by vacancy and helium (except the impurity, alloy element and transmutation). Void and dislocation loop is major sink which induced dimensional change. Fig 1. Shows characteristic of dislocation loop and void.



Fig. 1. Dislocation loops (a) and voids (b) in high-purity aluminum after irradiation at 50 °C to a fluence of 3.5 x  $10^{24}$ nm<sup>2</sup> (E > 0.1 MeV) [1].

However, in many case, alloy element are widely used for the mechanical and chemical properties improvement. And also transmutation are generated by various radiation interaction mechanism. Therefore, microstructure are change with various element. In generally, facetted Si particle attached to the outside of voids. In Fig 2, void are exaggerated at the grain boundary rims.



Fig. 2. Denuded grain boundary and associated void enhanced regions in 4–9 purity aluminum after irradiation at 50 °C to a fluence of  $3.4 \times 10^{26}$  nm<sup>2</sup> (E > 0.1 MeV) [1].

## 2.3 Assumption of defect and transmutation behavior

For the understanding of irradiation defect behaviors, every possible reactions should be defined in this research. In the previous research, the simplified reaction mechanism was reviewed by neglecting primary cluster and silicon atom transmutation [4].

Briefly summary this simple mechanism, it was assumed that all of cascade induced vacancy cluster are developed into staking fault tetragonal whilst interstitial cluster are developed into interstitial loop. In case of bubble and void, which are assumed that generated by diffusion behavior of the single vacancy and helium atom. These extended sink (void bubble, STF and loop) behavior are analyzed by the KMC modeling.

Fig 3 shows simple reaction kinetic of irradiation defect. Although this mechanism could explain in detail about extended sink growth behavior, it could not explain about the generation of sink behavior. Therefore, for precisely prediction of this sink behavior, sink generation should be considered by using theoretical generation modeling.



Fig. 3. Simplified defect reaction mechanism in the aluminum matrix [4].

#### 3. Summary and conclusions

This study is focused on the understanding of radiation effect on sink behavior. Mechanism of defect reaction and generation are briefly reviewed. From this research, it was confirmed that limitation of recent research. Transmutation and primary cluster effect are neglected previous research and alloy element effect also is ignored. Therefore, from the KMC modeling, these extended defect behavior will be examined next research step.

#### 4. Acknowledgement

This work was financially supported by the Korean Nuclear R&D program organized by the National Research Foundation (NRF) in support of the Ministry of Science, ICT and future Planning (MSIP).

## 5. Reference

[1] K. Farrell, Performance of aluminum in research Reactors, Comprehensive Nuclear Materials, 5, pp. 143-175 (2012)

[2] McLane, V., Dunford, C.L., Rose, P.F., Eds. ENDF-6 Formats Manual, version of June 1997; IAEA-NDS-76, (1997)

[3] M. Soukieh and N. Ghazi, Radiation damage estimation in the Al-alloy cladding of the MNSR reactor, Radiation Effects & Defects in Solids, Vol. 169, pp 522–528, (2014)
[4] M.J. Caturla, T. Diaz de la Rubia, M. Fluss, Radiation growth of HCP metals under cascade damage conditions,

Journal of Nuclear Materials, 323, pp 163–168, (2003)