Monte Carlo Evaluation of Fast Neutron Irradiation Damage for Al_2O_3/SS316L

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1. Introduction

Hydrogen and hydrogen isotope (D, T) dissolves and penetrates into most metals, and the causes a embrittlement destroying the material without structural deformation.

Nuclear fusion reactor produces the energy by D-D and D-T reaction and are constructed with various metals. Therefore, reducing of the hydrogen permeation of nuclear fusion structural materials is very important.

The application of hydrogen isotope permeation barriers of nuclear fusion reactor structural materials have been studied to reduce the hydrogen isotope permeability. The ceramic penetration barrier works as reducing the risk by hydrogen isotope due to its high temperature stability, high hardness and strong chemical bonding.

Among the various ceramic materials, Al_2O_3 is the most important candidate to improving the permeation reduction factor. According to the DFT calculation, the defected Al_2O_3 structure shows different behavior for the hydrogen permeation. The hydrogen penetration through the defected area of materials is easier than the perfect surface due to the lower barrier.

Neutron irradiation causes defect of materials. Therefore, it is necessary to analyze the hydrogen isotope permeability of the Al_2O_3 depending on the neutron irradiation damage. In this study, we calculated the activity and neutron irradiation damage of the Al_2O_3/ SS316L as a pre-investigation.

2. Neutron activity calculation

For the similar analysis of the neutron irradiation damage under similar energy range of neutrons, which generated by nuclear fusion, the neutron spectrum calculation for $^9Be(p,n)^9B$ reaction was considered. The proton source was assumed to be using the MC-50 cyclotron at Korea institute of radiological medical sciences. The neutron spectrum and flux was calculated by MCNP (Monte Carlo N-Particle) 6 transport code based on the model of the neutron irradiation experimental room of the MC-50 cyclotron. The initial energy, beam current of the proton and irradiation time were set to 30 MeV, 10 μA and 3,000 sec with diameter of the 2 cm.

The activity of the radionuclide by neutron irradiation can be calculated by the equation as following

$$A = N_0\sigma_0\phi\left(1-e^{-\lambda t_i}\right)\left(e^{-\lambda t_c}\right)$$

where, N_0 is the number of mother nuclide, σ_0 is the neutron absorption cross section corresponding to 14.1 MeV of neutron, ϕ is the neutron flux calculated by MCNP6, λ is the decay constant, t_i is the neutron irradiation time, t_c is the cooling time, respectively. The values of the neutron cross section and the decay constant were determine by ENDF/B-VIII.0 library. To simplify the calculation, Fe, Cr and Ni concentrations were normalized to 100 at. %, with exception of the trace elements, for SS316L. The types of radionuclides that can be generated neutron irradiation of Al_2O_3/ SS316L and the natural abundance of their mother nuclides are shown in table.1.

Table.1. Radionuclides for Al_2O_3/ SS316L

Mother nuclide	at. %	Reaction	Radionuclide
Fe-54	5.845	(n,p)	Mn-54
		(n,g)	Fe-55
Fe-56	91.754	(n,p)	Mn-56
Fe-58	0.282	(n,g)	Fe-59
Cr-50	4345	(n,g)	Cr-51
Cr-52	83.789	(n,2n)	Cr-51
Cr-53	9.501	(n,2n)	Cr-52
		(n,p)	V-53
		(n,α)	Sc-49
Cr-54	2.365	(n,g)	Cr-55
Ni-58	68.077	(n,g)	N-59
		(n,p)	Co-58
Ni-60	26.223	(n,p)	Co-60
Ni-62	3.635	(n,p)	Ni-63
Ni-64	0.9255	(n,g)	Ni-65
Al-27	100	(n,g)	Al-28
		(n,p)	Mg-27
		(n,2n)	Al-26
O-16	99.757	(n,p)	N-16
O-17	0.038	(n,p)	N-17

The neutron cross section for the nuclides of the Al_2O_3/ SS316L are shown in Fig.1.

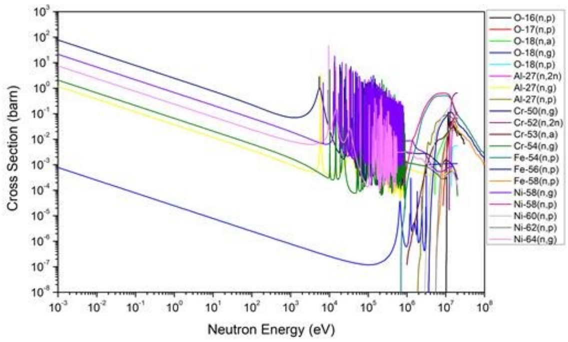

Fig. 1. Neutron cross section of the nuclides of Al_2O_3/ SS316L

Based on the neutron irradiation time of the 3,000 sec, the change of the specific activity of the nuclides of Al_2O_3/ SS316L are shown in Fig. 1. The radionuclides of Al_2O_3 are decayed within 2.5 hours. Besides, the mother nuclides of SS316L produces the radionuclides with long half-life, such as ^{51}Cr, ^{55}Cr, ^{56}Fe, ^{59}Fe, ^{59}Ni, ^{63}Ni.

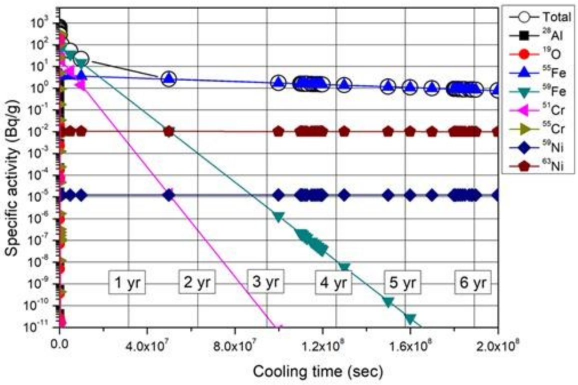

Fig.2. Specific activity of the Al_2O_3/ SS316L depending on the cooling time after the neutron irradiation of 3,000 sec

3. Collision heating by neutron irradiation

Collision heating was calculated to evaluate the possible damage of the Al_2O_3/ SS316L by temperature increasing due to the neutron irradiation. Through the quantification of the collision heat, the thermal expansion of the Al_2O_3 and SS316L can be estimated as calculating the temperature increasing. The density, specific heat and thermal expansion coefficient for the temperature changing and thermal expansion of the materials are shown in table.2.

Table.2. Density, specific heat and thermal expansion coefficient of the Al_2O_3 and SS316L

Mat	Density (g/cm³)	Specific heat (J/g℃)	Thermal expansion coefficient (/℃)
Al_2O_3	3.95	0.77	7.50E-6
SS316L	8.00	0.46	1.60E-5

To calculate the collision heating according to the different neutron fluences, the +F6 tally was calculated by varying the distance to the Be target, and the results are shown in table.3. It is assumed that all collision heating is used for the temperature increasing of the samples, As the results, the damage of the sample by temperature increasing is negligible.

Table.3. Density, specific heat and thermal expansion coefficient of the Al_2O_3 and SS316L

(cm)	Φ(n/cm²s)	MeV/gs	Mat	ΔT(℃)
3.45	6.07E9	2.63E-5	Al_2O_3	3.41E-5
			SS316L	5.71E-5
12.75	5.50E8	3.25E-7	Al_2O_3	4.22E-7
			SS316L	7.06E-7
32.25	9.00E7	1.57E-8	Al_2O_3	2.03E-8
			SS316L	1.00E-9

4. Calculation of DPA

A damage of the material by neutron irradiation is defined by transferred energy to the sample and the displacements of atoms in the materials. The neutron irradiation damage of the sample can be quantified by DPA (Displacement Per Atom) and its equation is as following

$$DPA_{total} = \int_0^t \int_0^\infty \sigma_{dpa}(E)\phi(E)dEdt$$

where, σ_{dpa} is the DPA cross section depending on the neutron spectrum, $\phi(E)$ is the differential neutron flux, respectively. A DPA value of the neutron irradiated Al_2O_3/ SS316L samples were calculated by PHITS (Particle and Heavy Ion Transport System) code and the results are shown in table.4. The DPA values of the Al_2O_3 and SS316L with neutron flux of 6.07E9 were 1.38E-28 and 1.75E-25, and these DPA values decrease as increasing the distance. Consequently, the DPA rate of the Al_2O_3/ SS316L by fast neutron irradiation is very low.

Table.4. DPA values of the Al_2O_3 and SS316L depending on the neutron fluence

(cm)	Φ(n/cm²s)	Mat	DPA/sec
3.45	6.07E9	Al_2O_3	1.38E-28
		SS316L	1.75E-25
12.75	5.50E8	Al_2O_3	1.01E-29
		SS316L	1.7E-26
32.25	9.00E7	Al_2O_3	3.59E-27
		SS316L	2.38E-31