Modeling of Irradiation Hardening in Reactor Pressure Vessel Steel Based on a Rate Theory

Gyeong-Geun Lee*, Yong-Bok Lee, Junhyun Kwon
Nuclear Materials Division, Korea Atomic Energy Research Institute,
989-111 Daedeok-daero, Yuseong-gu, Daejeon, 305-353, Korea
**Corresponding author: gglee@kaeri.re.kr*

1. Introduction

It is a common issue that neutron irradiation to reactor pressure vessel (RPV) steels causes a decrease in fracture toughness and an increase in yield strength while in service. A number of models have been proposed to account for the embrittlement of RPV steels [1, 2]. It is generally accepted that the growth of point defect cluster (PDC) and copper-rich precipitate (CRP) affects radiation hardening of RPV steels. The theoretical model developed by Stoller mathematically described the evolution of radiation-induced microstructures of ferritic steels under neutron irradiation. In this work, we modified the rate theory model for PDC and CRP, and estimated the magnitude of hardening induced by irradiation defects.

2. Methods and Results

The details of the mathematical model for PDC evolution are described in other references [3,4]. A number of time-dependent differential equations were established and integrated numerically, which contained the interstitial and vacancy concentrations, the number density of interstitial and vacancy clusters with varying sizes, and the size of CRP in matrix. The amount of radiation hardening caused by PDC and CRP was calculated using the simple Orowan's model.

2.1 Evolution of copper-rich precipitates

Microstructural studies have revealed that CRPs in RPV are distributed with high density ranging from 10^{17} to 10^{18} n/cm^3, and the size of CRP is very small (2-6 nm) [1]. In this work, the density of CRP was fixed in the calculations from the beginning, and growth of CRP is dominated by diffusion of vacancies. The detailed description of the CRP size calculation can be found elsewhere [5].

2.2 Basic model parameters

It is very crucial to determine the kinetic and material parameters as accurately as possible in order to solve the rate equations. The basic parameters used in this work are listed in Table 1. These values represented the base case for ferritic steels [6]. Although the parameters are less than ideal, it seems that the calculation results are useful to expect a trend for a quantitative prediction of the amount of radiation hardening.

Table I: Kinetic and material parameters

Parameter	Value
Vacancy migration energy (E_v^m)	
Vacacny formation energy (E_v^f)	1.25 eV
Vacancy pre-exponential factor (D_o^v)	1.55 eV
Effective grain diameter (d_g)	0.5 cm^2/s
Interstitial migration energy (E_m^i)	0.001 cm
Interstitial pre-exponential factor (D_o^i)	025 eV 0.05 cm^2/s
Dislocation density (ρ_{dis})	1×10^{11}/cm^2
Dislocation interstitial bias (z_i^{dis})	1.25
Dislocation vacancy bias (z_v^{dis})	1
Lattice constant of Fe (a_L)	2.87×10^{-8} cm
Cascade efficiency (η)	0.1
Vacancy clustering fraction (f_{vcl})	0.3
Insterstitial clustering fraction (f_{icl}^2:f_{icl}^3:f_{icl}^4)	0.15:0.1:0.05
Interstitial cluster binding energy (E_2^B:E_3^B:E_4^B)	0.5:0.75:1.25 eV
Initial number of vacancies per cluster (n_v)	5
Surface free energy (γ)	$2.947-(4.5\times10^{-4})\times T$(°C) J/m^2 2.7 eV
Copper migration energy (E_{Cu}^m)	300 cm^2/s
Copper pre-exponential factor (D_o^{Cu})	

2.3 Calculation results

Fig. 1. shows the concentration change in vacancies and interstitials with irradiation time. The final value of C_i is very lower than C_v because an interstitial has a very low migration energy than vacancies, and they are absorbed into the sinks rapidly. The difference between the C_i and C_v can be changed drastically by varying the migration energy of the species.

Fig. 2. shows the evolution of various interstitial cluster concentrations. The operating temperature of LWR is about 300°C, and the mobility of the vacancies is low, and voids grow very slowly at the temperature. In contrast, interstitials can move promptly and grow to defect clusters in this condition. As can be seen from Fig. 2, the concentrations of the defect clusters increased with time and showed plateaus. After

reaching to the plateaus, the concentrations increased very slowly.

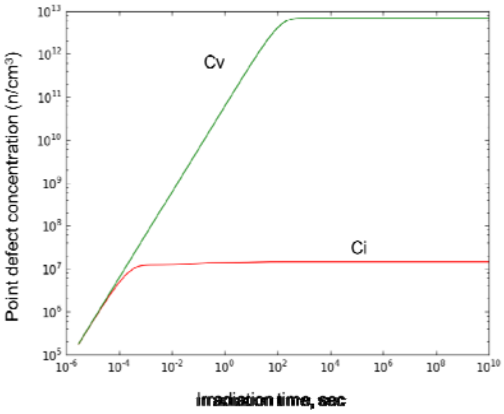

Fig. 1. Concentration changes of vacancies and interstitials with increasing irradiation time.

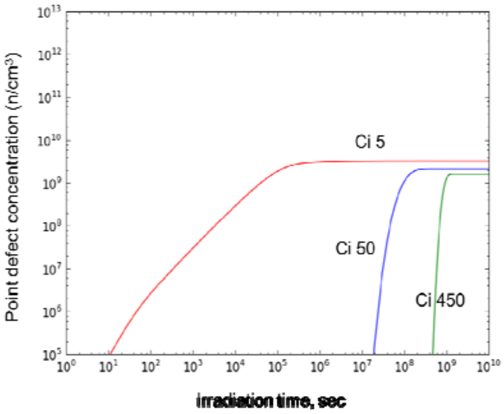

Fig. 2. Concentration changes of interstitial clusters with increasing irradiation time. The number represents the number of interstitials in the cluster.

Fig. 3. shows the comparison of the yield strength changes between calculated value and surveillance test data of YG 3. The yield strength increase includeed incremental changes from the PDC and CRP contributions. The calculated value is similar to the experimental data. However, it is required to consider various parameters to get a more accurate results.

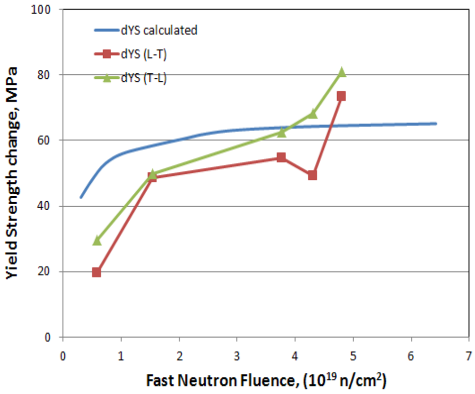

Fig. 3. Comparison of calculated and measured values of radiation hardening in YG2 data.

3. Conclusions

A theoretical evaluation of radiation hardening in RPV steels were carried out and compared to the measured values in RPV data. This results was sensitive to model parameters, however the calculated amount of hardening shows a fair agreement with the measured one with the uncertainties of the parameters. It is essential to determine the accurate parameters related to displacement cascade and to develop an elaborate model in the future.

REFERENCES

[1] S. B. Fisher, J. E. Harbottle, and N. Aldridge, Radiation Hardening in Magnox Pressure-Vessel Steels, Philosophical Transactions of the Royal Society of London, Vol. A 315, p. 301, 1985.

[2] S. B. Fisher and J. T. Buswell, A model for PWR pressure vessel embrittlement, International Journal of Pressure Vessels and Piping, Vol. 27, p. 91, 1987.

[3] R. E. Stoller, Modeling the Influence of Irradiation Temperature and Displacement Rate on Hardening Due to Point Defect Clusters in Ferritic Steels, Effects of Radiation on Materials: 16th International Symposium (ASTM STP 1175), p. 394, 1993.

[4] J. Kwon and A. T. Motta, Effect of Radiation Damage on BWR Core-shroud Cracking, Materials Research Society Symposium Proceedings, Vol. 540, p. 483, 1999.

[5] G. E. Lucas, G. R. Odette, P. M. Lombrozo, J. W. Sheckherd, Effects of Composition, Microstructure, and Temperature on Irradiation Hardening of Pressure Vessel Steels, Effects of Radiation on Materials: 12th International Symposium (ASTM STP 870), p. 900, 1985.

[6] R. E. Stoller, Pressure Vessel Embrittlement Predictions Based on a Composite Model of Copper Precipitation and Point Defect Clustering, Effects of Radiation on Materials: 17th International Symposium (ASTM STP 1270), p. 25, 1996.