Estimation of Radiation Hardening in Ferritic Steels Using the Cluster Dynamics Models

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1. Introduction

Evolution of microstructure under irradiation brings about the mechanical property changes of materials, of which the major concern is radiation hardening in this work. Radiation hardening is generally expressed in terms of an increase in yield strength as a function of radiation dose and temperature. Cluster dynamics model for radiation hardening has been developed to describe the evolution of point defects clusters (PDCs) and copper-rich precipitates (CRPs). While the mathematical models developed by Stoller focus on the evolution of PDCs in ferritic steels under neutron irradiation [1], we slightly modify the model by including the CRP growth and estimate the magnitude of hardening induced by PDC and CRP. The model is then used to calculate the changes in yield strength of RPV steels. The calculation results are compared to measured yield strength values, obtained from surveillance testing of PWR vessel steels in France [2].

2. Methods

A number of time-dependent differential equations are integrated numerically, which consist of the interstitial and vacancy concentrations, the population of interstitial and vacancy clusters, and the CRP size. In order to quantify the amount of radiation hardening caused by PDC and CRP, the simple Orowan's model was applied.

2.1 Point Defect Cluster Dynamics

The basic mechanism of PDC evolution is the nucleation and growth by diffusive reactions between PDC and point defects. It is probable that random collisions between the same types of point defects can lead to homogeneous nucleation of PDC. For interstitial clusters, it is assumed to begin with the formation of small clusters (up to tetra-interstitials) created directly from displacement cascades. The detailed information about primary damage resulting from displacement cascade can be obtained from molecular dynamics (MD) simulations [3]. The vacancy cluster concentration is described by a simple creation and decay model. The vacancy clusters are assumed to form in the displacement cascade as microvoids with a given radius. Taking into account such irradiation conditions as low temperature (< 300°C) and dose rate, these microvoids tend to shrink at a rate governed by the absorption of point defects and vacancy emission.

2.2 Copper-Rich Precipitate Evolution

The CRP model is based on the presumption that nucleation takes place instantly under irradiation and that the kinetics are dominated by the diffusion-controlled process. A fixed density of CRP is included in the calculations from the beginning, which is given by:

$$N_{crp} = C_o \sqrt{Cu_o} \exp\left\{ \frac{E_p}{k} \left(\frac{1}{T} - \frac{1}{561.16} \right) \right\} \qquad (1)$$

where C_{uo} is the initial copper contents contained in the matrix, k the Boltzmann constant, T temperature in K, E_p~0.35 eV, and C_o is an adjustable constant in the range 0.5 to 2.25 x 10^{23} /m^3.

A copper-precipitate of radius r_p can be regarded as the spherical agglomerate containing $(4\pi r_p^3/3)/\Omega_{Cu}$ Cu atoms, where Ω_{Cu} is the atomic volume of Cu. Under the assumption of diffusion-limited growth, the rate of change of the CRP size can be written as;

$$\frac{d r_p}{dt} = \frac{\Omega_{Cu}}{r_p} D_{Cu}^{+} \left(Cu_o - \frac{N_{crp}}{\Omega_{Cu}} \frac{4\pi r_p^3}{3} \right) \qquad (2)$$

where D_{Cu}^+ stands for the radiation-enhanced diffusivity for copper in iron. The equations for single point defect and PDC concentrations, as well as the CRP size, are solved simultaneously using the FORTRAN subroutine *dlsode* [4].

2.3 Dislocation Barrier Model

The strength of a crystalline material is increased by introducing barriers to dislocation motion within the material. Thus, hardening of alloys resulting from irradiation can be estimated by a dislocation barrier model which describes the interaction forces of various defects as they impede the mobile dislocation motion along the slip planes. Such a model is based on Orowan's theory for the bending of dislocations around precipitates. Its use presents the simple way of investigating the potential significance of defects.

3. Calculation Results

In solving the cluster dynamics equations, it is of great importance to determine the kinetic and material parameters as accurately as possible. The major parameters used in this calculation are listed in Table 1, which are believed to represent the base data for ferritic steels.

Table 1. Kinetic and material parameters for ferritic steel

Parameter	Value
Vacancy migration energy (E_v^m)	1.25 eV
Vacacny formation energy (E_v^f)	1.55 eV
Vacancy pre-exponential factor (Do^v)	0.5 cm^2/s
Effective grain diameter (d_g)	0.001 cm
Interstitial migration energy (E^i_m)	0.25 eV
Interstitial pre-exponential factor (Do^i)	0.05 cm^2/s
Dislocation density (ρ_{dis})	$1x10^{11}$ $/cm^2$
Dislocation interstitial bias (z_i^{dis})	1.25
Dislocation vacancy bias (z_v^{dis})	1
Lattice constant of Fe (a_L)	$2.87x10^{-8}$ 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)	$2.947-(4.5x10^{-4})$ x T[°C] J/m^2
Copper migration energy (E_{Cu}^m)	2.7 eV
Copper pre-exponential factor (D_o^{Cu})	300 cm^2/s

We employed the results of surveillance testing of French PWR vessel steels in comparing between the calculated and measured yield strength. The French surveillance data contain a number of tensile and fracture properties in irradiated RPV steels along with irradiation conditions. The RPV steel used in the surveillance test was forged low-alloy 16 MND 5, which is similar to the ASME SA 508 cl.3. Among the mechanical test results, the data of interest in this study are the changes in yield strength of irradiated RPV steels as a function of copper contents and total dose. Using the theoretical model described previously, the increase in yield strength for French RPV steels is calculated. Two variables of consideration are the initial copper contents and the dose rate in the unit of dpa/s. Fig. 1 illustrates the difference in yield strength changes between the calculated and measured values. The calculated data are close to the measured ones as the data point are located near the diagonal line. In general, most of the calculation results tend to over-predict the measured ones. Except the three data points located on the ordinate in Fig.1, which represent 'no changes in measured yield strength', the calculation results show a fair agreement with the test data in spite of the use of estimated irradiation input parameters.

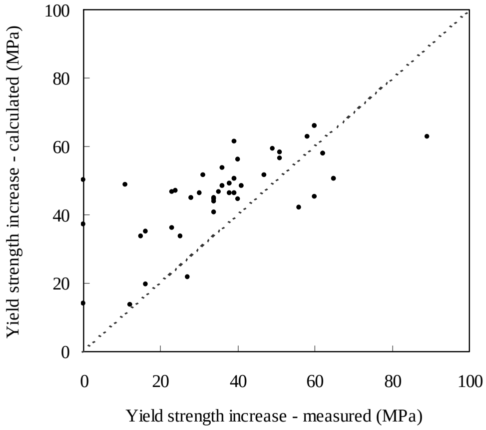

Figure 1. Comparison between measured and calculated yield strength changes.

4. Conclusions

We have performed a theoretical evaluation of radiation hardening in RPV steels and compared the calculation results with measured ones. The results of calculation show that the copper-rich precipitates are major sources of radiation hardening, while the contribution of the point defect clusters to hardening is relatively minor. Although the calculation results are model-dependent, the calculated amount of hardening shows a fair agreement with measured one within the uncertainties of parameters.

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