Model Calculation of the Damage Rate Dependence of Yield Stress Change in an Irradiated Fe–Cu Model Alloy

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The damage rate dependence of the yield stress change in a neutron-irradiated Fe–Cu model alloy was analyzed by a model calculation. The model was based on the rate theory, and focused on the description of the nucleation and growth of point defect clusters and copper clusters. The binding between copper atoms and vacancies and the effect of cascade damage which directly creates small point defect clusters were incorporated in this model. The instability of small point defect clusters caused by thermal dissociation was also included. From the result of the calculation, the yield stress changes were estimated using the Orowan model and the Russel-Brown model. As a result of this calculation, it was clarified that copper clusters are the main factor of yield stress change in almost all irradiation stages below 0.1 dpa. The contribution of copper-vacancy binding but by the sink strength, which changes dynamically throughout irradiation.

(Received December 25, 2001; Accepted May 1, 2002)

Keywords: copper-vacancy binding, damage rate dependence, iron-copper alloy, model calculation, point defect cluster, radiation effect, yield stress change

1. Introduction

The clustering of copper atoms is one of the main factors of irradiation-induced embrittlement in the aging reactor pressure vessels of first generation nuclear plants. Understanding this clustering is important in order to accurately estimate the property changes of reactor pressure vessel steel. To obtain information on the property changes of materials in advance, accelerated irradiation tests have been performed. In these tests, specimens are irradiated at a higher damage rate which is two or more orders higher than that in the normal operation of power reactors. However, it has been pointed out that the high damage rate in the accelerated irradiation tests may cause a different result. This effect of the damage rate on the property changes of materials was suspected when the results of irradiation tests using the Gundremmingen reactor¹⁻³ were reported. However, no reasonable explanation for the results has yet been found. From these reports, it was clear that there are various irradiation factors which influence the property changes of materials. The damage rate, which is the focus of this study, is one of them.

Model calculations have been used to examine the effect of damage rate.⁴⁻⁶) Previously we also performed a model calculation for neutron-irradiated Fe–Cu alloy based on the rate theory⁷) and demonstrated the obvious existence of damage rate dependencies in various properties, e.g., the concentration of point defect clusters and the yield stress change. But the binding of copper atoms with vacancies was not considered in the previous model. This ignorance of the copper-vacancy binding may change the damage rate dependence. The volume size factor of a copper atom in an iron matrix is reported by +17.55%,⁸) so copper atoms tend to bind with vacancies. As the copper-vacancy pair is the dominant mechanism in the migration of copper atoms, the incorporation of copper-vacancy binding is necessary for improvement of the calculation model.

In this study, we made an improved model which included the copper-vacancy binding and analyzed the effects of damage rate on yield stress change.

2. Description of the Model

The calculation model is based on rate theory. The target alloy composition is Fe–0.6 at%Cu. The model describes the reaction rates among various point defect reactions, e.g., the reaction rates between the mobile defects and the immobile defects, the formation and growth rates of point defect clusters and copper clusters, the mutual annihilation rate of point defects, etc. In this model, the defect species considered are point defects, point defect complexes and point defect clusters.

Interstitials and vacancies are created as a form of the Frenkel pair with a damage rate $P$. Interstitials, vacancies and copper-vacancy pairs are assumed to be mobile in this model. Compared with the previous model, copper atoms cannot move unless copper-vacancy pairs are created. We assume that a copper-vacancy pair acts as a point defect and that all of the values of the number of reaction site $Z$ are the same as a single vacancy. The copper-vacancy binding energy ($E_{\text{CuV}}^B$) is set to 0.1 eV (1 eV = 1.60218 × 10⁻¹⁹ J) from recent reports of the calculations.⁹⁻¹¹)

We denote a defect which consists two (di-) or three (tri-) point defects or copper atoms as a point defect complex. We assume that point defect complexes cannot move. To describe the cascade damage and the thermal instability of the defects created by the cascade damage, tri-interstitials and tri-vacancies are assumed to be created directly by the cascade damage. The point defect complex production rates by the cascade damage ($P_{\text{IC}}$ for interstitial clusters and $P_{\text{VC}}$ for vacancy clusters) are assumed to be proportional to the damage rate $P$, where $P_{\text{IC}} = P_{\text{VC}} = r_{\text{CP}} P$. The constant (cascade damage formation ratio, $r_{\text{CP}}$) was taken to 1 × 10⁻³ which
was assumed from the results of the PKA (primary knock-on atom) energy spectrum analysis.\textsuperscript{12} In contrast to the point defect complexes, direct production of copper complexes by the cascade damage is not considered because the copper concentration of the target alloy (0.6 at%) is low enough to omit such reactions for copper complexes.

A defect which contains four or more point defects and copper atoms is named a point defect cluster. As the shape of the clusters, we assume a disc for interstitial clusters and a sphere for vacancy clusters and copper clusters. The clusters are assumed not to dissociate, and the changes of cluster size are considered. We also assume that the clusters act as the sink of the point defects and copper atoms. The number of reaction sites \( Z \) for the clusters is assumed to be proportional to the circumference for interstitial clusters and to the surface area for vacancy clusters and copper clusters.

Equations of concentrations of the point defects are given as follows:

\[
\frac{dC_1}{dt} = P_1 - C_1 M_1 C_1 - Z_1 V (M_1 + M_V) C_1 C_V - 2Z_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1 - Z_{1VC} C_V C_M C_1 C_1
\]

\[
- Z_{12} C_1 C_1 M_1 C_1 - Z_{132} C_2 V_2 M_1 C_1 + Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1
\]

\[
+ 2Z_{12} C_1 C_1 M_1 C_1 + Z_{13} C_1 C_1 M_1 C_1 - Z_{1VC} C_1 C_1 M_1 C_1 + Z_{1VC} C_1 C_1 M_1 C_1
\]

\[
\frac{dC_V}{dt} = P_V - C_1 M_1 C_1 - Z_1 V (M_1 + M_V) C_1 C_V - 2Z_1 V (M_1 + M_V) C_1 C_V - Z_{1VC} C_V C_V C_V - Z_{1VC} C_V C_V C_V
\]

\[
- Z_{132} C_2 V_2 C_V C_V - Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1
\]

\[
+ 2Z_{12} V (M_1 + M_V) C_1 C_V + Z_{13} C_1 C_1 M_1 C_1 - Z_{1VC} (M_1 + M_V) C_1 C_V + Z_{1VC} (M_1 + M_V) C_1 C_V
\]

\[
+ Z_{1VC} C_1 C_1 M_1 C_1 + Z_{1VC} C_1 C_1 M_1 C_1 + Z_{1VC} C_1 C_1 M_1 C_1 + Z_{1VC} C_1 C_1 M_1 C_1
\]

\[
- Z_{1VC} C_1 C_1 M_1 C_1 - Z_{1VC} C_1 C_1 M_1 C_1 - Z_{1VC} C_1 C_1 M_1 C_1 - Z_{1VC} C_1 C_1 M_1 C_1
\]

\[
\frac{dC_{CA}}{dt} = Z_{1VC} C_1 C_1 C_1 C_1 + Z_{1VC} C_1 C_1 C_1 C_1 + Z_{1VC} C_1 C_1 C_1 C_1 + Z_{1VC} C_1 C_1 C_1 C_1 + Z_{1VC} C_1 C_1 C_1 C_1
\]

\[
- Z_{1VC} C_1 C_1 M_1 C_1 - Z_{1VC} C_1 C_1 M_1 C_1 - Z_{1VC} C_1 C_1 M_1 C_1 - Z_{1VC} C_1 C_1 M_1 C_1
\]

\[
+ Z_{1VC} C_1 C_1 M_1 C_1 - Z_{1VC} C_1 C_1 M_1 C_1 - Z_{1VC} C_1 C_1 M_1 C_1 - Z_{1VC} C_1 C_1 M_1 C_1
\]

\[
+ Z_{1VC} C_1 C_1 M_1 C_1 + Z_{1VC} C_1 C_1 M_1 C_1 + Z_{1VC} C_1 C_1 M_1 C_1 + Z_{1VC} C_1 C_1 M_1 C_1
\]

Equations for concentrations of the point defect complexes are given as follows:

\[
\frac{dC_{C1}}{dt} = Z_{13} C_1 C_1 M_1 C_1 - Z_{132} C_2 V_2 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1
\]

\[
+ Z_{13} C_1 C_1 M_1 C_1 + Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1
\]

\[
+ Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1
\]

\[
\frac{dC_{C2}}{dt} = Z_{132} C_2 V_2 M_2 C_2 V_2 - Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1
\]

\[
+ Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1
\]

\[
+ Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1
\]

\[
\frac{dC_{C3}}{dt} = Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1
\]

\[
+ Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1
\]

\[
+ Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1
\]

\[
\frac{dC_{C4}}{dt} = Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1
\]

\[
+ Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1
\]

\[
+ Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1
\]

\[
+ Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1 - Z_{13} C_1 C_1 M_1 C_1
\]
Thermal dissociations of the point defect complexes are included as terms which contain $B$, e.g. term 4 of the right side in eqs. (5) and (8). The effect of cascade damage is included at term 5 of the right side in eqs. (8) and (9).

Equations for concentration of the point defect clusters are given as follows:

$$\frac{dC_{IC}}{dt} = Z_{1IC}C_{IC}M_{IC}C_{I} - Z_{CuV,IC}C_{IC}M_{CuV}C_{CuV}$$  \hspace{1cm} (11)

$$\frac{dC_{VC}}{dt} = Z_{V,VC}C_{VC}M_{VC}C_{V} + Z_{CuV,VC}C_{VC}M_{CuV}C_{CuV}$$  \hspace{1cm} (12)

$$\frac{dC_{CaC}}{dt} = Z_{CaV,CaC}C_{CaC}M_{CaV}C_{CuV}$$  \hspace{1cm} (13)

Equations for concentration of the point defects forming the point defect clusters are given as follows:

$$\frac{dR_{I}}{dt} = Z_{IIC}C_{IC}M_{I}C_{I} - Z_{V,IC}C_{IC}M_{VC}C_{VC} + 4\frac{dC_{IC}}{dt}$$ \hspace{1cm} (14)

$$\frac{dR_{V}}{dt} = Z_{V,VC}C_{VC}M_{VC}C_{V} - Z_{I,VC}C_{VC}M_{IC}C_{I} + 4\frac{dC_{VC}}{dt}$$ \hspace{1cm} (15)

$$\frac{dR_{Ca}}{dt} = Z_{CaV,CaC}C_{CaC}M_{CaV}C_{CuV} + 4\frac{dC_{CaC}}{dt}$$ \hspace{1cm} (16)

The size and volume of the point defect clusters can be calculated using $R$ by assuming the shape of the clusters.

The symbols used in above equations are as follows,

$C_{j}$: concentration of defects of type $j$ ($j = I$ for interstitials, $j = I$ for di-interstitials, $j = I$ for tri-interstitials, $j = IC$ for interstitial clusters, $j = V$ for vacancies, $j = V$ for vacancy clusters, $j = VC$ for vacancy clusters, $j = Cu$ for copper atoms, $j = Cu2$ for di-copper atoms, $j = Cu3$ for tri-copper atoms, $j = CuC$ for copper clusters and $j = CuV$ for copper-vacancy pairs)

$R_{j}$: concentration of $j$-type point defects in their cluster

$Z_{1/2}$: number of reaction sites between $j$-type defects and $j$-type defects (see below)

$M_{j}$: jump frequency of $j$-type point defects

$B_{j}$: binding term of $j$-type defects

$C_{i}$: concentration of the static sinks.

$M_{j}$ and $B_{j}$ are expressed as $M_{j} = v_{0}\exp[-E_{m}^{j}/(k_{B}T)]$ and $B_{j} = \exp[-E_{b}^{j}/(k_{B}T)]$, where $k_{B}$ is the Boltzmann constant and $T$ is the temperature. Using them, the detrapping frequency of $j$-type point defects from $j$-type defects can be expressed as $M_{j}B_{j}$. The values of the miscellaneous parameters used in this model are summarized in Tables 1, 2 and 3. The same as $E_{m}^{V}$, the binding energies of the point defect complexes ($E_{m}^{I}$, $E_{m}^{IC}$, $E_{m}^{V}$, $E_{m}^{VC}$ and $E_{m}^{CaC}$) are taken from the results of the recent calculations.\(^{9-11}\) We assume that this calculation is performed at the center of a grain which radius is $1 \times 10^{5}$ atomic distance. In this assumption, the average number of jumps of the defects from the center of the grain to the grain boundary is considered to $1 \times 10^{10}$. So $C_{i}$ is set to the inverse of that value. For the reactions between the point defects and the point defect clusters which contain $n$ point defects are given as follows.

|| Parameter | Symbol | Value |
|---|---|---|
| Migration energy (I) (eV) | $E_{m}^{I}$ | 0.3 |
| Migration energy (V) (eV) | $E_{m}^{V}$ | 1.0 |
| Migration energy (CuV) (eV) | $E_{m}^{CuV}$ | 1.1 |
| Binding energy (di-I) (eV) | $E_{b}^{I}$ | 0.75 |
| Binding energy (tri-I) (eV) | $E_{b}^{I}$ | 1.5 |
| Binding energy (di-V) (eV) | $E_{b}^{V}$ | 0.2 |
| Binding energy (tri-V) (eV) | $E_{b}^{V}$ | 0.5 |
| Binding energy (di-Cu) (eV) | $E_{b}^{Cu}$ | 0.05 |
| Binding energy (tri-Cu) (eV) | $E_{b}^{Cu}$ | 0.1 |
| Vacancy formation energy (eV) | $E_{f}^{V}$ | 1.5 |
| Bias factor | $f$ | 1.1 |
| Cascade damage formation ratio | $r_{CP}$ | $1 \times 10^{-3}$ |
| Concentration of the static sinks | $C_{i}$ | $1 \times 10^{-10}$ |
| Jump frequency (s$^{-1}$) | $v_{0}$ | $1 \times 10^{-13}$ |

The software package CVODE,\(^{13}\) which solves simultaneous ordinary differential equations by the Gear method, was used for the calculation. The irradiation temperature ($T$) was set to 573 K for all calculations to simulate the operation temperature of nuclear power plants. Each calculation was performed using a dose of 0.1 dpa. The unit “dpa” means a probability of knock-on of an atom, and the dose 0.1 dpa is the dose of a reactor pressure vessel at the end of the lifetime of a nuclear power plant.

Based on the result of the calculation, the yield stress changes of the model alloy were calculated by using the Orowan model\(^{14}\) and the Russell-Brown model,\(^{15}\) and the damage rate dependences of the yield stress change were ex-
7) In the previous model, a binding energy of each cluster to the yield stress change at 0.1 dpa is illus-

dependence almost disappears at 0.1 dpa. The contribution for lower damage rate irradiation. However, the damage rate change. Below 1

number of jumps in lower damage rate irradiation. 

Fig. 3 clearly indicates the increase of the total number of jumps in lower damage rate irradiation. 

The migration and clustering of copper are caused by the migration of vacancies. The close relationship between vacancy and copper can be observed in comparison of Fig. 1(b) and Fig. 4. So the total number of jumps of vacancies during irradiation is directly proportional to the amount of copper clusters. Figure 3 clearly indicates the increase of the total number of jumps in lower damage rate irradiation.

Figure 6 shows the damage rate dependence of yield stress change. Below $1 \times 10^{-2}$ dpa the yield stress change is larger for lower damage rate irradiation. However, the damage rate dependence almost disappears at 0.1 dpa. The contribution of each cluster to the yield stress change at 0.1 dpa is illustrated in Figs. 7 and 8. Figure 8 is the result obtained by the previous model. In the previous model, a binding energy between copper and vacancy is set to zero and a migration energy of copper atom is equal to that of vacancy. For example, an absorption of copper atom toward copper cluster is expressed as $Z_{Cu,Cu} C_{Cu} M_{Cu} C_{Cu}$ in the previous model, whereas $Z_{Cu,V,Cu} C_{Cu} M_{Cu} C_{Cu} V$ in this model. Other parameters and assumptions are the same as this model. Figures 7 and 8 clearly show that the damage rate dependence of copper clusters to the yield stress change is inverse to the dependences of interstitial clusters and vacancy clusters. This is due to the difference in the dominant nucleation process between copper clusters and the point defect clusters. The nucleation of copper clusters only occurs by the migration of copper-vacancy pairs. In such a case, the concentration of copper clusters is greater in lower damage rate irradiation (see above), the effects of copper clusters on the yield stress change increase with decreasing damage rate. On the other hand, almost all of the nuclei of the point defect clusters are formed directly by the cascade damage. The production rate of the point defect complexes is proportional to the damage rate. As can be seen in Fig. 2, the concentrations of the clusters increase throughout irradiation and the concentrations are higher in higher damage rate irradiation. We can say that the effects of the point defect clusters on the yield stress change increase with increasing damage rate. At 0.1 dpa, the yield stress change by copper clusters at lower damage rate irradiation is close to that by the point defect clusters at a higher damage rate. As a result, the damage rate dependence of the

Table 3 Values of the number of reaction sites.

<table>
<thead>
<tr>
<th>Reaction</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Interstitial-interstitial</td>
<td>$Z_{11}$</td>
<td>6</td>
</tr>
<tr>
<td>Interstitial-di-interstitial</td>
<td>$Z_{12}$</td>
<td>22</td>
</tr>
<tr>
<td>Interstitial-tri-interstitial</td>
<td>$Z_{13}$</td>
<td>24</td>
</tr>
<tr>
<td>Interstitial-vacancy</td>
<td>$Z_{1v}$</td>
<td>100</td>
</tr>
<tr>
<td>Interstitial-di-vacancy</td>
<td>$Z_{1v2}$</td>
<td>33</td>
</tr>
<tr>
<td>Interstitial-tri-vacancy</td>
<td>$Z_{1v3}$</td>
<td>37</td>
</tr>
<tr>
<td>Interstitial-CuV</td>
<td>$Z_{CuV}$</td>
<td>100</td>
</tr>
<tr>
<td>Vacancy-di-interstitial</td>
<td>$Z_{v12}$</td>
<td>20</td>
</tr>
<tr>
<td>Vacancy-tri-interstitial</td>
<td>$Z_{v13}$</td>
<td>22</td>
</tr>
<tr>
<td>Vacancy-vacancy</td>
<td>$Z_{vV}$</td>
<td>7</td>
</tr>
<tr>
<td>Vacancy-di-vacancy</td>
<td>$Z_{vV2}$</td>
<td>33</td>
</tr>
<tr>
<td>Vacancy-tri-vacancy</td>
<td>$Z_{vV3}$</td>
<td>37</td>
</tr>
<tr>
<td>Vacancy-copper</td>
<td>$Z_{vCu}$</td>
<td>7</td>
</tr>
<tr>
<td>Vacancy-di-copper</td>
<td>$Z_{vCu2}$</td>
<td>33</td>
</tr>
<tr>
<td>Vacancy-tri-copper</td>
<td>$Z_{vCu3}$</td>
<td>37</td>
</tr>
<tr>
<td>Vacancy-CuV</td>
<td>$Z_{vCuV}$</td>
<td>7</td>
</tr>
<tr>
<td>CuV-di-interstitial</td>
<td>$Z_{CuV12}$</td>
<td>20</td>
</tr>
<tr>
<td>CuV-tri-interstitial</td>
<td>$Z_{CuV13}$</td>
<td>22</td>
</tr>
<tr>
<td>CuV-di-vacancy</td>
<td>$Z_{CuVv2}$</td>
<td>33</td>
</tr>
<tr>
<td>CuV-tri-vacancy</td>
<td>$Z_{CuVv3}$</td>
<td>37</td>
</tr>
<tr>
<td>CuV-copper</td>
<td>$Z_{CuVv}$</td>
<td>7</td>
</tr>
<tr>
<td>CuV-di-copper</td>
<td>$Z_{CuVvCu2}$</td>
<td>33</td>
</tr>
<tr>
<td>CuV-tri-copper</td>
<td>$Z_{CuVvCu3}$</td>
<td>37</td>
</tr>
<tr>
<td>CuV-CuV</td>
<td>$Z_{CuVvCuV}$</td>
<td>7</td>
</tr>
</tbody>
</table>

Fig. 1 Dose dependences of interstitial concentration (a) and vacancy concentration (b).
yield stress change “disappear” at 0.1 dpa.

When comparing Fig. 7 and Fig. 8, there is a difference in the contribution of copper clusters to the yield stress change. Figure 9 shows a comparison of the calculation results of the total yield stress change between the previous model\(^7\) and this model at the doses of \(1 \times 10^{-3}\) dpa and 0.1 dpa. From Fig. 9, it is considered that results of the modified model are lower than those of the previous model for all irradiation levels. It is obvious that the existence of the copper-vacancy binding causes a decrease in the contribution of copper clusters. The copper-vacancy binding makes the migration of copper atoms slower. Since the yield stress change is sensitive to the concentration of obstacles, the result in Fig. 7 shows that the copper cluster concentration in the modified model is lower than that in the previous model at the same dose. This difference also suggests that the clustering of copper atoms continues until the latter stage of irradiation in the modified model.

It should be noted that the yield stress changes by the point defect clusters are almost the same between Fig. 7 and Fig. 8. Since the existence of copper-vacancy pairs makes the isolated vacancy concentration in the matrix high, it is expected that in the modified model the mutual annihilation of the point defects prevents the growth of the point defect clusters and the contribution to the yield stress change consequently becomes smaller. The reason why the contributions of the point defect clusters do not show any difference is that the magnitudes of the sink strength of the point defect clusters are almost the same in two models. The concentration of the point defect clusters is determined mainly by the cascade damage. Once the clusters are created, they act as strong sinks of the point defects. The copper-vacancy binding does not influence this tendency.

It is also observed in Fig. 9 that both results show similar damage rate dependences although the previous model did not consider the copper-vacancy binding. Previously we argued that the origin of the damage rate dependence was in the difference of the sink strength.\(^7\) Figure 9 supports this conclusion, and the damage rate dependence is not affected by the incorporation of the copper-vacancy binding. As mentioned above, the migration of the point defects and copper-vacancy pairs is ruled by the sink strength of the point defect clusters. However, the damage rate dependence of the sink strength is almost the same in both models. And since the sink strength to copper-vacancy pairs is assumed to be the same as
Dose dependences of copper cluster concentration.

Fig. 6 Damage rate dependences of yield stress change. Numbers in the figure are the total dose (units in dpa).

the strength to single vacancies, the point defect clusters regard copper-vacancy pairs as single vacancies. The total number of jumps of vacancies, which influences the clustering of copper, is thus not so different between the two models. Note that the damage rate dependence of the yield stress change does not change if Z of a copper-vacancy pair is modified because the "true" Z of the pair is expected to be lower than that of single vacancies due to the relaxation volume of the pair.

4. Conclusions

An irradiation model for Fe–Cu alloy which incorporated copper-vacancy binding was developed. The model was based on rate theory, and copper atoms were assumed to move only in the form of copper-vacancy pairs. The effects of the cascade damage and the thermal instability of small point defect clusters were also considered in the model. We compared the result from this model to that from the previous model which did not incorporate the copper-vacancy binding, to clarify the origin of damage rate dependence in the yield stress change. The modified model has a tendency for the nucleation of copper clusters to continue until the latter stage of irradiation. This is the direct effect of the copper-vacancy binding, where the binding makes the migration of copper atoms slower. On the other hand, the damage rate dependences of yield stress change in this model were similar to the dependences in the previous model. It is concluded that the origin of the damage rate dependence is not affected by the copper-vacancy binding and that the origin is in the difference of the sink strength.

Acknowledgement

This work has been carried out in part under the Visiting Researcher’s Program of the Research Reactor Institute, Kyoto University.

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Fig. 9 Comparison of the results of calculation between the modified model and the previous model at $10^{-3}$ dpa and 0.1 dpa. 