Prediction of the micro-thermo-mechanical behaviors in dispersion nuclear fuel plates with heterogeneous particle distributions

Yijie Jiang\textsuperscript{a}, Qiming Wang\textsuperscript{a}, Yi Cui\textsuperscript{a}, Yongzhong Huo\textsuperscript{a}, Shurong Ding\textsuperscript{a,b,\textsuperscript{⇑}}, Lin Zhang\textsuperscript{b}, Yuanming Li\textsuperscript{b}

\textsuperscript{a}Department of Mechanics and Engineering Science, Fudan University, Shanghai 200433, China
\textsuperscript{b}Science and Technology on Reactor System Design Technology Laboratory, Nuclear Power Institution of China, Chengdu 610041, Sichuan, China

\textbf{Abstract}

Dispersion nuclear fuel elements have promising prospects to be used in advanced nuclear reactors and disposal of nuclear wastes. They consist of fuel meat and cladding, and the fuel meat is a kind of composite fuel in which the fuel particles are embedded in the non-fissile matrix. Prediction of the micro-thermo-mechanical behaviors in dispersion nuclear plates is of importance to their irradiation safety and optimal design. In this study, the heterogeneity of the fuel particles along the thickness direction in the fuel meat is considered. The 3D finite element models have been developed respectively for two cases: (1) variation of fuel particle–particle (PP) distances for the particles near the mid-plane of the fuel meat; (2) variation of the particle-cladding (PC) distances for the fuel particles near the interface between the fuel meat and the cladding. The respective finite strain constitutive relations are developed for the fuel particle, metal matrix and cladding. The developed virtual temperature method is used to simulate irradiation swelling of the fuel particles and irradiation growth of the metal cladding. Effects of the heterogeneous distributions of the fuel particles on the micro temperature fields and the micro stress–strain fields are investigated. The obtained results indicate that: (1) as a whole, the maximum Mises stress, equivalent plastic strain and first principal stress at the matrix between the two closest particles increase with decreasing the particle–particle (PP) distance; existence of large first principal stresses there may be the main factor that induces the matrix failure; (2) variation of the particle-cladding (PC) distance has remarkable effects on the interfacial normal stress and shear stress at the interface between the fuel meat and the cladding; the first principal stress at the cladding near the interface increases dramatically when the fuel particle is closer and closer to the cladding. Thus, the proper distance between the fuel particles and the one between the fuel particle and the cladding should be considered in the optimal design; (3) the micro temperature distribution in the fuel element is hardly affected.

\textcopyright\ 2011 Elsevier B.V. All rights reserved.

1. Introduction

Due to accumulation of greenhouse gases in fossil-fueled energy, nuclear energy becomes one promising option (perhaps the only option) to replace the fossil fuels in a large-scale with the energy demand all over the world increasing to support the growing populations and economies. With development of nuclear energy, a large amount of nuclear wastes \cite{1} with heavy radioactivity have been produced and will be produced. Transmutation of the long-lived actinides to reduce the radioactivity of nuclear wastes is necessary. Besides, the nuclear fuels should be adequately burned down to improve the economy. Thus, the advanced GEN IV nuclear reactors should be designed to meet the needs of being highly economical, of enhanced safety, of minimized wastes and of proliferation resistance.

Compared to the traditional fuel elements in the present nuclear plants, dispersion nuclear fuel elements have much higher thermal conductivity and thus can reach high burnup. As a result, they have promising prospects to be used in GEN IV reactors \cite{2}, and they are studied to dispose of nuclear wastes \cite{3,4}.

Besides, the dispersion nuclear fuel elements have been widely used in the research and test reactors since the Reduced Enrichment for Research and Test Reactors (RERTR) program started in 1970s. In order to fulfill the demands of RERTR program, relative researches \cite{5,6} are focused on developing new fuels with very high density.

Dispersion nuclear fuel elements consist of cladding and the internally wrapped fuel meat. And the fuel meat is a kind of composite fuel with the fuel particles embedded in the non-fissile matrix. In the nuclear reactors, the components of nuclear fuel elements are exposed to severe environment. The nuclear fission of
uranium in the fuel particles results in complex irradiation effects [3]. Firstly, it is responsible for generating heat that can be subsequently transformed into electricity. Secondly, fuel particle swelling occurs due to the generated solid and gaseous fission products, which leads to the intense mechanical interactions with the surrounding matrix; and generation of fission products will degrade the thermal conductivity of fuel particles. Thirdly, the fission gas will release into the free volume, thus additional pressure will be subjected to the surrounding matrix and cladding. Above all, in the harsh environment, the fission fragments and fast neutrons with high energy will exchange the energy with the lattice atoms until they come to rest. So, the atoms of the metal matrix and cladding are displaced from their original lattice positions, which results in vacancies and interstitials, and on a macroscopic scale the above irradiation damages [7] of the metal materials appear as irradiation-induced hardening, embrittlement, creep and growth.

If the fuel element loses its integrity, the nuclear leakage will take place; and if the size variations are large enough to affect the normal flowing of the coolant between the fuel elements, the accident will happen. Preventing failure is of primary concern for dispersion nuclear fuel elements, and must be focused on in the design. And the design should consider the complex interactions of the irradiation effects.

Besides the irradiation experimental researches [8], the numerical simulations are playing a more and more important role in explaining the experiment results and in the optimal design because they can supply the engineers with a predictive tool and shorten the design period. Recently, the relative researches on because they can supply the engineers with a predictive tool and explain the experiment results and in the optimal design of the irradiation effects.

The developed virtual temperature method is used to simulate irradiation swelling of the fuel particles and irradiation growth of the metal cladding. Effects of the heterogeneous distribution of the fuel particles along the thickness in the fuel meat on the micro temperature fields and the micro stress-strain fields are investigated.

2. The three-dimensional finite-strain constitutive relations

In the nuclear fuel element, the thermal–mechanical behaviors are mainly induced by the high temperature differences at the initial stage of burnup. Thus, the relative small-deformation constitutive relations for the internal materials are used, with the thermal-elastic one for the fuel particles and the thermal-elasticplastic ones for the metal matrix and the cladding.

With increasing burnup, at higher burnups the relative volume variations of the particles due to the fission products can reach high. And irradiation growth of the metal cladding will be enhanced with increasing burnup. Then the mechanical interactions between the fuel particles and the matrix will be enhanced and large deformation will appear. In the three-dimensional constitutive relations for the fuel particles, the matrix and the cladding, the finite strain forms should be considered. In this study, the real temperature variation after the obtained steady-state temperature field at the initial stage is not considered. In the following, the finite strain constitutive relations for the fuel particles, the metal matrix and the cladding at the increasing stage of burnup are developed.

2.1. The three-dimensional constitutive relation for the fuel particles

The total deformation rate of the fuel particle is assumed to be the sum of the elastic one and the irradiation swelling one, which can be denoted as

\[ \dot{d}_{ii} = \dot{d}_{ii}^e + \dot{d}_{ii}^sw \] (1)

where \( \dot{d}_{ii}^e \) is the elastic deformation rate. \( \dot{d}_{ii}^sw \) is the swelling deformation rate for the current configuration; it is the instantaneous variation rate of the swelling true strain at the current configuration. The irradiation swelling only brings the volumetric variation without shape changes, which is quite similar to the thermal expansion strain for the isotropic material. So, only the linear strain \( \varepsilon^b \) which is the same along all directions exists without the shear strain components.

The fuel particle swelling is usually characterized by the relative volume variations. A kind of swelling coefficient \( \beta^sw \) can be introduced as the volume swelling rate by

\[ SW(BU) = \frac{\Delta V}{V_0} = \int_0^{BU} \beta^sw d(BU) \] (2)

where \( V_0 \) is the reference volume, \( \Delta V \) is the volume variation measured after a period of fission reactions. \( BU \) is called burnup with a unit % FIMA, which is defined as the ratio of the number of the fissioned U atoms to the original number of U atoms.

The swelling rate \( \beta^sw \) (swelling per 1% FIMA) has three contributions from the fission gas-bubbles \( \beta^gb \), the solid fission products \( \beta^sp \) and the fission densification \( \beta^fd \). Namely,

\[ \beta^sw = \beta^gb + \beta^sp + \beta^fd \] (3)

According to the definition of the irradiation swelling, the particle swelling at time \( t \) can be expressed as
If the plastic flow potential is associated, the plastic flow potential deformation rate is along the outer normal direction of the yield surface equation becomes

\[ \dot{\epsilon}_p = \dot{\epsilon}_p^H = \dot{\epsilon}_p - H(\dot{\epsilon}_p) = 0 \]  

(16)

where \( \dot{\epsilon}_p \) is the Mises equivalent true stress, \( \dot{\epsilon}_p \) is the equivalent plastic true strain. For the large-deformation analysis, the yield surface equation must be expressed with the true stress and the true strain. And \( \dot{\epsilon}_p = \sqrt{3/2} s_{ij} s_{ij} \), where \( s_{ij} \) are the components of the deviatoric tensor of the Cauchy stress.

According to the associated flow rule, the plastic deformation rate is given as

\[ \dot{\epsilon}_p = \frac{1}{2} \frac{\partial F}{\partial \sigma_y} = \frac{1}{2} \frac{\partial \dot{\sigma}}{\partial \sigma_y} \]  

(17)

According to the plastic work rate as

\[ W_p = \sigma_y \dot{\epsilon}_p \]  

(18)

Together with \( \dot{\epsilon}_p = \sqrt{3/2} s_{ij} s_{ij} \), \( s_{ij} = \sigma_{ij} - \delta_{ij} \tau_{ij} \), and \( \tau_{ij} = \frac{1}{2} \sigma_{ij} \), it can be obtained that \( \lambda = \dot{\epsilon}_p \). Thus, the plastic deformation rate (17) can also be expressed as

\[ \dot{\epsilon}_p = \dot{\epsilon}_p \frac{\partial \sigma}{\partial \sigma_y} \]  

(19)

According to the yield surface equation as Eq. (16) and the consistent condition (that is, the point located at the yield surface will remain at the yield surface through the plastic loading), we have

\[ F = \frac{\partial \sigma}{\partial \sigma_y} \sigma_y - \frac{\partial H}{\partial \epsilon_p} \dot{\epsilon}_p = 0 \]  

(20)

Using Eqs. (13) and (19) yields

\[ \sigma_y = D_{ijkl} (\dot{d}_{ijkl} - \dot{\epsilon}_p \frac{\partial \sigma}{\partial \sigma_y}) \]  

(21)

The Mises yield function is the isotropic function of the stresses, and thereby it is the function of the invariant of the stresses. So, the following relation is obeyed [24]

\[ \frac{\partial \sigma}{\partial \sigma_y} \sigma_y - \frac{\partial H}{\partial \epsilon_p} \dot{\epsilon}_p = 0 \]  

(22)

Substituting Eq. (22) into (20) gets

\[ \frac{\partial \sigma}{\partial \sigma_y} \sigma_y - \frac{\partial H}{\partial \epsilon_p} \dot{\epsilon}_p = 0 \]  

(23)

Substitution of Eq. (21) into (23) yields

\[ \dot{\lambda} = \dot{\epsilon}_p = \frac{1}{2} \frac{\partial \sigma}{\partial \sigma_y} D_{ijkl} \dot{d}_{ijkl} \]  

(24)

The three-dimensional constitutive relation for the metal matrix can be deduced through substituting Eq. (24) into (21),

\[ \sigma_y = D_{ijkl} (\dot{d}_{ijkl} - \dot{\epsilon}_p \frac{\partial \sigma}{\partial \sigma_y}) \]  

(25)

where \( D_{ijkl} \) is the tangent elastoplastic stiffness tensor which can be denoted as

\[ D_{ijkl} = D_{ijkl} - D_{ijkl}^{\psi} = \frac{1}{2} \frac{\partial \sigma}{\partial \sigma_y} D_{ijkl} \]  

(26)

\[ D_{ijkl}^{\psi} = D_{ijkl} - D_{ijkl}^{\psi} = \frac{1}{2} \frac{\partial \sigma}{\partial \sigma_y} D_{ijkl} \]  

(27)

According to the definition of the irradiation growth rate of the cladding.
\[
[d^e_{ij}] = \begin{bmatrix}
  i^e_{xz} & 0 & 0 \\
  0 & i^e_{yz} & 0 \\
  0 & 0 & i^e_{zx}
\end{bmatrix}
\] (28)

In the same way as that for the matrix in Section 2.2, the three-dimensional constitutive relation for the cladding can be deduced as
\[
\sigma_{ij}^C = D^C_{ijkl}d_{kl} + \sigma_{ij}^{r0}
\] (29)
where \( D^C_{ijkl} \) is the tangent elastoplastic stiffness tensor which is the same to Eq. (26), and
\[
\sigma_{ij}^{r0} = D_{ijkl}^{\delta} \frac{\partial \sigma_{kl}}{\partial \sigma_{pq}} D_{pqmn}^{\delta} \frac{\partial \sigma_{mn}}{\partial \sigma_{rs}} + D_{ijkl}
\] (30)

When the elastic loading or the unloading is carried out, \( D^C_{ijkl} = D_{ijkl}^{\delta} \).

3. Simulation of the coupled irradiation effects

The total burnups can be divided into two stages: the initial stage of burnup and the increasing stage of burnup. The temperature distribution and the induced thermo-mechanical behaviors are mainly concerned at the initial stage. The solution of the above thermo-mechanical coupling behaviors is the focus of the first analysis step. For the second analysis step corresponding to the increasing stage of burnup, irradiation swelling of the fuel particles and irradiation growth of the cladding are the main contributions to the evolution of the micro stress–strain fields. According to the constitutive relations in the above section it can be obtained that irradiation swelling of the fuel particles and irradiation growth of the cladding are the initial strains similar to the thermal expansion strains. Thus, the method of virtual temperature increase is used to represent the effects of fuel particle swelling and cladding irradiation growth. The virtual temperature method is given as follows based on the Updated Lagrange Method in numerical simulation of finite strain problems.

3.1. The simulation method for irradiation swelling of the fuel particles

The total swelling \( SW(BU) \) of the fuel particles include three parts: gas-bubble swelling, solid fission product swelling and densification due to the variation of the porosity \([21]\).

The total calculation process is divided into \( n \) virtual time steps. At an arbitrary time step from \( t-1 \) to \( t \), the ratio of the volume change is
\[
\frac{V_t}{V_{t-1}} = \frac{V_{t-1} + \Delta V_t}{V_{t-1}} = (1 + \Delta \varepsilon)^3
\] (31)
where \( \Delta \varepsilon \) denotes the strain increment induced by the irradiation swelling at every step. Then

![Fig. 1. The temperature load at each burnup.](image)

![Fig. 2. (a) The sketch map, (b) RVE and (c) finite element model of the dispersion fuel plate.](image)
The total temperature load at certain burnup is

\[ T_{\text{load}} = \left(1 + \Delta_t^3 \right) T_{\text{ref}} - 1 \]

where \( T_{\text{ref}} \) is the base temperature.

The mesh grids, node and element information for different PP distances.

### Table 1

<table>
<thead>
<tr>
<th>Particles distances PP (( \mu m ))</th>
<th>105</th>
<th>110</th>
<th>120</th>
<th>130</th>
<th>140</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of elements</td>
<td>25,216</td>
<td>25,416</td>
<td>25,416</td>
<td>25,616</td>
<td>26,024</td>
</tr>
<tr>
<td>Number of nodes</td>
<td>114,665</td>
<td>115,589</td>
<td>115,589</td>
<td>116,513</td>
<td>118,387</td>
</tr>
</tbody>
</table>

3.2. The simulation method for cladding irradiation growth

The irradiation growth of cladding is anisotropic, which means to stretch along the length direction and to contract along the width and thickness direction. The model [25] is adopted as the following

\[ \Delta \epsilon_i^x = \frac{\epsilon_i^x}{\alpha} \Delta T \]

\[ \epsilon_{gr}^x = 4.942 \times 10^{-20} \phi \]

\[ \epsilon_{gr}^y = -0.059 \epsilon_{gr}^y \]

\[ \epsilon_{gr}^z = -0.941 \epsilon_{gr}^z \]

where the growth rates \( \epsilon_{gr}^x, \epsilon_{gr}^y \) and \( \epsilon_{gr}^z \) are the components along the length, width and thickness direction respectively. \( \phi \) is the fast neutron flux rate in n/cm² s. Such irradiation growth can be simulated by using anisotropic thermal expansion.

Considering a constant fission rate, irradiation growth strain can be obtained from Eq. (37).

\[ \epsilon_{gr}^x = \epsilon_{gr}^x t \]

The virtual temperature can be obtained as described below

\[ \Delta T_{\text{virtual}} = \frac{n}{\alpha} \left[ \sqrt{\epsilon_{gr}^x + 1} - 1 \right] \]

where the thermal expansion coefficient is set as \( 5.58 \times 10^{-6}/K \), \( n \) is the number of all the time steps which should be set as a large number.

The thermal expansion coefficients along the other two directions can be obtained by solving the following equations

\[ \Delta T_{\text{virtual}} = \frac{n}{\alpha} \left[ \sqrt{0.059 \epsilon_{gr}^y + 1} - 1 \right] \]

\[ \Delta T_{\text{virtual}} = \frac{n}{\alpha} \left[ \sqrt{0.941 \epsilon_{gr}^z + 1} - 1 \right] \]

3.3. The simulation method for the coupled irradiation effects

Set the initial stage of burnup as a load step. At the initial stage of burnup, the heat generation rate 3.204 W/mm³ is applied in the fuel particles. With the boundary conditions clarified in the following section, the real temperature \( T_{\text{base}} \) can be solved firstly.

For the increasing burnup stage, the temperature loads in the fuel particles and cladding should be the sum of real temperature \( T_{\text{base}} \) and the virtual temperature \( \Delta T_{\text{virtual}} \); and the temperature loads in the matrix remain constant. This process can be divided into six steps (Fig. 1) with respect to each burnup (BU = 5%, 10%, 15%, 20%, 25% and 30% FIMA). In Fig. 1, the applied temperature loads with APDL language for the typical nodes in the fuel particles, cladding and matrix are shown.

4. The finite element model

According to the periodicity and the actual plate geometry shape that the sizes along the length direction and the width direction are much larger than the one along the thickness direction (Z direction) shown in Fig. 2a, the representative volume element...
(RVE) is selected as Fig. 2b. The finite element model is developed as Fig. 2c, according to the symmetry, as 1/8 of the RVE. The thickness of the meat is 1.408 mm and the one of the cladding is 0.4 mm. The radius of the fuel particle is set as 0.05 mm with the volume fraction 25%.

The distance between the lowest two particles in Fig. 2c, from center to center, PP varies as PP = 105 μm, 110 μm, 120 μm, 130 μm and 140 μm. The convergent mesh grids, node and element information of the developed finite element models are presented in Fig. 3 and Table 1. The distance from the center of the top particle to the cladding PC varies as PC = 55 μm, 60 μm, 65 μm and 70 μm. The thickness H remains the same when PP or PC changes. The models and the convergent grid information are shown in Fig. 4 and Table 2. The proper material models [23] are applied.

Due to the geometric structure of the plate whose sizes along the length or width direction are much larger than the one along the thickness, the coolant takes away the fission heat mainly from the upper and lower surfaces. Meanwhile, the upper and lower surfaces will bear the liquid pressure of the coolant. Thus, they are the main boundaries and should be considered in the finite element models.

The boundary conditions to determine the temperature field are given as

1. Except the upside surface \( Z = H/2 \), the other surfaces of the finite element models all satisfy: \(-k \frac{\partial T}{\partial n} = 0\).
2. The upside surface \( Z = H/2 \) satisfy the convective boundary condition: \(-k \frac{\partial T}{\partial n} = h(T - T_f)\), where the temperature of the periphery fluid \( T_f \) is 573 K and the heat transfer coefficient used is \(2 \times 10^{-2} \text{ W/mm}^2 \text{ K}\).

The boundary conditions to determine the structural fields are as the following:

<table>
<thead>
<tr>
<th>Particle to cladding distances PC (μm)</th>
<th>55</th>
<th>60</th>
<th>65</th>
<th>70</th>
</tr>
</thead>
<tbody>
<tr>
<td>Number of elements</td>
<td>25,416</td>
<td>25,516</td>
<td>25,616</td>
<td>25,716</td>
</tr>
<tr>
<td>Number of nodes</td>
<td>115,589</td>
<td>116,051</td>
<td>116,513</td>
<td>116,975</td>
</tr>
</tbody>
</table>

Fig. 4. The mesh grids for different PC distances: (a) 55 μm, (b) 60 μm, (c) 65 μm and (d) 70 μm.

Fig. 5. The temperature distribution (a) PP = 105 μm, (b) PP = 120 μm, (c) PP = 140 μm and (d) the maximum matrix temperatures for different PP cases.
The symmetric boundary condition is applied at all the surfaces of the finite element models, except the upper surface $Z = H/2$. The coolant pressure at the upper surface is 15 MPa.

The continuous displacement conditions are met at the interfaces between the fuel particles and the matrix and the ones between the meat and the cladding.

5. Results and discussion

For the two different cases: (1) variation of PP (particle–particle distance) and PC (particle-cladding distance), the temperature field and the resultant irradiation-induced mechanical behaviors with increasing burnup are calculated. Effects of variations of particle distances on the micro-thermo-mechanical behaviors are obtained and analyzed.

5.1. Effects of variation of the particle distance PP

5.1.1. Effects on the micro temperature distributions

For different PP distances, the obtained contour plots of the micro temperature distributions are illustrated as Fig. 5. It can be observed that the matrix region with higher temperatures is concentrated with decreasing the distances between the two particles close to the mid-plane; however, the actual temperature values hardly change. The maximum temperatures in the matrix with variations of PP distances are depicted in Fig. 5d, and it can be apparently found that almost no differences exist. This is due to the relatively high heat conductivity of the metal matrix.

5.1.2. Effects on the micro stress–strain fields

The lowest part of matrix in the finite element model (Fig. 2c) is to be investigated. The contour plots of the Mises stresses, equivalent plastic strains and first principal stresses at 20% FIMA for different PP distances are shown in Figs. 6 and 7, respectively.

It can be found that the maximum Mises stresses and equivalent plastic strains exist at the interface between the matrix and the fuel particles. Meanwhile, the maximum first principal stresses occur at the metal matrix between the two closest particles along the thickness direction. The variations of the distances between the two particles will locally influence the actual stress and strain.

![Fig. 6.](image1.png) (a) The Mises stress (MPa), (b) equivalent plastic strain and (c) first principal stress (MPa) at 20% FIMA for PP = 130 μm.

![Fig. 7.](image2.png) (a) The Mises stress (MPa), (b) equivalent plastic strain and (c) first principal stress (MPa) at 20% FIMA for PP = 110 μm.

![Fig. 8.](image3.png) Result output paths.
values and distributions, and it can be seen that the first principal stresses are remarkably affected.

Thus, Path 1 (BC) and Path 2 (AB) are selected as indicated in Fig. 8 to depict the effects of the PP distance variations on the micro mechanical behaviors at the matrix.

The maximum Mises stresses and equivalent plastic strains along Path 1 with increasing burnup are shown as Fig. 9a and b, and the maximum first principal stresses along Path 2 with increasing burnup are denoted in Fig. 10.

It can be seen from Fig. 9a that the maximum Mises stresses increase with burnup, while the increasing rates decrease. With decreasing the particle distances, the Mises stresses at different burnups tend to be larger. When PP varies from 140 to 120 μm, the Mises stress varies little. When the distance decreases to 110 μm, the Mises stresses show relatively obvious change. However, when the PP distance decrease from 110 μm to 105 μm, the maximum Mises stresses at higher burnups are lowered. This might result from the lowered differences among the three principal stresses. At the initial stage of burnup, it can be found obviously that the maximum Mises stresses jump from PP = 120 μm to PP = 110 μm, which can result from that the distance variation makes the interaction between the two particles and the relative matrix have a jump. The above phenomena can be explained from the obtained results of three principal stresses: for PP = 110 μm, \( \sigma_1 = 166.4 \text{ MPa}, \sigma_2 = 23.1 \text{ MPa} \) and \( \sigma_3 = -117.6 \text{ MPa} \); and for PP = 120 μm, \( \sigma_1 = 136.4 \text{ MPa}, \sigma_2 = -0.0077 \text{ MPa} \) and \( \sigma_3 = -127.4 \text{ MPa} \). It can be observed that the maximum tensile

\[
\sigma = \sqrt{\frac{1}{2}[(\sigma_1 - \sigma_2)^2 + (\sigma_1 - \sigma_3)^2 + (\sigma_2 - \sigma_3)^2]}
\]

Fig. 9. The maximum (a) Mises stress (MPa) and (b) equivalent plastic strain.

Fig. 10. The maximum values of the first principal stresses.

Fig. 11. The appearance of cracks in the dispersion nuclear fuel [26].

Fig. 12. The output paths of the computation results.
stress for PP = 110 μm is larger than the one for PP = 120 μm, and it can be worked out that the differences between two principal stresses for PP = 110 μm all get larger than the ones for PP = 120 μm. Thus, the Mises stresses have a jump from PP = 120 μm to PP = 110 μm. The equivalent plastic strains have the similar changing rules as indicated in Fig. 9b. For the cases with shorter distances, the increase of the equivalent plastic strains is more obvious, and the main reason for this is that the interaction between the two particles is strengthened. With increasing burnup, the effects of variation of PP distances become more and more obvious.

The maximum first principal stresses at the matrix along Path 2 are indicated in Fig. 10. It can be found that the maximum first principal stresses increase with burnup and the variation of particle distance has great influence on them. When the distance is small (105 μm), the maximum first principal stress can be up to 989.27 MPa. Apparently, the interaction of particles with matrix and the one between the adjacent particles will be intensified if the particle distance decreases sharply. Due to irradiation damage resulting from the fission fragments and fast neutron flux, the metal matrix along Path 2 will be easier to be hardened and become brittle. Thus, the brittle failure (Fig. 11) may be the main failure mode. Based on the reasons above, it can be drawn that, when the particle distance is typically small, the large value of the first principal stress may be the main reason for the appearance of cracks in the matrix [26].

5.2. Effects of variation of the particle to cladding distance PC

In this study, four cases of PC = 55 μm, 60 μm, 65 μm and 70 μm are considered. In order to obtain the detail effects of variation of PC, Path 3, Path 4 and Path 5 as shown in Fig. 12 are selected respectively to output the computation results.

The maximum Mises stresses and equivalent plastic strains along Path 3 are shown in Fig. 13. It can be observed from Fig. 13 that both of the above mechanical variables increase with burnup and have almost no changes when PC distances vary. The reason for this phenomenon is as follows: (1) the matrix material is the same to the one of the cladding, thus the effects of the slight shift of the fuel particle to the cladding can be ignored; (2) the interaction between the fuel particle and the matrix and the one between the fuel particles are scarcely affected.

Fig. 14 denotes the maximum interfacial tensile stresses and shear stresses along Path 4 at the interface between the fuel meat and the cladding. When the distance is smaller (PC = 55 μm and 60 μm), the maximum interfacial normal stresses decrease before 10% FIMA and then increase with burnup. For the cases with PC = 65 μm and 70 μm, the maximum interfacial tensile stresses monotonously increases with burnup as a whole. The interfacial tensile stresses are caused by non-homogeneous interaction between the fuel meat and the cladding. The displacement along the thickness direction at Point F and G (shown in Fig. 12) tend to be different, which induces existence of interfacial tensile stres-
ses. According to the simulation results of PC = 60 μm, 65 μm and 70 μm in Fig. 14a, it can be obtained that the closer the particle to the cladding is, the larger the interfacial tensile stress is at higher burnups. Specially, the maximum interfacial tensile stresses of PC = 55 μm are smaller than those of PC = 60 μm. This might be caused by the complex interaction among the fuel particles, the metal matrix and the cladding due to swelling of the fuel particles and the thermal expansion effects within them.

The maximum interfacial shear stresses appear in the middle of Path 4 near Point F as shown in Fig. 12. Fig. 14b depicts the maximum interfacial shear stresses for different PC cases at different burnups. For PC = 60 μm, the interfacial shear stresses increase with burnup monotonously and have much larger values than those in the other cases. However, for the three cases with PC = 60, 65 or 70 μm, the maximum interfacial shear stresses hold smaller values at all the considered burnups. So, the distance from the particle center to the cladding should be a considerable factor for optimal design of the dispersion nuclear plate.

The maximum Mises stresses and equivalent plastic strains along Path 5 with increasing burnup can be found in Fig. 15. Both of them increase with burnup. The influence of PC variation can be only seen when the distance get very close (PC = 55 μm) at higher burnup. It can be drawn that variation of PC would have little effects on the maximum Mises stresses and equivalent plastic strains at the cladding.

6. Conclusions

In this study, the method of virtual temperature increase has been adopted in the simulation of the irradiation effects within the nuclear fuel element. The three-dimensional models have been established based on different particle to particle (PP) distances and particle to cladding (PC) distances. The interactions between the fuel particles and the matrix and the one between the fuel meat and the cladding in the dispersion nuclear fuel element have been considered. The effects of the micro-geometric variations in the fuel meat on the micro-thermo-mechanical behaviors have been calculated and analyzed. The main conclusions are drawn as follows:

For the cases of varying the particle to particle (PP) distances:

1. Decreasing the particle distances will lead to the increment of the maximum Mises stress and equivalent plastic strains at the matrix between the closer two particles. But the data indicate that the apparent influence can be observed only when the distance is small enough.

2. The first principal stresses at the matrix between the closer and closer two particles increase remarkably with decreasing the particle distances, which would be the main reason for the matrix failure there.

For the case of varying the particle to cladding (PC) distances:

1. Variation of PC distances has very slight effects on the maximum Mises stresses and equivalent plastic strains, no matter at the nearby matrix or the cladding.
(2) The interfacial normal and shear stresses between the fuel meat and the cladding can be dramatically affected when the fuel particle becomes closer to the cladding.

(3) The maximum first principal stresses at the cladding near the interface between the fuel meat and the cladding increase with decreasing the PC distance. When the fuel particle is very close to the cladding, the first principal stress will increase strongly. Large value of the first principal stress at the cladding would be one of the main reasons for cladding failure and should be avoided.

In the future studies, more precious fuel swelling models considering the coupling effects with the macroscopic thermo-mechanical behaviors should be take into consideration. And the heterogeneity of the time and spatial distribution of irradiation hardening together with irradiation creep effects should be further introduced into the research.

Acknowledgements

The authors thank for the supports of the Natural Science Foundation of China (10772049, 11072062), Research and Development Program of China (863 Program, 2009AA04Z408), the Natural Science Foundation of Shanghai (06ZR14009), the Pujiang Scholar Program, and the Wangdao Scholar Program (08076) of Fudan University.

References