The DART Dispersion Analysis Research Tool: A Mechanistic Model for Predicting Fission-Product-Induced Swelling of Aluminum Dispersion Fuels


by J. Rest

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Energy Technology Division

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Abstract

This report describes the primary physical models that form the basis of the DART mechanistic computer model for calculating fission-product-induced swelling of aluminum dispersion fuels; the calculated results are compared with test data. In addition, DART calculates irradiation-induced changes in the thermal conductivity of the dispersion fuel, as well as fuel restructuring due to aluminum fuel reaction, amorphization, and recrystallization. Input instructions for execution on mainframe, workstation, and personal computers are provided, as is a description of DART output. The theory of fission gas behavior and its effect on fuel swelling is discussed. The behavior of these fission products in both crystalline and amorphous fuel and in the presence of irradiation-induced recrystallization and crystalline-to-amorphous-phase change phenomena is presented, as are models for these irradiation-induced processes.
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Executive Summary

DART, a thermomechanical model for the prediction of fission-product-induced swelling in aluminum dispersion fuels, has been applied to the analysis of $\text{U}_3\text{Si}$ and $\text{U}_3\text{Si}_2$ dispersion fuel swelling in plate, tube, and rod fuel element geometries for research reactor applications. The model calculates irradiation-induced swelling of fission gas bubbles as a function of fuel morphology. The DART mechanical model calculates the behavior of a rod, tube, or plate during closure of as-fabricated porosity, during which the fuel particle swelling is accommodated by the relatively soft aluminum matrix flowing into the existing porosity; it also calculates the subsequent macroscopic changes in rod diameter or plate/tube thickness caused by additional fuel deformation processes. DART also includes a calculation for the effect of irradiation on the thermal conductivity of the dispersion fuel, and for fuel restructuring due to the aluminum fuel reaction, amorphization, and recrystallization.

This report describes the primary physical models that form the basis of the DART mechanistic computer model for calculating fission-product induced-swelling of aluminum dispersion fuels. In addition, it compares calculated results with test data. Input instructions for execution on mainframe, workstation, and personal computers are provided, as is a description of DART output. The theory of noble-gas behavior and its effect on fuel swelling is discussed. The behavior of the fission products in both crystalline and amorphous fuel and in the presence of irradiation-induced recrystallization and crystalline-to-amorphous-phase change phenomena is presented, as are models for these irradiation-induced processes.
DART, a thermomechanical model for the prediction of fission-product-induced swelling in aluminum dispersion fuels, has been applied to the analysis of U$_3$Si and U$_3$Si$_2$ dispersion fuel swelling in both plate and rod fuel element geometries for research reactor applications. The model calculates irradiation-induced swelling of solid fission products and of fission gas bubbles as a function of fuel morphology. The DART mechanical model calculates the behavior of a rod, tube, or plate during closure of as-fabricated porosity, during which the fuel particle swelling is accommodated through the relatively soft aluminum matrix flowing into the existing porosity; it also calculates the subsequent macroscopic changes in rod diameter or plate/tube thickness caused by additional fuel deformation processes. DART also includes a calculation for the effect of irradiation on the thermal conductivity of the bulk material.

This report describes the primary physical models that form the basis of the DART mechanistic computer model for calculating fission-product-induced swelling of aluminum dispersion fuels. In addition, it compares calculated results with test data. Input instructions for execution on mainframe and personal computers are provided, as is a description of DART output. The theory of noble-gas behavior and its effect on fuel swelling is discussed. The behavior of the fission products in the presence of irradiation-induced recrystallization and crystallin-to-amorphous phase change phenomena is presented, as are models for these irradiation-induced processes.

The DART fission gas swelling model is based on the mechanistic Steady-State and Transient-Gas Release and Swelling Subroutine (GRASS-SST) [1]. Models are included for the effects of fission-product generation, atomic migration, bubble nucleation and re-solution, bubble migration and coalescence, bubble pinning and growth on dislocations and grain boundaries, grain growth and grain boundary sweeping, channel formation on grain faces, the existence of a fixed density of nodes that are identified as grain edge corners or triple points, porosity interlinkage on the grain edges, irradiation-induced recrystallization (grain subdivision), and irradiation-induced crystallization. Bubble-size distributions are calculated as a function of fuel morphology and microstructure, as is the fuel swelling and gas release. DART incorporates algorithms for calculating the densities of bubbles in each of a number of bubble-size classes. Each bubble-size class is characterized by an average number of atoms per bubble, the value of which differs from that of the preceding size class by a constant multiplier. The number of size classes is a variable that is determined dynamically during a computer run. Changes in the bubble-size distribution, caused by bubble coalescence and irradiation-induced re-solution, for example, are determined by solving a large number of integral/differential equations for each time-step. Solutions are carried out for intragranular bubbles, bubbles along dislocations, and intergranular bubbles (bubbles on grain faces and edges). DART utilizes an iterative solution of a relatively large number of coupled equations.

During irradiation, fuel rods increase in diameter, and fuel plates and tubes increase in thickness as a result of swelling of the fuel core. The swelling is a direct result of the accumulation of fission product elements in the fuel. Although this accumulation is, to the first order, directly proportional to the burnup of the fissionable uranium, the resultant swelling is also affected by several microstructural changes that occur in the fuel core during irradiation.
An important factor in reducing the overall amount of net swelling is radiation-enhanced sintering of fabrication voids. In U$_3$O$_8$, this effect was first demonstrated by Reinke [2] and was later confirmed by an experiment of Martin et al. [3] in which U$_3$O$_8$ dispersion fuel made with depleted uranium was irradiated. The fabrication voids within the U$_3$O$_8$ particles, as well as cracks and gaps resulting from fabrication, sintered to spherical cavities after irradiation. It is well established that an increase in dispersant loading also increases the number of fabrication voids. Inasmuch as a substantial fraction of the sintered porosity can be taken up by the swelling fuel, a large volume of fabrication voids can substantially reduce the net swelling.

The DART mechanical analysis, based on the work of Blake [4], addresses the mechanical behavior of both dispersion fuel plates and fuel rods. The model examines a system of spherical fuel particles surrounded by a large spherical shell of matrix material bonded to an outer shell of aluminum cladding. The approach treats the inner sphere as a mechanically deforming body and the spherical shell as perfectly plastic. The DART swelling models provide the driving force for mechanical deformation.

DART does not currently model the thermal performance of the fuel element (aside from the calculation of the thermal conductivity of the dispersion material). Thus, fuel temperature and linear power are required input into the analysis. In a fully coupled model, the calculation of fuel deformation and thermal conductivity is interactive with the thermal analysis.

The DART model includes several assumptions. Among these is the assumption that no swelling of the aluminum matrix is assumed to occur during reactor operation. This assumption is based on the relative swelling rates of the aluminum matrix and the fuel. From these swelling rates, it can be shown that fuel swelling is several orders of magnitude greater than aluminum matrix swelling. Inclusion of aluminum matrix swelling would lead to a slight increase in predicted rod diameter or plate thickness.

The fuel particles are assumed to be identical in size and to have a uniform spherical shape. The size of actual fuel particles varies and their shape is irregular. However, irregular particle shapes are difficult to handle mathematically, and because the orientation of the particles is random, an assumption of uniform overall behavior seems reasonable. In addition, particle-particle interactions are ignored. Including particle-particle interactions will result in a greater degree of swelling than predicted by the model.

No change in aluminum yield stress with respect to fluence is assumed. Using the usual time-dependent deformation methodology, we did not include the effects of the creep of the fuel and matrix. These phenomena are modeled by including a factor that multiplies the aluminum yield strength. This factor differs, depending on whether the fuel element is in a plate/tube or a rod geometry.

In addition to uncertainties involving model assumptions, various uncertainties exist in the experimental data. Physical measurements are subject to errors induced by oxide layers. Measurements are made at various points on the plate or rod to yield an overall thickness and/or diameter measurement, which is an average and is subject to error. Measurement of fabricated porosity is subject to uncertainties. Likewise, it is difficult to accurately measure
matrix dimensions after fabrication. Actual interface conditions between both fuel particles and matrix, and between the matrix and the cladding are not precisely known, and are presumably not orderly and homogeneous as assumed in the model. All of these uncertainties will contribute to deviations between model predictions and experimental data.

This User's Guide includes and describes a typical DART input file, a dictionary of variables in COMMON/PROG/PROG(250), and a typical DART output file in Appendixes A-C, respectively.

2 DART Theory of Fission Gas Behavior in Crystalline Fuel

The DART code predicts atomic and bubble behavior of fission gas in aluminum dispersion fuels under steady-state and transient conditions. Included are models that assess the effects of fission product generation, atomic migration, bubble nucleation and re-solution, bubble migration and coalescence, channel formation on grain faces, porosity interlinkage on grain edges, the existence of a fixed density of nodes that are identified as grain edge corners or triple points, and grain growth/grain boundary sweeping on both the amount of released fission products and on their distribution within the fuel. DART solves a set of coupled nonlinear differential equations for the intra- and intergranular concentrations of fission-product atoms and gas bubbles of the form

\[
\frac{dC_{i}^{\alpha}}{dt} = -a_{i}^{\alpha} C_{i}^{\alpha} C_{i}^{\alpha} - b_{i}^{\alpha} C_{i}^{\alpha} + e_{i}^{\alpha} \quad (i = 1, ..., N; \alpha = 1,2,3,4),
\]

where \(C_{i}^{\alpha}\) is the number of \(\alpha\)-type bubbles in the \(i\)-th size class per unit volume; \(\alpha = 1,2,3,4\) represents the lattice, dislocation, grain face, and grain edge distributions, respectively; and the coefficients \(a_{i}^{\alpha}\), \(b_{i}^{\alpha}\), and \(e_{i}^{\alpha}\) obey functional relationships of the form

\[
a_{i}^{\alpha} = a_{i}^{\alpha}(C_{i}^{\beta}).
\]

\[
b_{i}^{\alpha} = b_{i}^{\alpha}(C_{i}^{\beta}, ..., C_{i-1}^{\beta}, C_{i+1}^{\beta}, ..., C_{N}^{\beta}).
\]

The variables in Eq. 1 are defined in Table 1. \(a_{i}^{\alpha}\) represents the rate at which \(\alpha\)-type bubbles are lost from (grow out of) the \(i\)-th size class because of coalescence with bubbles in that class; \(b_{i}^{\alpha}\) represents the rate at which \(\alpha\)-type bubbles are lost from the \(i\)-th size class because of coalescence with bubbles in other size classes, migration out of the structural region, change in bubble type (i.e., by acquiring a different value of \(\alpha\)) due to bubble migration processes and re-solution; and \(e_{i}^{\alpha}\) represents the rate at which bubbles are being added to the \(i\)-th size class because
of fission gas generation, bubble nucleation, bubble growth resulting from bubble coalescence, migration processes, and bubble shrinkage due to gas atom re-solution.

The bubbles are classified by an average size, where size is defined in terms of the number of gas atoms per bubble. This method of bubble grouping significantly reduces the number of equations needed to describe the bubble size distributions. The bubble classes are ordered so that the first class refers to bubbles that contain only one gas atom. If \( S_i \) denotes the average number of atoms per bubble for bubbles in the \( i \)-th class (henceforth called \( I_b \) bubbles), then the bubble size classes are defined by

\[
S_i = mS_{i-1},
\]

where the integer \( m \geq 0.5 + \sqrt{1.25} \), \( i \geq 2 \), and \( S_1 = 1 \). The \( i = 1 \) class is assumed to consist of a single gas atom associated with one or more vacancies or vacancy clusters. In general, the rate of coalescence \( \Gamma_{ij} \) of \( i \) bubbles with \( j \) bubbles is given by

\[
\Gamma_{ij} = t_i^j C_i^a C_j^a,
\]

where \( P_{ij} \) is the probability in \( m^3 \text{s}^{-1} \) of an \( i \) bubble coalescing with a \( j \) bubble. For \( i = j \), \( \Gamma_{ii} \) becomes

\[
\Gamma_{ii} = \frac{1}{2} P_{ii} C_i^a C_i^a
\]

so that each pairwise coalescence is counted only once.

Coalescence between bubbles results in bubbles growing from one size class to another. The probability that a coalescence between an \( i \) bubble and a \( j \) bubble will result in a \( k \) bubble is given by the array \( T_{ijk} \). The number of gas atoms involved in one such coalescence is \( S_i + S_j \). The array \( T_{ijk} \) is defined by three conditions:

1. \( \sum_k T_{ijk} = 1 \) (the total probability of producing a bubble is unity).
2. \( \sum_k T_{ijk} S_k = S_i + S_j \) (the number of gas atoms, on average, is conserved).
3. For a given pair \( ij \), only two of the \( T_{ijk} \) array elements are nonzero. These elements correspond to \( k \) and \( k+1 \), where \( S_k \leq S_i + S_j \leq S_{k+1} \).

From these three conditions, it follows that \( k = i \), and

\[
T_{ij} S_k + (1 - T_{ijk}) S_{k+1} = S_i + S_j.
\]
Thus, the probability that a coalescence between an i bubble and a j bubble will result in a k bubble is given by

\[ T_{jk} = \frac{S_{k+1} + S_j - S_k}{S_{k+1} - S_k} = 1 - \frac{S_j}{S_{k+1} - S_k}, \]  

and the probability that the coalescence will result in a k+1 bubble is given by

\[ T_{jk+1} = \frac{S_j + S_k - S_k}{S_{k+1} - S_k} = \frac{S_j}{S_{k+1} - S_k}. \]  

The array \( T_{ijk} \) may be considered the probability that an i bubble will become a k bubble as a result of its coalescence with a j bubble. The rate \( N_{ik} \) at which i bubbles become k bubbles is given by

\[ N_{ik} = \sum_{j \neq i} \Gamma_{ij} T_{jk}. \]  

The j bubble is assumed to disappear because gas atoms are absorbed into the i bubble. The rate of disappearance \( \chi_j \) is given by

\[ \chi_j = \sum_{j \neq i} \Gamma_{ij}. \]  

The rate \( N_{ik} \) at which i bubbles become k bubbles, with k = i+1, is reduced by various processes such as the re-solution of gas atoms. Re-solution is the result of collisions (direct and/or indirect) between fission fragments and gas bubbles. From Eqs. 7 and 8,

\[ N_{ik} = \sum_{j \neq i} \Gamma_{ij} T_{jk} \]

\[ = \sum_{j \neq i} P_{ij} C_i C_j \frac{S_j}{S_k - S_i} \]

\[ = \frac{C_i}{S_k - S_i} \sum_{j \neq i} P_{ij} C_j S_j. \]  

The expression \( \sum_{j \neq i} P_{ij} C_j S_j \) is the rate at which gas atoms are added to an i bubble. Re-solution causes an i bubble to lose gas atoms at a rate given by \( b_i S_j \), where \( b_i \) is the probability that a gas atom in an i bubble is redissolved. The reduced \( N_{ik} \) becomes
\[ N_{ik} = \frac{C_i}{S_i - S_j} \sum_{j \neq i} (P_j C_j S_j - b_j S_j). \] (11)

If the expression within the parentheses is negative, then \( N_{ik} \) is zero, and \( N_{ik} \), the rate at which \( i \) bubbles become \( i-1 \) bubbles, with \( k = i-1 \), is defined as

\[ N_{ik} = \frac{C_i}{S_i - S_j} \left( b_j S_j - \sum_{j \neq i} P_j C_j S_j \right). \] (12)

Equations 11 and 12 are proportional to the probabilities that any particular \( i \) bubble will become an \( i+1 \) or an \( i-1 \) bubble, respectively; the ratio of the probabilities is equal to the ratio of the rates. Clearly, the above definitions of \( N_{ik} \) and \( N_{ik} \) are consistent with the conservation of the total number of gas atoms.

The components of the basic equations (i.e., Eq. 1) solved in DART are described below.

### 2.1 Intragrahronic Fission Gas and Fission Gas on Dislocations

The flux of gas atoms diffusing to the grain boundaries in a concentration gradient is obtained by solving for the concentration of gas atoms \( C_g \) within a spherical grain that satisfies the equation

\[ \frac{\partial C_g}{\partial t} = \frac{1}{r^2} \frac{\partial}{\partial r} \left( D_g r^2 \frac{\partial C_g}{\partial r} \right) + \alpha f. \] (13)

where \( D_g \) is the gas atom diffusion-coefficient, \( f \) is the fission rate, \( \alpha \) is the average number of rare-gas atoms produced per fission, and \( r \) is the radial distance from the grain center.

In general, Eq. 13 is solved with the boundary conditions

\[ C_g = 0 \quad \text{at} \quad t = 0 \quad \text{for} \quad 0 \leq r \leq d_g / 2. \] (14)

\[ C_g = 0 \quad \text{at} \quad r = d_g / 2 \quad \text{for} \quad t_0 \leq t \leq t_0 + \Delta t, \] (15)

\[ \frac{\partial C_g}{\partial r} = 0 \quad \text{at} \quad r = 0 \quad \text{for} \quad t_0 \leq t \leq t_0 + \Delta t, \] (16)

where \( \Delta t \) is an increment of time.
Table 1. Definition of variables in Eq. 1, $\frac{dC_i^\alpha}{dt} = -a_i^\alpha C_i^\alpha C_i^\alpha - b_i^\alpha C_i^\alpha + e_i^\alpha$

<table>
<thead>
<tr>
<th>$\alpha$</th>
<th>$i$</th>
<th>$C_i^\alpha$</th>
<th>$a_i^\alpha C_i^\alpha C_i^\alpha$</th>
<th>$b_i^\alpha C_i^\alpha$</th>
<th>$e_i^\alpha$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1,2</td>
<td>1</td>
<td>Concentration of intragranular gas atoms ($\alpha = 1$), and gas atoms on dislocations ($\alpha = 2$)</td>
<td>Rate of gas atom loss due to gas bubble nucleation</td>
<td>Rate of gas atom loss due to diffusive flow to grain boundaries, grain boundary sweeping, and diffusion into gas bubbles</td>
<td>Rate of gas atom gain due to atom re-solution and fission of uranium nuclei</td>
</tr>
<tr>
<td>1,2</td>
<td>2,...,N</td>
<td>Concentrations of intragranular gas bubbles ($\alpha = 1$), and gas bubbles on dislocations ($\alpha = 2$)</td>
<td>Rate of gas bubble loss due to bubble coalescence with bubbles within the same size class</td>
<td>Rate of gas bubble loss due to coalescence with bubbles in other size classes, diffusive flow to grain boundaries ($\alpha = 1$), grain boundary sweeping, and gas atom re-solution</td>
<td>Rate of gas bubble gain due to bubble nucleation and coalescence, and diffusion of gas atoms into bubbles</td>
</tr>
<tr>
<td>3</td>
<td>1,...,N</td>
<td>Concentrations of grain face gas atoms ($i = 1$) and gas bubbles ($i &gt; 1$)</td>
<td>Rate of gas loss due to gas bubble nucleation ($i = 1$) and bubble coalescence with bubbles within the same size class ($i &gt; 1$)</td>
<td>Rate of gas bubble loss due to coalescence with bubbles in other size classes, venting to grain edges, and microcracking, and rate of gas atom loss due to capture by gas bubbles</td>
<td>Rate of gas bubble gain due to bubble nucleation and coalescence, diffusion of gas atoms into bubbles, and intragranular migration to grain faces</td>
</tr>
<tr>
<td>4</td>
<td>1,...,N</td>
<td>Concentrations of grain edge gas atoms ($i = 1$) and gas bubbles ($i &gt; 1$)</td>
<td>Rate of gas loss due to gas bubble nucleation ($i = 1$) and bubble coalescence with bubbles within the same size class ($i &gt; 1$)</td>
<td>Rate of gas bubble loss due to coalescence with bubbles in other size classes, long-range grain edge bubble interconnection, and microcracking, and rate of gas atom capture by bubbles</td>
<td>Rate of gas bubble gain due to bubble nucleation and coalescence, diffusion of gas atoms into bubbles, and the venting of gas from the grain faces</td>
</tr>
</tbody>
</table>
The concentration of gas atoms in a spherical grain described in Eq. 13 is

\[
\frac{1}{r^2} \frac{d}{dr} \left( D_r r^2 \frac{dC_g}{dr} \right) - \frac{C_g'}{\delta t} + \frac{C_g''}{\delta t} + \alpha f = 0. \tag{17}
\]

Euler's theorem may now be used to obtain a variational principle equivalent to Eq. 17:

\[
\delta \int_0^{1/2d_g} 4\pi \left[ \frac{D_r}{2} \left( \frac{dC_g}{dr} \right)^2 + \frac{C_g^2}{2\delta t} - \left( \frac{C_g'}{\delta t} + \alpha f \right) C_g \right] r^2 dr = 0, \tag{18}
\]

which assumes that Dirichlet boundary conditions are to be applied. An approximate solution to the problem may now be obtained by choosing a trial function that satisfies the boundary conditions and minimizes the integral in Eq. 18 in terms of free parameters in the function. Many types of trial function could be chosen, but it is easier to work with piecewise functions than global functions. Quadratic functions are attractive because they allow an exact representation of Eq. 13 for long times. To meet the objective of a realistic level of accuracy with a minimum of computer storage and running time, the spherical grain is split into two concentric regions of approximately equal volume, as shown in Fig. 1. In each region, the gas concentration is represented by a quadratic function constrained to have \( dC_g/dr = 0 \) at \( r = 0 \). In the outer Region II (Fig. 1), the concentration function is constrained to a value of \( C_g = 0 \) at \( r = d_g/2 \). The two functions are also constrained to be continuous at the common boundary of the two regions. This leaves three free parameters. Matthews and Wood [5] chose these

\[
\rho_1 = 0.4, \quad \rho_2 = 0.8, \quad \rho_3 = 0.9
\]

Fig. 1. Configuration of two-zone model.

...
For Region I,

\[ C_x = C_1^0 \left( 0.64 - \rho^2 \right) / 0.48 + \left( \rho^2 - 0.16 \right) / 0.48. \]  \hfill (19)

For Region II,

\[ C_y = C_1^0 \left( 0.64 - \rho^2 \right) / 0.48 + \left( \rho^2 - 0.16 \right) / 0.48. \]  \hfill (20)

Eqs. 19 and 20 are substituted for \( C_g \) in Eq. 18 and an extremum is found by differentiating with respect to \( C_1^0, C_2^0, \) and \( C_3^0 \) in turn. The following three linear equations are thus obtained:

\[
\begin{align*}
\left( \frac{q_1 D_x}{d_x^2} + q_2 a \right) C_1^0 &= K_g q_1 + \left( C_1^0 q_2 + C_2^0 q_4 \right) / \delta, \\
\left( \frac{q_3 D_x}{d_x^2} + q_4 a \right) C_1^0 &= K_g q_2 + \left( C_1^0 q_3 + C_2^0 q_5 \right) / \delta, \\
\left( \frac{q_9 D_x}{d_x^2} + q_8 a \right) C_1^0 &= K_g q_3 + \left( C_1^0 q_9 + C_2^0 q_10 \right) / \delta,
\end{align*}
\]

where \( C_1^0, C_2^0, \) and \( C_3^0 \) are the values of the concentrations at the evaluation points at the start of the time increment. The various \( q \) coefficients are integrals, which, when directly evaluated, are, to four figures,

\[
\begin{align*}
q_1 &= 4.552, \quad q_2 = 0.06935, \quad q_3 = -4.552, \\
q_4 &= 0.02167, \quad q_5 = 0.09102, \quad q_6 = 37.78, \\
q_7 &= 0.07615, \quad q_8 = -38.72, \quad q_9 = 0.008456, \\
q_{10} &= 0.01008, \quad q_{11} = 87.04, \quad q_{12} = 0.08656, \\
q_{13} &= 0.1083.
\end{align*}
\]

Equations 21a-c can be directly solved to obtain concentrations \( C_1, C_2, \) and \( C_3 \) as follows:
\[ C_1^e = \frac{X_1 - F_2 C_2^e}{F_1}, \quad (22a) \]
\[ C_2^e = \frac{\frac{F_2}{F_1} X_1 + \frac{F_4}{F_5} X_4 - X_2}{\frac{F_2}{F_1} F_2 + \frac{F_4}{F_5} F_4 - F_3}. \quad (22b) \]

and

\[ C_3^e = \frac{(X_3 - F_2 C_2^e)}{F_5}. \quad (22c) \]

where

\[
\begin{align*}
F_1 &= q_1 D_{g_1} / d_g^2 + q_2 / \delta t, \\
F_2 &= q_3 D_{g_2} / d_g^2 + q_4 / \delta t, \\
F_3 &= q_5 D_{g_3} / d_g^2 + q_6 / \delta t, \\
F_4 &= q_7 D_{g_4} / d_g^2 + q_8 / \delta t, \\
F_5 &= q_9 D_{g_5} / d_g^2 + q_{10} / \delta t, \\
X_1 &= \dot{f} q_2 + (C_{10} q_2 + C_{11} q_4) / \delta t, \\
X_2 &= \dot{f} q_4 + (C_{12} q_4 + C_{13} q_6 + C_{14} q_8) / \delta t, \\
X_3 &= \dot{f} q_6 + (C_{15} q_6 + C_{16} q_8) / \delta t.
\end{align*}
\]

The flux of gas atoms to the boundary (in units of atoms/m$^3$/s) is given by

\[ J = -\left. \frac{6 D_{g_1}}{d_g} \frac{\partial C}{\partial r} \right|_{rad./2}, \quad (23) \]

or

\[ J = -\left. \frac{D_{g_1}}{d_g^2} \right( -60 C_2^e + 240 C_3^e \right). \quad (24) \]
For proper coupling of the diffusive flow process with other processes that affect fission gas behavior, (e.g., gas atom re-solution, gas atom trapping by bubbles, and gas bubble nucleation and coalescence) information about the average concentration of fission gas within the grain is required.

Matthews and Woods [5] determined that the best expression for the average concentration within the grains, \( \overline{C_g} \), is given by

\[
\overline{C_g} = 0.2876C_i^g + 0.2176C_s^g + 0.4261C_j^g.
\]

At the end of an iteration, the concentrations \( C_i^g, C_s^g, \) and \( C_j^g \) in Eq. 25 are scaled by imposing the condition that the average concentration calculated with Eq. 25 is equal to the average concentration calculated with Eq. 1, i.e., that the modified \( C_i^g, C_s^g, \) and \( C_j^g \) then become the initial values of the concentrations (i.e., \( C_i^0, C_s^0 \) and \( C_j^0 \)) that are to be used for the next iteration. The diffusive flow of fission gas bubbles is treated in a manner analogous to that for fission gas atoms, but with \( f = 0 \) in Eq. 13. This method of coupling diffusive flow with other processes that affect fission gas behavior (e.g., gas atom re-solution, gas atom trapping by gas bubbles, gas nucleation and coalescence) is computationally efficient and has been benchmarked against various analytical solutions.

Re-solution causes an i bubble to lose gas atoms at a rate given by \( b_i \dot{S}_i \) (see Eq. 11), where the rate at which gas atoms are ejected from the bubble, \( \dot{b}_i \), is calculated under the assumption that gas atom re-solution from a spherical bubble is isotropic and proceeds by the ejection of single gas atoms. Thus,

\[
b_i = \frac{3b_0 \dot{S}_i}{R_i^3} \int_{R_i - \lambda}^{R_i} \left( \frac{1 + \cos \theta}{2} \right) r^2 dr,
\]

where \( R_i \) is the radius of an i bubble and \( \cos \theta_i = \left( R_i^2 - \lambda^2 - r^2 \right) / 2r\lambda \). A straightforward integration of Eq. 26 results in

\[
b_i = \frac{3b_0 \dot{S}_i}{R_i^3} \left\{ R_i^2 \left[ \frac{R_i}{6} + \frac{R_i^2}{16\lambda} + \frac{1}{8} \left( \frac{R_i - \lambda}{\lambda} \right) \right] - \right. \]

\[
\left. \left( R_i - \lambda \right)^2 \left[ \frac{R_i - \lambda}{6} + \frac{(R_i - \lambda)^2}{16\lambda} + \frac{1}{8} \left( \frac{R_i - \lambda}{\lambda} \right) \right] \right\},
\]

where \( \lambda \) is the average distance an ejected atom travels, \( b_0 \) is a measurable property of the material, and \( \dot{S}_i \) is a measure of the “strength” of gas atom re-solution from grain boundary bubbles.
The atom fission gas diffuses by random migration to dislocations at a rate governed by

\[ R_i^d = \frac{2\pi D_i \rho C_i}{\ln(r_c / r_i)}, \]  

(28)

where \( \rho \) is the dislocation density (mm/mm\(^3\)), \( r_i \) is the mathematical radius of a single gas atom, and \( r_c \) is the radius of the cylindrical capture volume; i.e.,

\[ (\frac{r_c^2}{\ln(r_c / r_i)}) \rho = 1. \]  

(29)

Once the fission gas is pinned to dislocations, the gas can coalesce with both lattice and dislocation bubbles (re-solution causes gas atoms to be knocked back into the lattice), and the gas can be pulled back into the lattice by the force of a temperature gradient if the fission-gas bubbles grow beyond a specified critical size. In the lattice, the probability, \( P_i \), of an \( i \) bubble coalescing with a \( j \) bubble by random motion is given by

\[ P_{ij} = 4\pi (R_i + R_j) (D_i + D_j), \]  

(30)

Coalescence probabilities for bubbles on dislocations can be derived based on a solution of the one-dimensional, time-independent diffusion equation and are given by

\[ P_{ij}^d = \left( D_i^d + D_j^d \right) / \sqrt{\rho}, \]  

(31)

where \( D_i^d \) is the average dislocation \( i \)-bubble diffusion coefficient. The coalescence probabilities for dislocation bubbles coalescing with lattice bubbles is given by Eq. 30 with the diffusivity of the dislocation bubble equal to zero; i.e., the bubble on the dislocation is assumed pinned and immobile.

### 2.2 Intergranular Fission Gas: Grain Faces

DART calculates fission gas saturation in the grain face by directly addressing the calculated distribution of fission gas bubble sizes. The projected areal coverage of the grain face by these bubbles, per unit volume, is given by

\[ A_j = \pi f_j(\theta) \sum_i \left( R_i^{j'} \right)^2 C_i^{j'}, \]  

(32)

where \( f_j(\theta) \) is a geometrical factor that accounts for the lenticular shape of the grain face bubbles, and \( R_i^{j'} \) is the radius of a grain face \( i \) bubble. If the gas is assumed to be made up of equal, closely packed, touching bubbles, the maximum areal coverage per unit area of grain face is \( A_j^* = 0.909 \). (Under conditions where this assumption is
not valid, i.e., \( A'_f < 0.909 \), the DART code utilizes a nominal value of \( A'_f = 0.5 \). Grain face saturation (i.e., the initiation of gas channel formation) occurs when

\[
A_f \geq A'_f S^{\alpha o}_v ,
\]

where \( S^{\alpha o}_v \) is the grain face area per unit volume.

Equations 32 and 33 do not account for local variations in fuel microstructure. To include these effects in the calculation of grain face channel formation, it is assumed that the local variations in fuel microstructure can be represented by the width \( \sigma_f \) of a distribution of \( A_f \) (Eq. 32) such that the probability fraction of grain face channel interlinkage \( P_{A_f} \) is given by

\[
P_{A_f} = \frac{1}{\sigma_f \sqrt{2 \pi}} \int_{x = A'_f S^{\alpha o}_v}^\infty \exp\left[\frac{(-x - A_f)^2}{2 \sigma_f^2}\right] dx.
\]

The width of the distribution in Eq. 34 is a function of erratic structural parameters, depending on local fuel condition and heterogeneity; in principle, it can be determined experimentally.

### 2.3 Intergranular Fission Gas: Grain Edges

The DART model for calculating the probability of long-range grain edge tunnel interconnection is based on the assumption that long-range interconnection is a function of the swelling of grain edge bubbles. This assumption is supported by experiment [6] and theory [7]. To account for local fluctuations in fuel microstructure and gas bubble morphology, the grain edge/porosity interlinkage fraction \( P_I \) is assumed to be a statistical distribution around an average value of the grain edge swelling \( B_{\text{edge}} \), thus,

\[
P_I = \frac{1}{\sigma_e \sqrt{2 \pi}} \int_{x = B_{\text{edge}}}^\infty \exp\left[\frac{-(x - B_{\text{edge}} - B_{\text{por}})^2}{2 \sigma_e^2}\right] dx,
\]

where \( B_{\text{edge}} = \frac{4 \pi \sigma_e}{3} \sum_{i=1}^{n_{\text{max}}} \left( R_i \right)_e C_i^e \) and \( \sigma_e \) is the width of a distribution of \( P_I \) that accounts for local fluctuations in fuel microstructure and gas bubble morphology (e.g., the ellipsoidal shape of grain edge bubbles). The value of the grain edge swelling at which long-range interconnection would take place if the fuel microstructure and gas bubble morphology were homogeneous is \( B_{\text{crit}} = 0.05 \); the fractional as-fabricated grain edge porosity is \( B_{\text{por}} \). Retained grain edge fission gas causes the deformation of grain edges (i.e., grain edge swelling of fission gas bubbles), and subsequent increased long-range interconnections of grain edge tunnels. This interconnection of
grain edge tunnels provides the pathways for fission gas release to triple points. The DART intergranular swelling model has been benchmarked against experimental results [8].

2.4 Intergranular Fission Gas: Dead-End Nodes

A striking aspect of the observed bubble population is that it is uniformly distributed and noninteracting. As discussed in Section 6 (see Fig. 7), the total number of bubbles in the second (large bubble) peak of the measured bimodal distribution remains relatively constant for all of the examined samples.

It is assume here that the large bubble population inhabits fixed sites. These sites are formed upon grain recrystallization and are associated with nodes that are formed by the intersection of grain edges within the subgrain boundary structure. Upon intersection, fission gas that collects along grain edges vents to these nodes, where it is trapped. Gas bubbles at these “dead-end” nodes grow as they continue to collect additional gas. If the grains are assumed to be cubes, and the dead-end nodes are taken to be grain corners formed by the intersection of six grain edges, the number of nodes per cubic centimeter $C_N$ is given by the inverse of the cube root of the grain diameter, i.e., $C_N = d^{-1/3}$.

2.5 Fission Gas Release

Contributions to fission gas release come from the venting of grain face gas into interconnected grain edge tunnels, and from the venting of previously trapped grain edge gas through newly interconnected tunnels. The fission gas release rate (atoms.m$^{-3}$.s$^{-1}$) is given by

$$\frac{df_{gr}}{dt} = \sum P_i C_i S_i P_i / h + \sum \frac{dP_i}{dt} C_i S_i.$$  

(36)

For a multinode calculation, the various gas release contributions from each individual node, given by Eq. 37, are summed up to obtain the total gas released during the time step $h$.

2.6 Options for Calculating Bubble Radii

Whereas intragranular bubbles are assumed to be spherical, the intergranular gas bubbles are assumed to be lenticular on the grain faces and ellipsoidal along the grain edges. Grain corner bubbles are assumed to be spherical. The diffusional growth of nonequilibrium intragranular bubbles is based on an analysis by Gruber [9]. The rate of change of the lattice i bubble radius is given by

$$\frac{dR_i}{dt} = D_i \left[ 1 - \exp\left( \frac{P_i - P_h - 2\gamma}{R_i} \right) \frac{\Omega}{kT} \right].$$  

(37)
where \( D_v \) is the vacancy diffusion coefficient, \( \Omega \) is the atomic volume, \( kT \) is the thermal energy, \( P_i^e \) is the internal gas pressure in the lattice i bubble, \( P_h \) is the external hydrostatic pressure, and \( \gamma \) is the surface energy. For ease in calculating, an approximation is utilized for the relaxation time; it is of the form

\[
R_i' = R_i'(0) + \left[ R_i^{eq} - R_i'(0) \right] \left[ 1 - e^{-t'/\tau_i'} \right],
\]

where \( \tau_i' \) is defined by the initial growth rate calculated with Eq. 37. In DART, \( R_i^{eq} \) is obtained by solving an approximate equation of state simultaneously with the capillarity relationship.

The diffusional growth of nonequilibrium intergranular bubbles is taken from Speight and Beere [10]. Accordingly, the rate of volume change of grain boundary pores is given by

\[
\frac{dV_i}{dt} = 2D_{gb} \frac{W}{kTL} \left( \frac{P_i - 2\gamma}{\rho_i} - P_h \right),
\]

where \( V_i \) is the volume of the pore, \( \rho_i \) is the radius of curvature of the pore, \( L \) is a function of the fraction of the grain boundary area occupied by pores, \( D_{gb} \) is the grain boundary diffusion coefficient, and \( W \) is the boundary thickness. DART provides three choices for the Xe equation of state: Van der Waals, Harrison’s extrapolation, and a perturbed hard-sphere model. The perturbed hard-sphere model also provides an equation of state for Kr and Ar.

### 3 DART Model for Irradiation-Induced Changes in Thermal Conductivity of Dispersion Fuel

The DART thermal conductivity model accounts for the dependence of thermal conductivity on both as-fabricated and irradiation-induced porosity. For dispersion fuels, two distinct classes of pores exist, namely, fission gas microbubbles generated within the \( \text{U}_3\text{Si}_2 \) fuel particles and as-fabricated voids contained within the aluminum matrix. Where pore geometry and physical properties are of prime importance, the analytical treatment of such pores is, however, similar. Pore geometry is defined by its size, shape, and orientation with respect to the direction of heat flow. Physical properties of importance are the emissivity of the pore surface and the thermal conductivity of the gas trapped within the pore. Figure 2 can be used to establish a geometric relationship for the thermal conductivity of a solid material containing a gas pore. The unit cell can be represented as a cube of solid material surrounding a spherical pore. The most important variable considered, and the one that appears in all theoretical models [11-13], is the volume porosity \( P \), defined as

\[
P = \frac{\text{Pore Volume}}{\text{Pore Volume} + \text{Volume of Solid}}.
\]
Assuming that heat flows in the y direction only, the effective thermal conductivity $k_e$ of the unit cell in the y direction is given by the expression

$$ k_e = P_c k_{ap} + (1 - P_c) k_s, $$

(41)

where $k_e =$ effective thermal conductivity, $k_s =$ thermal conductivity of solid material, $k_{ap} =$ apparent thermal conductivity of the pore tube, and $P_c$ is the fraction of the cross-sectional area of the x–z face of the unit cell that is occupied by the pore. To assess the conductance over the path length in the y direction, we define a pore tube length $L$ that considers both the pore and the solid material that occupies the remaining tube length. The apparent thermal conductance of the pore tube (pore plus solid material in the path length) can be evaluated by considering the thermal resistance of these two regions; it can be expressed as

$$ \frac{1}{k_{ap}} = \frac{P_L}{k_p} + \frac{1 - P_L}{k_s}, $$

(42)

Fig. 2. Representation of unit cell of a porous body for which effective thermal conductivity is assessed.
where \( P_L \) = fractional length of pore and \( k_p \) = effective pore thermal (gas conductivity plus radiation). By eliminating \( k_{dp} \) between Eqs. 41 and 42, we obtain the following expression [14,15]:

\[
\frac{k_s}{k_s} = 1 - P_c \left( 1 - \frac{k_s}{k_s} \right). \tag{43}
\]

In Eq. 43, the effect of volume porosity on thermal conductance is contained in the quantities \( P_c \) and \( P_L \). For the case of fission gas bubbles within U3Si2 fuel particles, it is assumed that the bubbles are spherical, with a radius \( R \), and uniformly spaced in the material. Under these assumptions, the following expressions apply:

\[
P_c = \pi \frac{R^2}{l^2} = \pi \phi^2 \frac{R^2}{\rho} \left( \frac{\rho}{\rho} \right)^{2/3}, \tag{44}
\]

\[
P_L = 2\frac{R}{l} = 2\phi \frac{R}{\rho} \left( \frac{\rho}{\rho} \right)^{1/3}, \tag{45}
\]

where \( \rho \) is the bubble density (bubbles/cc), \( l \) is the interbubble spacing, and \( \phi \) is a geometric factor that relates the average interbubble spacing to the bubble density, i.e., \( l = \phi \rho^{1/3} \). For uniformly spaced gas bubbles, \( \phi = 1.26 \).

The thermal conductivity of a pore filled with gas is given by the expression [16]

\[
k_p = k_g + 4 \varepsilon \sigma RT^3, \tag{46}
\]

where \( k_g \) = bulk thermal conductivity of the gas, \( \varepsilon \) = emissivity, \( \sigma \) = Stefan–Boltzmann constant, and \( T \) = temperature.

For the size pores and range of temperatures under consideration, the second term in Eq. 46, representing radiative heat transfer, can be neglected. Thus, Eq. 43, when applied to gas bubbles, reduces to the form

\[
k_p / k_f = 1 - \left[ \frac{\pi R^2}{\rho} \left( \frac{\rho}{\rho} \right)^{2/3} \right] \left[ 1 - k_g / (2k_f R \rho^{1/3}) \right], \tag{47}
\]

where \( k_p \) = effective thermal conductivity of fuel particles that contain fission gas, and \( k_f \) = thermal conductivity of bulk U3Si2.

Equation 47 can be written in the form

\[
k_p / k_f = 1 - \pi \left( \frac{R}{l} \right)^2 + \frac{\pi k_g}{2k_f} \left( \frac{R}{l} \right), \tag{48}
\]
where the ratio of the bubble radius \( R_g \) to interbubble spacing \( l_g \) can be expressed as

\[
R_g / l_g = \phi^{-1} R_g \rho_p^{1/3} = \phi^{-1} \sum_\alpha \sum_i R_i^\alpha \left( C_i^\alpha \right)^{1/3},
\]
where \( \alpha \) sums over the various morphological fuel regions (e.g., bulk, dislocations, faces, and edges) and \( i \) sums over the bubble size distribution.

The geometric condition for bubble interconnection is given by \( l_g = 2R_g \). Equations 47 and 48 represent expressions for \( k_g^i / k_f \) in terms of average properties of the fission gas bubble size distribution that evolves within the \( \text{U}_3\text{Si}_2 \) fuel particles during irradiation. The expression for \( k_g \) that is used to evaluate Eqs. 47 and 48, as given in Ref. 13, is

\[
k_g(\text{xenon}) = \left( 4.0288 \times 10^5 \right) T^{0.872} \text{ (W / mK)}. \tag{49}
\]

To include the effects of both as-fabricated and irradiation-induced porosity on the thermal conductivity of \( \text{U}_3\text{Si}_2 \) particles dispersed in an aluminum matrix, successive applications of a mixing formula of the form given by Eq. 48 have been utilized. For example, the thermal conductivity of aluminum containing a dispersion of \( \text{U}_3\text{Si}_2 \) particles (i.e., containing fission gas) with no as-fabricated porosity is given by

\[
k_c^f = 1 - \left( \pi R_f^2 \rho_f \right)^{2/3} \left[ 1 - k_c^g / \left( 2k_f R_f \rho_f^{1/3} \right) \right], \tag{50}
\]
where \( k_c^f \) = effective thermal conductivity of dispersion with no as-fabricated porosity, \( R_f \) = radius of particle, \( k_c^g \) = effective thermal conductivity of \( \text{U}_3\text{Si}_2 \) particles containing fission gas (given by Eq. 48), \( \rho_f \) = density of \( \text{U}_3\text{Si}_2 \) particles, and \( k_f \) = thermal conductivity of pure aluminum.

If as-fabricated porosity is now introduced into the material,

\[
\frac{k_c^m}{k_c^f} = 1 - \pi R_p^2 \rho_p^{2/3}, \tag{51}
\]
where \( k_c^m \) = thermal conductivity of dispersion, containing both as-fabricated and irradiation-induced porosity; \( R_p \) = radius of as-fabricated pores; and \( \rho_p \) = density of as-fabricated porosity.

In deriving Eq. 51, the thermal conductivity of an as-fabricated pore has been assumed to be zero. For particles dispersed in aluminum and for the distribution of as-fabricated porosity, \( \varphi = 1 \). Utilizing Eqs. 50 and 51, we can express \( k_c^m \) as

\[
k_c^m = k_a \left[ Z_1 + Z_2 F_f^{2/3} + Z_3 \left( k_c^f / k_a \right) F_f^{1/3} \left( 1 + Z_2 F_p^{2/3} \right) \right] + Z_2 F_p^{1/3} + Z_4 \left( F_f F_p \right)^{2/3}, \tag{52}
\]
where the fuel and pore volume fractions $F_f$ and $F_p$ are given by

$$F_f = \frac{4}{3} \pi R_f^3 \rho_f,$$  \hspace{1cm} (53)

$$F_p = \frac{4}{3} \pi R_p^3 \rho_p.$$ \hspace{1cm} (54)

and where $Z_1$–$Z_4$ are constants:

$$Z_1 = 1$$
$$Z_2 = -\pi (3/4\pi)^{3/4}$$
$$Z_3 = \pi / 2 (3/4\pi)^{3/4}$$
$$Z_4 = \pi^2 (3/4\pi)^{3/4}$$

Implicit in the derivation of Eq. 52 is the assumption of a homogeneous distribution of spherical particles (i.e., fission gas, as-fabricated pores, U3Si2 particles) within the respective host materials. To quantify the effects of deviations from this idealized geometry, such as nonspherical pores and particles, as-fabricated and irradiation-induced pores preferentially distributed along the particle/matrix interface (e.g., fission gas released from the grain interior can collect at the particle/matrix interface), the constant $Z_4$ was determined by regression analysis, based on unirradiated dispersion fuel data from Ref. 17, shown in Table 2 to be:

$$Z_4 = 0.6521.$$ 

Equation 52 is valid as long as the matrix aluminum is the continuous media. An analogous expression to Eq. 52 can be derived for cases where the fuel is the continuous media. This case is not considered here. In addition, $Z_4$ has been determined based on a comparison with plate-fuel conductivity measurements in the transverse (thickness) direction. As such, Eq. 52 is valid for thermal conductivity calculations in the transverse direction only. An extension of Eq. 52 to conductivity calculations in the longitudinal direction can be obtained by an appropriate utilization of measured anisotropy in U3Si2 ground-powder-based fuel plates.

The results of this analysis are shown in Table 2 and Figs. 3 and 4. Figure 3 shows the results of the regression analysis performed with Eq. 52 and with the data listed in Table 2. Figure 4 shows the thermal conductivity data and the results calculated for thermal conductivity with Eq. 52, plotted against the volume fraction of fuel plus voids. Figure 5 shows the DART-calculated thermal conductivity for U3Si fuel as a function of irradiation-induced porosity, and measured values [18] for irradiated and subsequently annealed bulk U3Si. The calculations shown in Fig. 5 were made utilizing $\phi = 1.33$, or a distribution closely approximating a distribution of equally spaced bubbles (given by $\phi = 1.26$). The effect of swelling porosity on the thermal conductivity of irradiated U3Si was deduced from electrical conductivity measurements on samples with pore volume fractions of 0.01-0.27. The
Table 2. Results of regression analysis from Eq. 52 and data from Ref. 17

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</tbody>
</table>
Equation 52 provides a physically based expression for the evolution of thermal conductivity in irradiated dispersion fuels. As such, even though the geometric constant \( Z_4 \) was determined from unirradiated data, Eq. 52 embodies physically realistic functional dependencies, e.g., the dependence of thermal conductivity on fuel and matrix volume fractions and on as-fabricated and irradiation-induced porosity, which allow for a reasonable extrapolation to irradiated materials.
Fig. 4. Thermal conductivity obtained from Eq. 52 and from data listed in Table 2, as a function of volume fraction of fuel + voids

4 DART Model for Mechanical Behavior of Aluminum Dispersion Fuels

During irradiation, the fuel rods, plates, and tubes increase in diameter (thickness) as a result of swelling of the fuel core. The swelling is a direct result of the accumulation of fission-product elements in the fuel. Although this accumulation is, in the first order, directly proportional to the burnup of $^{235}$U, the resultant swelling is also
Fig. 5. DART-calculated and measured (deduced from electrical conductivity measurements) change in thermal conductivity for U₃Si fuel as a function of irradiation-induced porosity in irradiated and subsequently annealed bulk U₃Si.

affected by several microstructural changes that occur in the fuel core during irradiation. An important factor in reducing the overall amount of net swelling is radiation-enhanced sintering of fabrication voids. In U₃O₈, this effect was first demonstrated by Reinke [2], and later confirmed by an experiment Martin et al. [3], in which U₃O₈ dispersion fuel made with depleted uranium was irradiated. The fabrication voids within the U₃O₈ particles, as well as cracks and gaps resulting from fabrication, were found to have sintered to spherical (or elliptical) cavities after irradiation. It is well established that an increase in dispersant loading also increases fabrication voids.
Inasmuch as a fraction of the sintered porosity can be taken up by the swelling fuel, the fabrication voids can substantially reduce the net fuel swelling.

Except for the calculation of thermal conductivity of the dispersion material described in Section 3, DART does not currently model the thermal performance of the fuel element. Thus, fuel temperature and linear power (i.e., fission rate), are required input into the analysis. In a fully coupled mode, the calculation of fuel deformation, fuel swelling, and thermal conductivity is interactive with the thermal analysis.

No matrix swelling is assumed to occur during reactor operation. This assumption is based on the relative swelling rates of the matrix and the fuel, from which it can be seen that fuel swelling is several orders of magnitude greater than matrix swelling. Inclusion of matrix swelling would lead to a slight increase in predicted rod diameter or plate/tube thickness.

The fuel particles are assumed to be identical in size and to have a uniform spherical shape. The actual fuel particles vary in size and are irregular in shape. However, because irregular particle shapes are difficult to handle mathematically, and because the orientation of the particles is random, an assumption of uniform overall behavior seems reasonable. In addition, particle-particle interactions are ignored. If particle-particle interactions are included, a greater degree of swelling than predicted by the model will occur.

No change in yield stress with fluence is considered. Evaluation of available data indicates that the change in yield stress due to fluence is negligible. Inclusion of this phenomenon will slightly reduce deformation estimates. In addition, the effects of irradiation-enhanced creep and irradiation hardening are not considered. Consideration of these phenomena would require time-dependent deformation analysis, which would add significantly to the complexity and execution efficiency of the DART code. The effects of irradiation-enhanced creep and hardening are accounted for by the inclusion of a phenomenological factor that multiplies the aluminum yield strength. The value of this factor depends on the geometry of the element, i.e., plate or rod.

The DART mechanical analysis addresses the mechanical behavior of dispersion fuel plates, tubes, and fuel rods. The model examines a system of spherical fuel particles surrounded by a large spherical shell of matrix material bonded to an outer shell of aluminum cladding. This approach treats the inner sphere as an elastically deforming body and the spherical shell as perfectly plastic [4]. The DART swelling models provide the driving force for mechanical deformation. The model is derived directly from the equations of equilibrium, compatibility, strain displacement, and the constitutive equations (stress-strain relationships) coupled with the assumption of incompressibility of plastic strains. The boundary conditions assume finite radial stresses at the center of the inner sphere, no discontinuity in the radial stress at the fuel/matrix interface, and no pressure on the outer surface of the spherical shell. It is also assumed that thermal expansion and swelling are not functions of radial position and that the outer radius of the spherical shell approaches infinity. This approach to thermal and swelling strains is based on calculations that indicate the temperature changes across a fuel plate or rod are small.
The model consists of the stress analysis of a hard sphere of radius $a$, assumed to behave elastically, surrounded by a spherical shell with outer radius $b$ of a softer material that is assumed to behave in a perfectly plastic manner ($b \gg a$). This plastic behavior is assumed to extend out to a plastic radius $r_c$ such that $a < r_c < b$. This procedure yields an equation for the interfacial pressure (radial stress) at the fuel/matrix interface in terms of fuel particle swelling and plastic deformation in the matrix (i.e., as the interfacial pressure increases, plastic flow is induced in the matrix out to some radius beyond which only elastic deformation occurs). Based on the results of a general solution to the problem, an approximation is introduced that avoids the simultaneous solution of the interfacial pressure and the radius of plastic deformation. For positive interface pressure $P_t$,

$$P_t = 2 \left[ \frac{1}{3} + \ln \left( \frac{r_c}{a} \right) \right] S_y,$$

(55)

where $S_y$ is the yield stress determined from the von Mises criterion for plastic flow. The results of the general solution indicate that $r_c$ increases rapidly to include most of the matrix aluminum. Thus, it appears reasonable to make the approximation that the fuel volume fraction is given by

$$\frac{V_f^t + \Delta V^t}{V_0^c} = \frac{4}{3} \pi a^3 \frac{4}{3} \pi r_c^3 = \left( \frac{a}{r_c} \right)^3,$$

(56)

where $V_f^t$ is the as-fabricated fuel volume fraction in the core and $\frac{\Delta V^t}{V_0^c}$ is the increase in fuel volume fraction due to processes such as as-fabricated pore closure and fuel particle swelling. Thus, from Eqs. 55 and 56,

$$P_h = P_t = 2 \left[ 1 - \ln \left( \frac{V_f^t + \Delta V^t}{V_0^c} \right) \right] \beta S_y,$$

(57)

where $P_t$ has been identified with the hydrostatic stress within the fuel particle $P_h$, and $\beta$ is a phenomenological factor (discussed above) that has been introduced to account for the effects of irradiation (e.g., irradiation-enhanced creep and hardening).

5 DART Model for Aluminum Silicide Fuel Reaction

$U_3Si_2$ reacts exothermally with aluminum to form the reaction product $U(Al, Si)_3$, a notation for $UA_{1.3}$ in which Si has been substituted for some of the aluminum atoms. Below the melting temperature, the reaction is diffusion controlled and proceeds quite slowly. Irradiation enhances diffusion rates. The interaction depth $y$ (μm) fits an
irradiation-enhanced diffusion correlation developed with irradiation data from the Oak Ridge Research Reactor (ORR) [19] and with irradiation data from the High-Flux Isotope Reactor (HFIR) [20]

\[ y = \left( D_0^{ie} \exp\left(-\frac{Q^{ie}}{kT}\right) \right)^{0.5}, \]  

where \( D_0^{ie} = 3.74 \times 10^{-17} \, \mu m^2/s \) and \( Q^{ie} = 7182 \) calories. At higher temperatures, thermally activated diffusion becomes measurable and the correlation developed is

\[ y = \left( D_0^{ie} \exp\left(-\frac{Q^{ie}}{kT}\right) + D_0^T \exp\left(-\frac{Q^T}{kT}\right) \right)^{0.5}, \]  

where \( D_0^T = 9.27 \times 10^{20} \, \mu m^2/s \), and \( Q^T = 83,357 \) calories.

6 DART Theory of Irradiation-Induced Recrystallization

6.1 Introduction

Experimental observations on low-temperature swelling of uranium silicide dispersion fuels (U3Si2) irradiated in the ORR have shown that the growth of fission gas bubbles is affected by fission rate [21-23]. The swelling of U3Si2 exhibits a distinct knee that shifts to a higher fission density with increased fission rate. Below the knee, no gas bubbles can be detected by scanning electron microscopy (SEM); if present, they must be below the resolution limit of the instrument, i.e., smaller than \( \approx 0.04 \, \mu m \) in diameter. Just at the knee, gas bubbles are first seen to form in a heterogeneous fashion. Above the knee, the bubble population rapidly multiplies and the bubble size increases with fission density. Bubble size distributions are clearly bimodal and bubble morphology of samples that have similar volume increase, albeit at different fission densities, is similar.

The bimodal distributions persist to very high fission densities for HEU at 9 and \( 16 \times 10^{27} \) fissions m\(^{-3}\). The second peak in the distribution shifts to a larger diameter as the bubbles acquire more fission gas. However, the total number of bubbles in the second part of the distribution remains relatively constant \( \approx 3 \times 10^{18} \, m^{-3} \) for all of the examined samples. This is interpreted to mean that the larger bubbles nucleate and grow on a fixed number of sites.
The bubble morphology retains its stable character up to the highest fission densities, i.e., bubble size and spacing are rather uniform, with no sign of bubble interlinking. The bubbles also form patterns suggestive of association with an underlying microstructural feature.

State-of-the-art models for fission gas behavior do not predict dependence of bubble growth on fission rate, and a bubble population with the observed bubble diameters can only be calculated [24] if microstructural features such as grain boundaries or dislocation networks are introduced. The original grain size of the fuel is large, i.e., approximately that of the fuel particles. Therefore, very few, if any, grain boundaries exist in the as-fabricated fuel. Indeed, the bubble patterns suggest bubbles associated with grain-boundarylike features, as discussed below, and there is evidence in the literature to support this interpretation.

Grain "subdivision" was observed by Bleiberg et al. [25] and Lambert [26] in uranium dioxide. Bleiberg et al. [25] showed that original 10–20-μm grains subdivided into unit sizes of <1 μm at a dose of ~2 \times 10^{21} \text{fissions m}^{-3} while retaining their crystalline structure. UO₂ swelling also increased in rate at this point (i.e., a knee in the UO₂ swelling curve) and the bubble morphology is similar to that observed in U₃Si₂. More recently, other investigators have observed that the peripheral region of light water reactor (LWR) fuel pellets reveals an increasingly porous microstructure with burnup [27-31]. At burnups above ~45 GWd/t U, a porous outer ring, with a typical thickness of 100-200 μm, is formed. Examination of this “rim effect” shows an extremely fine-grained structure, apparently formed by recrystallization of the original, much larger, UO₂ grains. Further evidence of this phenomenon has been found in ion bombardment studies on crystalline U₃Si [32]. In these studies, recrystallized grain sizes of ~100 Å were observed directly in a high-voltage electron microscope. It seems plausible that formation of small grains also occurs in U₃Si₂.

Evidence for a restructuring of U₃Si₂ that is undergoing high doses of low-temperature irradiation indicates that a subgrainlike structure exists in U₃Si₂ above the knee [23]. This preliminary observation, as well as observations from UO₂ irradiations and the ion bombardment studies mentioned above, leads us to speculate that at high burnup (corresponding to the knee in the swelling curve), a dense network of subgrain boundaries forms in these materials. Upon this network, gas bubbles nucleate and then grow at an accelerated rate relative to that in the bulk material.

The observation in U₃Si₂ that gas bubble swelling depends on fission rate has led to the theoretical formulation presented in Section 6.2, wherein the fission–induced stored energy in the material is concentrated on a network of recrystallization nuclei; this concentration diminishes with dose because of interaction with radiation-produced defects (i.e., vacancy–impurity pairs). Recrystallization starts when the energy per nucleus is high enough to offset creation of grain boundary surfaces by creating strain–free volumes, with a resultant net decrease in the free energy of the material. In Sections 6.3 and 6.4, the theory is applied, within the context of the DART mechanistic treatment of gas bubble behavior, to the interpretation of swelling in U₃Si₂. In Section 6.4, the theory is used to calculate UO₂ swelling, as well as to provide an interpretation of the rim effect in UO₂. Finally, the conclusions are summarized in Section 6.5.
6.2 Model for Grain Recrystallization

The recrystallization model proposed in this paper is derived from recrystallization in heavily cold-worked solids [33-35]. During deformation of metals, dislocations interact and tend to cluster into arrangements of high dislocation density that are separated by regions with relatively low dislocation density. Clustering of dislocations is a general observation in deformed single-crystal and polycrystalline metals and alloys [35-37]; typical dislocation configurations are dislocation tangles, two-dimensional dislocation boundaries (or walls), and three-dimensional dislocation cell structures. The different dislocation configurations derive from energy minimization, where glide–dislocation configurations increasingly approach the minimum energy per unit length of dislocation line as dislocation density, and hence interaction between dislocations, increases.

The concept that recrystallization ion nuclei [38] could originate from small preformed “strain-free” blocks in a crystal within the microstructure of a deformed state was proposed by Cahn [39] and Beck [40]. These strain-free blocks within a crystal are formed by the spatial rearrangement of dislocations into lower-energy arrays by polygonization. This model for recrystallization nuclei was further modified by Cottrell [41], who suggested that an additional need for the formation of a successful recrystallization nucleus was likely to be the development of a highly mobile bounding interface. These ideas have led to the low-angle boundary migration model, in which a viable recrystallization nucleus has a size advantage over the neighboring subgrain structure and is surrounded, at least in part, by a highly mobile interface. The mobility of this interface is affected by impurity atoms, which in an irradiated fuel are amply provided by fission products.

Recent transmission electron microscopy examination of the porous region of high–burnup LWR fuel has revealed networks on dislocations [29,30], and the cell size of these subgrain networks corresponds to the grain size of the rim material. An alternative mechanism to low–angle boundary migration, and a mechanism by which a subgrain of the above type can be formed, is the process known as subgrain coalescence [34]. In this process, the constituent dislocations of a low-angle boundary that separate two subgrains migrate along the plane of the boundary and are incorporated into the structure of surrounding low-angle boundaries. As a result, the low-angle boundary disappears and the two originally separated subgrains are joined as one much larger subgrain. The driving force for subgrain coalescence originates in the reduction in stored energy that accompanies the transfer of a dislocation from one low-angle boundary to another of higher angle; as a result, the interface accepting the dislocations will increase in misorientation. The increase in size of subgrains that are agglomerating by subgrain coalescence is obviously a favorable step toward the formation of a recrystallization nucleus, as is the accompanying increase in misorientation of a segment of the interface that surrounds the coalesced region.

Relatively few published reports have examined the phenomenon of radiation–enhanced recrystallization [42,43]. In a study of the microstructure of two copper alloys after heavy ion irradiation and thermal annealing [43], it was observed that some type of solute segregation/precipitation mechanism caused the pinning of subgrain boundaries in one of the alloys in the damage region. This alloy essentially retained the small polygonized subgrain structure in the damage region after irradiation at 773 K, while the unirradiated region of the crystal completely recrystallized. This is in contrast to the other alloy, which displayed no evidence of subgrain–boundary
pinning, completely recrystallized, and showed no discernible difference between irradiated and nonirradiated regions.

The model for radiation-induced recrystallization described below is based, in part, on the following assumptions:

- A cellular dislocation structure evolves relatively early in the irradiation period.
- Impurities formed during fissioning of the material diffuse to cell walls as vacancy/impurity complexes.
- The impurities effectively pin the wall, i.e., dislocation movement to and from the wall is retarded.
- Not all cell walls are uniformly affected by impurities; the walls that contain no impurities continued to undergo subgrain coalescence, which results in viable recrystallization nuclei.

Based on the above discussion, it is assumed that there exist a number $C_S$ of recrystallization nuclei per unit volume of material. We think that these nuclei form relatively early in the irradiation period at low values of stored energy and that they are associated with microstructural features such as subgrain-boundary triple points or walls of cellular dislocation structures. Recrystallization nuclei act as sinks for irradiation-produced defects. As the irradiation proceeds, the nuclei are eliminated by interaction with vacancy-solute pairs. In other words, the concentration of impurities reduces the mobility of the interface. Many potential solute atoms are produced during fission, e.g., gas atoms and rare earths. Thus, the available stored energy is concentrated on fewer and fewer nuclei (one can consider that the nuclei are holes in the material and that they act as stress concentrators), with a resultant increase in average energy per nucleus. Recrystallization is induced when the energy per nucleus is high enough to offset the creation of a grain boundary surface by creating a of strain-free volume, with a resultant net decrease in the free energy of the material.

It is assumed that the solute atoms require significant energy to become part of a dumbbell-shaped interstitial [44] and therefore do not migrate via an interstitial mechanism. It is further assumed that long-range diffusion of vacancy-solute pairs to the immobile nuclei eliminates the nuclei at a rate given by

$$\frac{dc_s}{dt} = -K_{sm} c_s c_m,$$  \hfill (60)

where $c_m$ is the pair concentration and $K_{sm}$, the reaction rate for the immobilization of recrystallization nuclei by vacancy-solute pairs, is defined as

$$K_{sm} = 4\pi r_{sm} D_{vi} / \Omega,$$  \hfill (61)
where \( r_{\text{sm}} \) is the annihilation radius of a recrystallization nucleus/vacancy-solute pair, \( D_{\text{v}} \) is the diffusivity of the vacancy-solute pair, and \( \Omega \) is the atomic volume. \( D_{\text{v}} \) consists of thermal and athermal components, i.e.,

\[
D_{\text{v}} = a^2 V_0 e^{-\epsilon/v_i/kT} + \chi \sqrt{\phi}.
\]

where \( a \) is the lattice parameter, \( V_0 \) is the vibration frequency factor for vacancies, \( \epsilon \) is the migration energy for a vacancy-solute pair, \( \xi \) is a preexponential factor that accounts for deviations from diffusion in a pure solvent, \( \phi \) is the fission rate (fissions/cm\(^3\)/s), \( \chi \) is a factor related to the strength of athermal diffusion, \( k \) is Boltzman's constant, and \( T \) is the absolute temperature.

The concentration of vacancy-solute pairs \( c_m \) is given by

\[
\frac{\partial c_m}{\partial t} = 12(K + 7\omega_0 c_v) c_i - c_m (\alpha c_i + 7\omega_\lambda).
\]

where \( K \) is the damage rate in displacements per atom per second; \( c_v \) and \( c_i \) are the concentrations of vacancies and interstitials, respectively; \( c_i \) is the solute concentration; \( \omega_\lambda \) and \( \omega_\lambda \) are the jump rates of vacancies away from and toward nearest-neighbor nuclei of solute atoms; and \( \alpha \) is the recombination coefficient given by

\[
\alpha = 12(\omega_0 + \omega_\lambda).
\]

where \( \omega_0 \) and \( \omega_\lambda \) are the jump frequencies of vacancies and interstitials, respectively, unperturbed by the presence of a solute atom.

If we assume that the concentration of vacancy-solute pairs is in steady state with the concentration of vacancies, interstitials, and solute atoms (i.e., \( \partial c_m/\partial t = 0 \)), we obtain

\[
12(K + 7\omega_\lambda) c_i = c_m (\alpha c_i + 7\omega_\lambda).
\]

This expression for the steady-state concentration of vacancy-solute pairs consists of the direct production of solute-defect pairs by irradiation (first term on the left side of Eq. 65), pair production due to interaction between vacancies and solute atoms (second term on the left side of Eq. 65), the loss of pairs through the interaction between vacancy-solute pairs and interstitials (first term on the right side of Eq. 65), and the loss of pairs due to dissociation (second term on right side of Eq. 65). In most cases, direct production of solute-defect pairs by irradiation should have only a small influence on the proportion of vacancies and interstitials trapped in vacancy-solute pairs. However, if the temperature is low, the dose rate is high, and the point-defect-solute binding energy is large, then recombination will be important. For the more general case, where recombination is important, the
equation for $c_m$ is obtained from Eq. 65 (neglecting the effect of direct production of vacancy-solute pairs by irradiation, i.e., the first term within parentheses on the right side of Eq. 65) as

$$c_m = \frac{84\omega_i^* c_v c_i}{(\alpha c_i + 7\omega_i^*)}.$$  

\hfill (66)

An equilibrium concentration of mobile defects is reached relatively early in the irradiation. Studies by Rest [45], who used a chemical rate theory of solute segregation for a solute concentration that depends on the fission (or dpa) rate, indicate that the above result (Eq. 66) for a fixed solute concentration is approximately true for the irradiation conditions of interest in this paper. In this case, the relevant solute concentration is that which is in dynamic solution within the fuel matrix and is thus able to participate in vacancy-solute pair formation. The equilibrium concentration of mobile point defects within the bulk material, $c_v$ and $c_i$, can be determined from the rate equations that describe point-defect behavior, which, for negligible bulk diffusion (e.g., to a surface) are given by

$$\frac{\partial c_i}{\partial t} = K_v c_v c_i - K_{sv} s_i c_v,$$  

\hfill (67)

and

$$\frac{\partial c_v}{\partial t} = K_v c_v c_i - K_{si} s_i c_i,$$  

\hfill (68)

where $K_v$, $K_{sv}$, and $K_{si}$ are the rate coefficients for mutual recombination and for the annihilation of vacancies and interstitials at sinks. Here the assumption is made that the overall effect of solute concentration on the steady-state concentration of point defects is small. The sinks, which occupy time-independent fractions of the lattice nuclei, are assumed to be inexhaustible and randomly distributed. The rate coefficients are

$$K_v = 4\pi r_v (D_v + D_i) / \Omega \equiv 4\pi r_v D_i / \Omega,$$  

\hfill (69)

$$K_{sv} = 4\pi r_s D_v / \Omega,$$  

\hfill (70)

$$K_{si} = 4\pi r_i D_i / \Omega.$$  

\hfill (71)

Here, $r_v$ is the radius of the recombination volume; $r_{sv}$ and $r_{si}$ are annihilation radii and depend on the type of sink, e.g., dislocation line, jog, or microvoid; and $D_v$ and $D_i$ are the random-walk diffusion coefficients of vacancies and interstitials given by

$$D_v = \xi a^2 \omega_0^*.$$  

\hfill (72)
\[ D_1 = \frac{2}{3} \xi a^2 \omega_0^i, \]  

(73)

where and \( \xi \) is a preexponential factor that accounts for deviations from diffusion in a pure solvent,

\[ \omega_0^i = v_i e^{-E_i/kT}, \]  

(74)

and

\[ \omega_0^i = v_i e^{-E_i/kT}, \]  

(75)

where \( E_v, E_i \) and \( v_v, v_i \) are the migration energies and vibration–frequency factors for vacancies and interstitials, respectively.

When we use Eqs. 2, 5, and 6 in Eq. 1, and because \( \omega_0^i \ll \omega_0^i \), we obtain

\[ \frac{1}{c_s} \frac{dc_s}{dt} = \frac{28\pi r_m c_i D_1 \omega_0^i c_s}{\Omega(c_i + 7\omega_0^v / 12\omega_0^i)\omega_0^i}. \]  

(76)

The concentration of viable recrystallization nuclei, which results from the integration of Eq. 76, is quite different from that given by classical nucleation theory in that the concentration decreases with fluence instead of increasing with irradiation, until the nucleation barrier is surmounted and the higher energy state of the crystal forms. In the present case, the nuclei are formed early in the irradiation by the damage process at relatively low values of strain energy. As the irradiation proceeds and the nuclei are eliminated by interaction with the vacancy-solute pairs, the available stored energy is concentrated on fewer and fewer nuclei, thus increasing the energy per nucleus. For a given value of stored energy \( E_s \), nucleation of a new crystal of material results in a net change in free energy \( \Delta G \), given by

\[ \Delta G = -E_s V + 8\pi \gamma \left( \frac{3}{4\pi} V^{2/3} \right). \]  

(77)

where \( V \) is the volume of the newly nucleated crystal (a spherical crystal shape has been assumed for simplicity), and \( \gamma \) is the surface energy density. The first term on the right side of Eq. 77 is the decrease in free energy due to the creation of a strain-free volume \( V \), and the second term is the work required to create the boundary surface. The maximum value of \( \Delta G \) occurs at a value of \( V \) given by

\[ V_{\text{max}} = \frac{4\pi}{3} \left( \frac{4\gamma}{E_s} \right)^{3}. \]  

(78)
where the value of $\Delta G$ at $V_{\text{max}}$ is

$$
(\Delta G)_{\text{max}} = \frac{128\pi \gamma^3}{3 E_s^2}.
$$

(79)

From Eqs. 78 and 79, we see that as $E_s$ increases, $V_{\text{max}}$ and $(\Delta G)_{\text{max}}$ shift to smaller values. When $(\Delta G)_{\text{max}}$ decreases to a value approximately equal to the thermal energy $kT$, a relatively small energy fluctuation can allow the system to jump over the energy barrier, and a new recrystallized grain of material will be created. As $(\Delta G)_{\text{max}}$ approaches $kT$, the rate of change in the stored energy (which, as discussed above, is taken to be concentrated on the network $cs$), of the nuclei with respect to a change in $cs$ is given by Boltzman's law, i.e.,

$$
\frac{dE_s}{dc_s} = -\frac{kT}{c_s}.
$$

(80)

Equation 76 provides a solution for $cs$ that is based on a kinetic analysis, whereas the equation for $cs$ provided by Eq. 80 is based on a thermodynamic analysis. By equating $cs$ obtained from Eq. 76 to the value of $cs$ determined from Eq. 80, where a relatively small energy fluctuation can allow the system to jump over the energy barrier and cause the creation of a relatively defect-free crystal of material, we obtain a relationship for the value of the fission density ($m^{-3}$) $FDX$ at which recrystallization will occur, i.e.,

$$
FDX = \frac{E_{sf} \Omega \left( c_s + 7 \omega_s^1 / 12 \omega_0^1 \right) \omega_0^1}{28\pi r_{sm} kT c_s D v \omega_s^1 c_v}.
$$

(81)

where $\dot{F} = BK$ (B is a conversion factor), $E_{sf} = E_s + E_f$, and $E_f$ is the formation energy of a viable nucleus. Equation 81 can be simplified to

$$
FDX = \frac{E_{sf} \left[ 9 \Omega \dot{F} + 7a \sqrt{\frac{\pi B_r}{\nu}} \xi \Omega \dot{F} e^{-\frac{(\varepsilon - \varepsilon_{\text{f}})/kT}{2}} \right]}{168 \pi r_{sm} kT c_s \left( \xi \nu \dot{F} + \varepsilon_{\text{f}} / kT + \chi \dot{F} \right)}.
$$

(82)

34
Equation 81 or 82 is the basic result of this generalized analysis.

Before proceeding, we must establish criteria to determine when mutual recombination of point defects dominates annihilation at internal sinks, and when the loss of vacancy-impurity pairs by recombination with interstitials dominates pair loss due to dissociation (i.e., vacancy emission). If the assumption is made that $s_v = s_i$, the solution to Eqs. 67 and 68 is given by

$$D_i c_v = D_v c_i = \left( \frac{K}{f_0^{1/2}} \right) \left[ (1 + Q)^{1/2} - Q^{1/2} \right].$$

(83)

where

$$Q = \frac{s_i^2 K_{s_i} D_v}{4KK',D_i},$$

(84)

and

$$f_0 = \frac{KK',D_i}{D_i D_v}.$$

(85)

For values of $K$ above a minimum value $K_{\text{min}}$ (e.g., those for ORR and HFIR irradiation conditions), $Q < 1$ and corresponds to mutual recombination that is dominant over annihilation at internal sinks, and leads to

$$D_i c_v = D_v c_i = \left( \frac{KD_v}{K_{i_v}} \right)^{1/2}.$$

(86)

At higher temperatures, $Q \gg 1$ and corresponds to annihilation at internal sinks dominant over mutual recombination, leading to

$$D_i c_v = D_v c_i = \frac{K D_v}{s_i K_{s_i}} = \frac{K D_v}{s_i K_{s_v}}.$$

(87)

Correspondingly, for vacancy-impurity pairs, if the temperature is low, dose rate high, and point-defect-impurity binding energy large, then $\alpha c_i \gg 7 \omega_i^v$ and the loss of pairs due to recombination will be important. In this case, Eq. 81 becomes

$$FDX = \frac{E_{st} \sqrt{f \omega_i c_v \Omega}}{28\pi \tau_{\text{sm}} k T c_i \chi \omega_i c_v}.$$

(88)
where, for these conditions, it is reasonable to assume (as will be quantified below) that athermal diffusion of the pair dominates over thermal diffusion, i.e., \( \xi a^2 v_e e^{-\epsilon_v/kT} < \chi \sqrt{f} \). On the other hand, if the temperature is high enough (e.g., as will be shown later for \( T \) in the intermediate-to-high temperature regime), the dissociation rates of the vacancy-impurity pairs are much higher than the loss rate of the vacancy in a vacancy-impurity pair by recombination with interstitials, and Eq. 81 becomes

\[
F_{DX} = \frac{E_F \dot{\Omega} \omega^*}{48\pi \rho_{sm} k T \xi a^2 v_e^* \omega^* c^v}, \tag{89}
\]

where, for these conditions, it is reasonable to assume (as will be quantified below) that thermal diffusion of the pair dominates athermal diffusion, i.e., \( \xi a^2 v_e e^{-\epsilon_v/kT} > \chi \sqrt{f} \).

Table 3. Values of various properties used in calculating recrystallization dose for U\(_3\)Si\(_2\)

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>( v_v )</td>
<td>( 5 \times 10^{13} \text{ s}^{-1} )</td>
<td>46</td>
</tr>
<tr>
<td>( \epsilon_v )</td>
<td>( 0.9 \text{ eV} )</td>
<td>47</td>
</tr>
<tr>
<td>( \epsilon_v )</td>
<td>( 1.3 \text{ eV} )</td>
<td>Present Calculations</td>
</tr>
<tr>
<td>( \chi )</td>
<td>( 6 \times 10^{-24} \text{ cm}^{7/2} \text{ s}^{-1/2} )</td>
<td>Present Calculations</td>
</tr>
<tr>
<td>( E_{sf} )</td>
<td>( 2.0 \text{ eV} )</td>
<td>Present Calculations</td>
</tr>
<tr>
<td>( c_1 )</td>
<td>( 1 \times 10^{-6} )</td>
<td>Present Calculations</td>
</tr>
<tr>
<td>( r_{IV} )</td>
<td>( 2 \times 10^{-10} \text{ m} )</td>
<td>48</td>
</tr>
<tr>
<td>( r_{sm} )</td>
<td>( 3 \times 10^{-10} \text{ m} )</td>
<td>48</td>
</tr>
<tr>
<td>( \xi )</td>
<td>( 0.1 )</td>
<td>Present Calculations</td>
</tr>
</tbody>
</table>
6.3 Recrystallization and Swelling in U₃Si₂

Figure 6 shows calculated values and measured data from Ref 23; the recrystallization dose for U₃Si₂ was calculated by solving Eq. 79 and the values of the material constants listed in Table 3 as a function of fission rate for an irradiation temperature of 373 K. Because many of the material constants for U₃Si₂ are not available, estimates of various parameters were taken from the references listed in Table 3. As is evident from Fig. 6, the above analysis provides a plausible interpretation of the observed knee in the U₃Si₂ swelling curve. Figure 6 also shows the analogous calculation and data for UO₂, which are discussed in the next section.

The DART code was used to calculate U₃Si₂ swelling. Fuel grain size was taken as the as-fabricated value until fuel burnup reached the recrystallization dose calculated with Eq. 79. Subsequently, the grain size used in the DART calculation was reduced to 0.5 μm (see below for details).

The following assumptions were made for the DART model:

1. Whole-bubble destruction is the physically realistic mechanism of gas atom re-solution from gas bubbles. Below a certain critical size, bubbles are completely destroyed when "hit" by a passing fission fragment; above the critical size, the bubbles survive the encounter.

2. The critical size for whole-bubble destruction is smaller for bubbles on grain surfaces than for bubbles in the bulk material because the gas-atom capture strength of the grain surfaces is strong. Here, a zero critical size is used for grain boundary bubbles.

3. Gas atoms diffuse from the bulk material to the grain surfaces by irradiation-enhanced diffusion.

4. The nucleation factor for bubbles on grain faces and grain edges is the same as that for bubbles within the grains (the nucleation factor is the probability that two interacting gas atoms will form a stable gas-bubble nucleus).

5. Gas atom diffusivity on grain surfaces is a factor of 10⁴ greater than in the bulk material.

6. Both grain faces and grain edges are included in the calculation. Gas on grain faces can vent to grain edges upon bubble interconnection. The observed bubble population is its uniformly distributed and noninteracting. As discussed in Section 6.1, the total number of bubbles in the second peak of the measured bimodal distribution remains relatively constant for all examined samples.

7. The large bubble population inhabits fixed sites. These sites are formed upon grain recrystallization and are associated with nodes formed by the intersection of grain edges within the subgrain boundary structure. Fission gas that collects along grain edges vents upon intersection with these nodes, where it is trapped. Gas bubbles at these dead-end nodes grow as they continue to collect additional gas.
The results of DART calculations made without Assumption 7 are not consistent with the measured distributions. First, the data show a bimodal bubble size distribution (very evident from the SEM photomicrographs), whereas the calculated distributions do not. (The calculated quantities do show a bimodal bubble size distribution if very small bubbles are included in the plot. However, these small bubbles are well below the limits of experimental resolution). Second, the calculated distributions are much broader than the measured quantities. If the grains are assumed to be cubes and the dead-end nodes are taken to be grain corners formed by
the intersection of six grain edges, the number of nodes per cubic centimeter is given by the inverse of the cube of the grain diameter.

Upon grain recrystallization, gas diffuses athermally (by irradiation-enhanced diffusion) from the bulk material to the grain faces, where it accumulates in gas bubbles that grow until the grain face is saturated. DART calculates fission gas saturation of the grain-face by directly addressing the calculated distribution of fission gas bubble sizes. Grain face saturation occurs when the projected areal coverage of the grain face by these bubbles exceeds the maximum areal coverage. If the gas is assumed to be made of equal, closely packed, touching bubbles, the maximum areal coverage per unit area of grain face is 0.907.

Once formed on the grain edge, the bubbles grow by accumulating additional gas that arrives from the grain faces. When long-range interconnection of the grain edge porosity occurs, the gas is vented to the dead-end nodes. The DART model for calculating the probability of long-range grain edge tunnel interconnection is based on the assumption that the long-range interconnection is a function of the swelling of the grain edge bubbles. This assumption is supported by both experiment and theory for oxide fuels [49]. The value of the grain edge bubble fractional swelling at which long-range interconnection takes place if the fuel microstructure and gas bubble morphology are homogeneous is 0.055. To account for local fluctuations in fuel microstructure and gas bubble morphology, the grain face saturation and the long-range grain edge interlinkage fractions are assumed to be statistical distributions around average values of these parameters.

The DART mechanical/stress model consists of spherical fuel particles surrounded by matrix aluminum. The model treats the inner fuel sphere as an elastically deformable body and the surrounding shell of aluminum matrix material as perfectly elastic. During irradiation, fission induces elastic deformation of the fuel particles. First, the as-fabricated pores in the matrix material close in response to expansion of fuel particle volume, then plastic flow/swelling of the aluminum occurs.

In Figs. 7a and b, the points connected by solid lines show DART-calculated bubble size distribution at fission densities of $9 \times 10^{27}$ m$^{-3}$ and $16 \times 10^{27}$ m$^{-3}$ when the dead-end nodes are included in the analysis and a recrystallized grain size of 0.6 µm is utilized. Grain recrystallization was calculated to occur at a fission density of $6.5 \times 10^{27}$ m$^{-3}$. Also shown in Figs. 7a and b are data obtained from SEM photomicrographs of the irradiated material. The calculated bubble distributions for bubble sizes below 0.4 µm and 0.6 µm (Figs. 7a and b, respectively), are due to the accumulated gas in the dead-end nodes. Currently, DART calculates only the growth of an average-sized node and does not account for the experimentally observed distribution of node bubble sizes. In addition, the observed density of node bubbles appears to decrease from $\approx 3.6 \times 10^{18}$ m$^{-3}$ at a fission density of $9 \times 10^{27}$ m$^{-3}$ to $\approx 2.4 \times 10^{18}$ m$^{-3}$ at a fission density of $16 \times 10^{27}$ m$^{-3}$. This decrease in density may be due to the consumption of smaller node bubbles by larger node bubbles. This process is currently not included in the DART calculations. Consequently, if we use 0.6-µm recrystallized grain size, which corresponds to a node density of $3.6 \times 10^{18}$ m$^{-3}$, the calculated size of the node bubbles at $16 \times 10^{27}$ m$^{-3}$ will be underpredicted, as seen in Fig. 7b. Given the above considerations, the DART calculations shown in Figs. 7a and b follow the trends of observed bubble size distribution in irradiated U$_3$Si$_2$ as a function of burnup and, as such, provide plausible
6.4 Recrystallization and Swelling in UO₂

In this section, we assess the theory of grain recrystallization as applied to high-burnup UO₂, where grain subdivision has also been observed directly. Postirradiation examination [25] of bulk UO₂ wafers irradiated to high burnup in pressurized hot-water loops have revealed that grain subdivision from =15 to <1 μm in diameter occurred in the burnup range of 24–31 x 10²⁰ fissions/cm³. Changes in fuel volume determined by immersion-density measurements also showed that the swelling rate of the material changed from an initial value of =0.16% to 0.5% ∆V per 10²⁰ fissions/cm³ in the burnup range of 17–36 x 10²⁰ fissions/cm³. This observation of a knee in the swelling curve and its association with grain recrystallization is qualitatively similar to that observed in U₃Si₂ [23]. In Fig. 6, we presented recrystallization-dose data for UO₂ from Refs. 25 and 26, and values calculated with Eq. 81 and the material constants listed in Table 4 for irradiation temperatures of 950 and 1000 K. As is evident from Fig. 6, the analysis provides a plausible interpretation of recrystallization in UO₂.

Figure 8 shows DART-calculated fractional fuel volume increase in bulk UO₂ as a function of fission density with and without recrystallization. The calculation with recrystallization utilized a recrystallized grain size of 0.5 μm. Various properties used in the calculation are listed in Table 4. Except for Eₜ, the ratio of the various...
Fig. 8. Calculated fractional fuel volume increase in bulk UO₂ as a function of fission density with and without recrystallization and a fit to data from Ref. 25.

energies in UO₂ to that in U₃Si₂ (see Table 3) is about the same as the ratio of the melting temperatures in the two materials. The radiation–enhanced diffusion parameter $\chi$ is a factor of 100 larger in UO₂ than in U₃Si₂. This is consistent with values of this property measured in other materials with higher thermal conductivity (as compared with UO₂, e.g., UC [31]). The solute concentration $c_1$ is a factor of 100 lower in UO₂ than in U₃Si₂. This finding is consistent with the higher activity of an ionic material when compared with that of a largely covalent compound. By theory, with the materials properties shown in Table 4, grain recrystallization is predicted to occur at $\approx 20 \times 10^{20}$ fissions cm$^{-3}$. The observed bubbles in the recrystallized material are relatively widely spaced because of the high value of the grain boundary area per unit volume and the existence of fixed-nucleus nodes associated with the intersection of grain edges within the subgrain texture. Thus, the bubbles are noninteracting and grow by accumulation of gas atoms. It is this growth mechanism that leads to the linear swelling behavior shown in Fig. 8. This predicted behavior is consistent with the observation of regularly spaced, noninteracting bubbles in the U₃Si₂.
As discussed in Section 6, Eq. 81 (or 82) provides an interpretation of recrystallization in UO\textsubscript{2} across a high-burnup cusp at the outer surface of the fuel rod, i.e., the so-called rim effect. This is seen more clearly in Fig. 9, which shows an example of the calculated burnup at which recrystallization will occur as a function of fractional radius and fuel temperature. Also shown in Fig. 9 are the fuel burnup and fission rate. When fuel burnup exceeds recrystallization burnup, calculated with Eq. 81 (or 82), recrystallization is predicted (hatched rectangle shown in Fig. 9). Also, the fission rate in this region, is enhanced by a factor of ~2.8 over the average. Values of various properties used in the calculation shown in Fig. 9 are listed in Table 4.

### Table 4. Values of various properties used in calculating the recrystallization dose for UO\textsubscript{2}

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>(v_v)</td>
<td>(5 \times 10^{13} \text{ s}^{-1})</td>
<td>24</td>
</tr>
<tr>
<td>(\epsilon_v)</td>
<td>2.4 eV</td>
<td>34</td>
</tr>
<tr>
<td>(\epsilon_{vi})</td>
<td>2.8 eV</td>
<td>Present Calculations</td>
</tr>
<tr>
<td>(\chi)</td>
<td>(6 \times 10^{-23} \text{ cm}^{7/2} \text{ s}^{-1/2})</td>
<td>34</td>
</tr>
<tr>
<td>(E_{sf})</td>
<td>2 eV</td>
<td>Present Calculations</td>
</tr>
<tr>
<td>(C_l)</td>
<td>(1 \times 10^{-7})</td>
<td>Present Calculations</td>
</tr>
<tr>
<td>(r_{lv})</td>
<td>(1 \times 10^{-10} \text{ m})</td>
<td>27</td>
</tr>
<tr>
<td>(r_{sm})</td>
<td>(3 \times 10^{-10} \text{ m})</td>
<td>27</td>
</tr>
<tr>
<td>(\xi)</td>
<td>0.1</td>
<td>Present Calculations</td>
</tr>
</tbody>
</table>
Fig. 9. Calculated burnup at which recrystallization will occur as a function of fractional radius (lower horizontal scale) and fuel temperature (upper horizontal scale). Also shown is fuel burnup and fission rate. When fuel burnup exceeds recrystallization burnup, calculated with Eq. 81 (or 82), recrystallization is predicted (hatched rectangle).

It is important to reiterate that a cellular dislocation structure has been observed within the porous band or rim [30]. This observation is consistent with the physical basis underlying the model presented in this paper. The results in Fig. 9 are intended to show that the trends of the calculation are consistent with observation. The predicted size of the porous band is a function of fuel temperature and fission rate, as well as of the properties listed in Table 4.
6.5 Discussion and Conclusions

Earlier in this section, we described a model for irradiation-induced recrystallization (grain subdivision) and swelling in $\text{U}_3\text{Si}_2$ and UO$_2$ fuels wherein the stored energy in the material is concentrated in a network of sinklike nuclei that diminish with dose because of interaction with radiation-produced defects. The sinklike nuclei were identified as a cellular dislocation structure that evolves relatively early in the irradiation period. Impurities formed during fissioning of the material diffuse as vacancy-impurity complexes to cell walls where they effectively pin the wall, i.e., dislocation movement to and from the wall is retarded. Not all cell walls are uniformly affected by impurities; walls that contain no impurities continue to undergo subgrain coalescence, which results in viable nuclei for recrystallization. Recrystallization is induced when the energy per nucleus is high enough to offset creation of grain-boundary surfaces by creating strain-free volumes, with a resultant net decrease in the free energy of the material. This formulation, applied within the context of a mechanistic treatment of fission gas bubble behavior, was shown to provide a plausible interpretation of the fission density at which grain subdivision begins, as well as the rate of fuel swelling, and the percentage of gas release in high-burnup UO$_2$ fuel.

In a recent paper [50], Nogita and Une describe their TEM observations of the formation mechanism of the recrystallized region (the so-called rim structure) in high-burnup UO$_2$ fuel. Dislocation density and the volume fraction of small intragranular fission gas bubbles increase with burnup. Low-angle boundaries begin to form above $7.5-8 \times 10^{26}$ fissions/m$^3$. Analyses of fuel irradiated to $2.1 \times 10^{27}$ fissions/m$^3$ show 20-30-mm subdivided grains, with high-angle boundaries due to the accumulation of an extremely high density of subboundaries; 50-200 nm recrystallized grains, adjacent to the subdivided grain region, that are presumably induced by the stored energy of the matrix; and the absence of bubbles within the recrystallized grains and the appearance of larger bubbles that most likely exist on the new grain boundaries. This is essentially the physical picture that we proposed as the basis of our theory of irradiation-induced recrystallization and swelling.

The observed dependence, at high burnup, of low-temperature swelling of irradiated uranium silicide dispersion fuels on fission rate is ascribed to the formation of grain boundaries in the material. Subsequently, fission gas atoms diffuse to the boundaries and nucleate fission gas bubbles that grow more rapidly on the boundaries than in the bulk material. We propose the existence of recrystallization nuclei (walls of a cellular dislocation network) on which stored energy is concentrated. Grain boundaries are formed when the density of recrystallization nuclei decreases to a level where the net change in free energy due to the creation of strain–free volumes (decrease in free energy) and boundary surfaces (increase in free energy) is approximately equal to the thermal energy $kT$. We further propose that the decrease in recrystallization nuclei density is due to interaction with mobile, irradiation–produced impurities (i.e., vacancy–impurity pairs).

The theory of grain recrystallization and gas–driven fuel swelling presented in this paper has been applied to the interpretation of the observed low-temperature swelling of irradiated uranium silicide dispersion fuels. The swelling rate of the material exhibits a distinct knee that shifts to higher fission density with increased fission rate. A subgrainlike structure has been observed in $\text{U}_3\text{Si}_2$ above the knee. No such structure is apparent in the material at fission densities below the knee. We propose that the basis for this kinetic phenomenon is the formation of
vacancy–solute pairs that, upon migrating to potential recrystallization nuclei, immobilize the nuclei and thereby increase the average value of the stored energy per nucleus. This theory was compared with data both swelling and bubble size distribution and provides a plausible interpretation of the phenomenon.

The theory was also applied to grain recrystallization in high-burnup UO₂, where grain subdivision was observed directly. Calculations for the onset of grain recrystallization, fuel swelling rate, and the size of the rim effect zone agree reasonably well with the data trends.

7 DART Theory of Gas Bubble Behavior in Amorphous Fuel

7.1 Introduction

Observations of certain low-enrichment, high-density, uranium-base intermetallic alloys, such as U₃Si and U₃Fe, have revealed extraordinarily large voids (breakaway swelling) at low and medium fuel burnup. This phenomenon of breakaway swelling does not occur in other fuel types, such as U₃Si₂ and U₃Al₁, where, instead, a distribution of relatively small, stable fission gas bubbles forms. The in-situ observations of ion-radiation-induced rapid swelling of intermetallic materials are consistent with growth by plastic flow.

In this section, we describe a microscopic theory of fission gas bubble behavior in irradiated amorphous compounds. The assumption underlying the overall theory is that the difference in the evolution of porosity in crystalline and amorphous U₃Si is due to a softening of the irradiated amorphous material, with a concurrent orders-of-magnitude increase in the effective gas bubble diffusivity due to plastic flow. The coupling of changes in shear modulus with radiation-induced softening of amorphous material and gas atom mobility within defect cascades is also discussed.

7.2 Model for Irradiation-Induced Softening of Amorphous Materials

The major differences between the crystalline and amorphous phases are due to changes in elastic properties. In the studies, substantial elastic softening of irradiated intermetallic compounds occurred in the crystalline phase and was associated with progressive destruction of the long-range chemical order. Brillouin scattering experiments and transmission electron diffraction studies have shown that single-crystal silicon and polycrystalline intermetallic compounds undergo dramatic elastic softening after irradiation with charged-particle beams. Measurements of the change in sound velocity show that the average shear constant decreases by as much as 30% in silicon and by as much as 50% in intermetallics [51]. These results point to a strong coupling between strain
and order parameters as a possible origin of the elastic softening and to strain accumulation as an important prerequisite for the amorphization of these intermetallics.

The degree of long-range atomic order $S$ is exponentially dependent on the total irradiation dose $\phi t$

$$S / S_0 = \exp(-K\phi t).$$ \hfill (90)

Measurements of the Zr$_3$Al lattice dilatation $\Delta a / a$ show that $\Delta a / a$ increases with increasing dose, reaches a maximum value of $\approx 0.8\%$ at the dose where amorphization starts, then drops abruptly to $-0.7\%$ ($S \approx 0$) and thereafter remains approximately constant [52]. For doses up to 0.2 dpa, the percentage lattice dilation is a quadratic function of $S$

$$\Delta a / a = (\Delta a / a)_m \left[ 1 - (S / S_0)^2 \right],$$ \hfill (91)

where $S / S_0 = \exp[-11.6\phi t]$ is the observed dose dependence of $S$, and $(\Delta a / a)_m = 0.775\%$ is the maximum lattice dilatation due to disordering. The results of postirradiation Brillouin scattering measurements of the same material show that a large ($\approx 50\%$) decrease in the shear constant occurs after chemical disordering. The decrease occurs before the onset of amorphization, and, hence, the elastic softening is a precursor effect rather than a consequence of amorphization. This result is significant because it strongly suggests that an elastic instability triggers the onset of amorphization. For doses up to 0.15 dpa, the shear constant is a quadratic function of $S$

$$C / C_0 = 0.5 \left[ 1 + (S / S_0)^2 \right].$$ \hfill (92)

The $S^2$ dependence described by Eqs. 91 and 92 implies that the shear constant is a linear function of volume dilatation, $3\Delta a / a$. Eliminating $(S / S_0)^2$ in Eqs. 91 and 92 yields

$$C / C_0 = 0.5 \left[ 1 - (3\Delta a / a + 4.65).$$ \hfill (93)

As described by Eq. 93, the shear constant decreases linearly with volume dilatation and extrapolates through the glass gap. That is, the change in density between the partially disordered crystalline phase and the amorphous phase $= 2.5\%$ at $3\Delta a / a = 4.7\%$, which is very close to the value of $4\pm1\%$ measured for total volume expansion of amorphous Zr$_3$Al [53]. The loss of resistance to shearing at a dilatation of $4.7\%$ indicates that the partially disordered material ($S = 0.2$) is mechanically unstable with respect to density fluctuations comparable in magnitude to the glass expansion gap. Because density fluctuations of comparable magnitude may occur in the cores of energetic cascades, the irradiation itself can provide the additional density fluctuation required to trigger an elastic-inelastic instability in the partially disordered material.

The elastic instability that occurs during irradiation is not one in which the entire crystal transforms catastrophically to an amorphous phase at some critical disorder. The glass expansion gap represents a nucleation
barrier against glass formation in the highly strained, metastable, disordered crystalline material. Although the dilatational strain will have a well-defined average value, local dilatation fluctuations result in regions of mechanical instability, that is, amorphization, and not everywhere simultaneously. In the context of the theory being developed in this section, the important point is that disorder results in a volume-dependent shear coefficient during irradiation similar to that associated with the heating and melting of metals.

### 7.3 Calculation of Gas Atom Diffusivities within Defect Cascades

Measurements of ion-beam mixing of tracer impurities in metallic glasses and in the pure crystalline elements that comprise the glasses [54] demonstrate that the ion mixing efficiency of the tracer impurities is greater in the metallic glasses than in either of the constituent elements. The radiation-enhanced diffusivities of the tracer impurities in the metallic glasses is within a factor of 10 of those measured in the crystalline materials. Although in the right direction, a factor-of-10 increase in the gas atom diffusivities is not sufficient to explain the breakaway swelling observed in irradiated U₃Si material. However, these results are consistent with the picture of cascade dynamics provided by molecular-dynamics computer simulations [55]. The simulations show that the cascade region exhibits a liquid-like structure during the thermal-spike phase of cascade evolution.

A simple picture for the relationship between the migration energy for diffusion and the elastic constants of the material can be developed on the basis of the following arguments. A diffusion jump introduces a lattice strain. One may expect the strain caused by the jump to be mainly a shear. The energy in this shear strain can be estimated by treating the material as a Hookeian solid. For Hookeian shear, the work done per unit volume of strain energy in the body is given by

\[ W = \frac{1}{2} \varepsilon^2 C', \quad (94) \]

where \( C' \) is the shear modulus and \( \varepsilon \) is the strain caused by the jump. The energy in the shear strain is obtained by multiplying \( W \) by the strained volume. Choice of a volume given by \( 4/3 \pi a^3 \), where \( a \) is the atomic spacing, results in

\[ E_m = \frac{2}{3} \pi a^3 C' \varepsilon^2. \quad (95) \]

which shows that a decrease in the shear modulus will result in a proportional decrease in the migration energy necessary for diffusion.

The thermally activated gas atom diffusivities in the amorphous phase can be described by an exponential dependence on temperature, i.e.,

\[ D_x = D_0 \exp\left(-E_m / RT\right). \quad (96) \]
Gas atom mobility in irradiated crystalline material at relatively low temperatures is dominated by radiation-enhanced diffusion. However, a decrease in $E_m$ may result in domination of the diffusion process by thermal activation. From Eqs. 93 and 95, the migration energy in the damaged material $E_d$ is given by

$$E_d = E_m[1 - (3\Delta a/a)/4.65],$$  \hspace{1cm} (97)

where $E_m$ is on the order of the migration energy in the undamaged material. Thus, the diffusivity in the damaged material is given by

$$D_d = D_0 \exp[(E_m/RT)(3\Delta a/a)/4.65].$$  \hspace{1cm} (98)

For a 3% volume dilatation, the diffusivity at 150°C would be enhanced by =11 orders of magnitude over thermal diffusion.

It is important to note that the gas atom diffusivity given by Eq. 98 is appropriate only for local regions of the amorphous (or crystalline) material. The dilatation $\Delta a/a$ in Eq. 98 applies to these damaged regions (for example, the volume of a damage cascade), and is estimated to have a lifetime on the order of the defect cascade ($10^{10}$ s). Equation 98 applies to damaged regions in partially disordered crystalline materials and in amorphous materials. The key difference between bubble behavior in most irradiated crystalline and in amorphous materials is that the amorphous materials can undergo substantial plastic flow due to an enhanced softening under irradiation. Some crystalline materials, however, behave very much like $U_3Si$ because of very low shear modulus values (e.g., the $\gamma$ phase of various uranium alloys). In irradiated amorphous materials that contain fission gas, overpressurized bubbles can provide the driving force for plastic flow. In addition, density fluctuations produced by damaging cascades can be a driving force for microscopic deformation. Plastic flow, in turn, results in enhanced bubble coalescence and bubble sweeping of gas atoms out of solution.

The calculation of bubble growth in irradiated amorphous materials is complicated by the interplay between bubble growth (driven by plastic flow) and plastic flow (e.g., driven by bubble overpressure). To provide for a computationally tractable description of this phenomenon, the assumption is made that bubble motion in a material that undergoes plastic flow can be described by an effective bubble diffusivity based on random motion in a liquid where the bubbles move by volume diffusion. The diffusivity of a bubble of radius $r_i$ migration by volume diffusion is given by

$$D_i = \frac{3\Omega}{4\pi r_i^3}D_0,$$  \hspace{1cm} (99)

where $\Omega$ is the molecular volume and $D_0$ is the diffusivity of the diffusing atoms. This diffusion is qualitatively described by the Stokes-Einstein equation.
\[ D_u = kT / (6\pi r_s \eta) \]  

where \( r_s \) is the radius of the diffusing species and \( \eta \) is the viscosity. A softening of the material produces a decrease in \( \eta \) and a corresponding increase in \( D_u \). The assumption is made here that, in irradiated amorphous materials, the effect of plastic flow can be described by using an effective atomic diffusivity \( D_u \) that is equal to \( D_u \) of Eq. 98.

8 Dart Methodology for Calculating Stress and Phase Gradients within U₃Si₂ Fuel Particles

As shown in Eqs. 35 and 37, the growth of fission gas bubbles depends on the hydrostatic pressure \( P_h \) in the fuel adjacent to the bubble surface. Equation 55 relates \( P_h \) to the overall fuel volume fraction and the aluminum yield stress and therefore provides an estimate of the average hydrostatic stress within the fuel particle. As seen in the above sections, a gradient in fuel composition will, in general, exist across fuel particle. This phase gradient will give rise to a gradient in swelling, and thus a gradient in stress. To realistically calculate the fission gas bubble size distributions (Eq. 1), and hence fuel swelling, we must introduce a mechanism for evaluating the stress gradient within the fuel particle.

DART employs a radial nodalization scheme to characterize temperature, stress, and phase gradients. As discussed in Section 3, a phenomenological factor has been introduced in the elastic/perfectly plastic analysis of fuel particle deformation within an aluminum matrix to account for the effects of irradiation (e.g., irradiation-enhanced creep and hardening) without resorting to a much more complicated time-dependent deformation analysis. This approach has been extended to the deformation analysis within the fuel particle. In particular, Eq. 55 is utilized for radial nodes that consist of a given phase surrounded by radial nodes that are composed of a different phase. In this case, the fuel volume fraction in Eq. 55, i.e., \( V_f^I + \Delta V_f^I / V_o^I \), is replaced by the volume fraction within the fuel particle that is occupied by the given fuel phase, and the effective yield strength \( \beta S_x \) of aluminum in Eq. 55 is replaced with the effective yield strength of the different fuel phase.

9 DART Validation for Behavior of U₃Si₂ Particles Irradiated in the HFIR

As discussed in the above sections, DART consists of models for the formation of various phases of U₃Si₂ (i.e., aluminide, recrystallized, amorphized), the evaluation of fission gas bubble morphology and swelling within various phases, aluminum diffusion into the U₃Si₂ particle, thermal conductivity, and mechanical deformation. A key assumption in the bubble morphology model is that within the recrystallized material, the observed large bubble population inhabits fixed sites. These sites are formed upon grain recrystallization and are associated with nodes that are formed by the intersection of grain edges within the subgrain boundary structure (e.g., grain
Fission gas that collects along the grain edges vents upon interconnection with these nodes, where it is trapped. The gas bubbles at these dead-end nodes grow as they continue to collect additional gas. Although the model is based on some assumptions that are derived from systems other than U$_3$Si$_2$, it represents a physically realistic interpretation of the observed irradiation behavior of U$_3$Si$_2$ over a wide rage of fission densities and fission rates.

Observations of photomicrographs of U$_3$Si$_2$ fuel particles dispersed in an aluminum powder and irradiated in the HFIR have revealed a microstructure of an outer aluminide shell (e.g., a UAl$_3$-type structure) that shows no evidence of grain recrystallization (Region 1 of Fig. 10F), an inner aluminide-type annulus that shows evidence of grain recrystallization (Region 2 of Figs. 10F, and Fig 10C), and a central region that shows swelling that is characteristic of an amorphous material (Region 3 of Fig. 10F). DART analyses of the evolution and swelling of this complex microstructure have identified the following phenomena. The formation of the outer aluminide shell acts as a restraint on the swelling of the inner fuel material. This is because the outer (unrestructured) aluminide shell contains predominantly small (not visible by SEM) intragranular bubbles (Fig. 10D). Thus, this outer shell has a relatively low swelling rate when compared with the interior regions (which are composed of recrystallized and/or amorphous-like material) and appears "hard," or stiff, when compared with the relatively "soft," or ductile interior regions. DART calculations show that if the outer aluminide shell does not form (e.g., for fuel particles irradiated in the absence of aluminum), fuel particle swelling rates increase significantly. It is conjectured (based on observation) that the aluminide material is stable against amorphization and recrystallization. Thus, for DART to generate an aluminide outer shell, aluminum diffusion into the material (i.e., through the outer fuel ring defined in the multinode configuration of the calculations) must occur before the recrystallization model predicts grain recrystallization in that node.

The inner nodes recrystallize prior to aluminum penetration, leading to an aluminide annulus with a refined grain structure (Region 2 of Figs. 10F and C). DART-calculated swelling rates in an annulus that has a refined grain structure are significantly higher (Fig. 10A) than what would occur in the absence of recrystallization (i.e., in the aluminide region, Fig. 10D) due to enhanced bubble growth on grain boundaries and on dead-end nodes. Subsequent to recrystallization, aluminum penetration of this inner annulus occurs, converting the material to a restructured (with a refined grain structure) aluminide region (Region 2 of Figs. 10F and C). The pre-exponential factor in the expression for the thermal diffusivity of aluminum was determined on the basis of a calculated amorphous annulus, which is consistent with the observations (Fig. 10B). As the simulation moves across the U-Si phase diagram, the code tests for whether the calculation has entered the unstable USi$_2$ phase. If so, models for the behavior of fission gas bubbles in irradiated amorphous U$_3$Si$_2$ are invoked. Swelling rates in the amorphous inner core (Fig. 10E) are higher than in the outer crystalline regions because of plastic nature of this amorphous material in the presence of irradiation. The outer, relatively hard, crystalline regions constrain the swelling of the inner, relatively soft, amorphous core.
Fig. 10. DART interpretation of $U_xSi_y$ particle irradiation in HIFR
Calculated bubble distributions result in an absence (by SEM) of visible bubbles in the outer unrecrystallized aluminide shell (Fig. 10D), visible intergranular bubbles in the inner recrystallized aluminide annulus (Fig. 10A), and relatively large bubbles in the inner amorphous core (Fig. 10E). As shown in Fig. 10, these results are in qualitative agreement with the observations. In addition, the DART-calculated fuel restructuring overlaid on a photomicrograph of a cross section of a fuel particle, shown in Fig. 10B, follows the trend of the observations.

10 DART Validation for Irradiation Behavior of Various Designs of Uranium Silicide Dispersion Fuel Elements

The DART mechanical (stress) model consists of a fuel sphere that deforms because of both solid fission product and fission gas bubble swelling. The fuel sphere is surrounded by an aluminum matrix shell, which is assumed to behave in a perfectly plastic manner and which deforms (yields) when fuel particle volume expands. The effects of cladding are included by a suitable adjustment of the effective aluminum volume fraction. Currently, the effects of creep are not included; instead, the stress relaxation is approximated by lowering the aluminum yield stress to an "effective" value. Different values of this effective yield stress are used for the rod, plate, and tube geometries to simulate the quite complicated time-dependent deformation behavior of the rod and plate with the rather simplistic DART stress model. The deformation of the matrix and cladding material generates stresses within the expanding fuel particles, which affect the swelling rate of the fission gas bubbles.

The swelling fuel particles push the matrix aluminum into as-fabricated porosities and simultaneously cause cladding deformation. The swelling rate primarily depends on the plastic yielding of the aluminum matrix and cladding. The hydrostatic stress $\sigma_i$ ($i = 1,2$ refers to plate or rod geometry), acting on the gas bubbles is given by (see Eq. 57)

$$\sigma_i = \frac{2}{3} \left[ 1 - \ln \left( \frac{V_o^F + \Delta V^F}{V_o^C} \right) \right] \beta_i \sigma_{\text{Al}}(T),$$

where $\sigma_{\text{Al}}(T)$ is the as-fabricated temperature-dependent yield strength of the aluminum, $\frac{V_o^F + \Delta V^F}{V_o^C}$ is the fuel volume fraction, and $\beta_i$ is a factor that accounts for the effects of irradiation (e.g., irradiation-enhanced creep). The values of $\beta_i$ used in DART are $\beta_1 = 7.5$ and $\beta_2 = 2.5$.

Results of DART calculations are shown in Figs. 11 and 12. The calculations shown in Figs. 11 and 12 were all performed at the same constant fuel temperature of 373 K. Figure 11 shows DART results for fuel swelling of $\text{U}_{x}\text{Si}_{1-x}\text{Al-Al}$ in plate, tube, and rod configurations as a function of fission density compared with data. The lower calculated fuel swelling in the rod-type element is due to an assumed biaxial stress state as compared with an assumed uniaxial stress state for the plate and thin-walled tube geometries. Fuel swelling in plates results in plate
thickness increase only, while plate width and length remain relatively unchanged. Likewise, in tubes, only the wall thickness increases and the overall diameter remains unchanged. Thus, cladding of these element designs contains minimal lateral or circumferential strain and consequently, much less restraint compared with the hoop stress state in a solid-clad rod. Irradiation experiments have shown that plate-type dispersion fuel elements can develop blisters or pillows at high \(^{235}\text{U}\) burnup when fuel compounds exhibiting breakaway swelling, such as U\(_3\)Si\(_2\)Al and U\(_3\)Si, are used at moderate to high fuel volume fractions. The U\(_3\)SiAl plate data shown in Fig. 11 exhibits this behavior at fission densities above about \(5 \times 10^{27} \text{ m}^{-3}\). Figure 12 shows DART-calculated results for fuel particle swelling of low-enriched U\(_3\)Si\(_2\)-Al fuel plates and rods as a function of fission density. The calculated values shown in Fig. 12 indicate that irradiation-induced recrystallization occurred at \(\approx 3.5 \times 10^{27} \text{ m}^{-3}\). Again, the fuel rods exhibit lower values of swelling than the plates because of the greater restraint imposed by the rod configuration.

Figure 13 shows DART-calculated results for pore closure of low-enriched U\(_3\)Si\(_2\) fuel plates fabricated to 50% and 13% fuel and pore volume fractions, respectively, compared with the measured values [56]. In Fig. 13, \(V_p^0\) and \(V_p\) are the initial and remaining values of the fraction of as-fabricated porosity in the dispersion. The DART calculations show the effects of fuel recrystallization (increased rate of pore closure) which is calculated to occur at a fission density of \(3.5 \times 10^{27} \text{ m}^{-3}\). Both the data and the calculations show that the as-fabricated porosity is completely removed by \(4.5 \times 10^{27} \text{ m}^{-3}\). As is evident from Figs. 11-13, DART calculated fuel swelling and pore closure is in reasonable agreement with observation.
Fig. 11. DART results for swelling of $\text{U}_3\text{SiAl-}\text{Al}$ in plate, tube, and rod configurations as a function of fission density compared with data.
Fig. 12. DART-calculated results for fuel particle swelling of low-enriched U₃Si₂-Al fuel plates and rods as a function of fission density.
Fig. 13. DART-calculated results for pore closure of low-enriched U$_3$Si$_2$ fuel plates as a function of fission density compared with the measured values.

11 DART Calculation of Dispersion Fuel
Thermal Conductivity

Figures 14 and 15 show the results of DART calculations of the bulk thermal conductivity and total fuel swelling, respectively, of a 3.5-g/cm$^3$ 35% enriched U$_3$Si$_2$ dispersion fuel containing 3.5% as-fabricated porosity for four values of fuel temperature. The calculations shown in Figs. 14 and 15 utilized a one-node mesh across the fuel plate, and a 20-node mesh across the fuel particle.
Fig. 14. DART calculated bulk thermal conductivity of a 3.5-g/cm³, 35% enriched U₃Si₂ dispersion fuel containing 3.5% as-fabricated porosity, at four fuel temperatures.

Each thermal conductivity curve shown in Fig. 14 exhibits a characteristic shape: initially, the thermal conductivity increases because of pore closure in response to fuel particle swelling; this is followed by a decrease in the thermal conductivity due to additional fuel particle swelling and a commensurate decrease in the volume fraction of aluminum; subsequently, an accelerated decrease in the thermal conductivity occurs because of the onset of grain subdivision, which leads to higher fuel particle swelling rates (see Fig. 15). Two predictions of the...
Fig. 15. DART calculated total fuel swelling (%) of a 3.5-g/cm³, 35% enriched U₃Si₂ dispersion fuel containing 3.5% as-fabricated porosity, at four fuel temperatures.

Temperature dependence of the thermal conductivity are shown in Fig. 14. First, for the initial phase of the irradiation that includes pore closure (up to the onset of grain subdivision), lower thermal conductivities are predicted for the irradiations at higher temperatures because of aluminide formation. Aluminide formation is faster at higher temperatures and results in an increase in fuel swelling (see Fig. 15) because the density of the aluminide is reduced beyond that of the original U₃Si₂. Second, for a constant fission rate, grain subdivision is predicted to occur earlier for irradiations at higher temperatures. As the swelling rate increases upon grain subdivision (see Fig. 15), the thermal conductivity starts an accelerated decrease earlier at the higher temperatures. This behavior is shown more clearly in Fig. 16, where the DART-calculated bulk thermal conductivity and total...
Fig. 16. DART-calculated bulk thermal conductivity and total fuel swelling of a 1.3-g/cm$^3$, 92.5% enriched U$_3$Si$_2$ dispersion fuel containing 0.7% as-fabricated porosity, irradiated at 373 K

Fuel swelling of a 1.3-g/cm$^3$, 92.5% enriched U$_3$Si$_2$ dispersion fuel containing 0.7% as-fabricated porosity are exhibited. As is clear from Fig. 6, increased fission rates (enrichments) result in higher thermal conductivity predictions (all other conditions remaining constant) because of the delay in the onset of grain subdivision. The calculations shown in Fig. 16 were performed at a constant fuel temperature of 373 K, and utilized a one-node mesh across the fuel plate, and a 20-node mesh across the fuel particle.

As described above, the thermal conductivity curve shown in Fig. 16 exhibits a characteristic shape: initially, the thermal conductivity increases as pore closure occurs; this is followed by a decrease in the thermal conductivity due to fuel particle swelling, an accelerated decrease in the thermal conductivity due to the onset of grain subdivision (grain refinement leads to higher fuel swelling rates); and, finally, at high burnup, we observe an additional accelerated decrease in the thermal conductivity due to the transformation of the interior of the fuel particles to an unstable phase (e.g., see Fig. 10).

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Appendix A: DART Input Description

Figure A-1 shows a typical DART input file: this file was used to generate Fig. 15. Table A-1 describes the driver input for DART.
INPUT DECK FOR DARTC

job
title
HIFR IRRADIATION SIMULATION U3S12,............................ .. 0

hifrr  hifrw

grs fl  igs nf lf kf idis nxo
0.0  0.10 1  1  1 5  0 1 0 1 1

prog changes

i  PROG(i)
47  0.05
48  0.532
49  2.2285d-23
50  12.2
83  1938.d0
86  253.667
118  7.5
195  10.
233  1.
0 0

geom =1. :rod =.5 :plate
0.5

prsol vfm0 vpm0 tmtp cvf0 poros
15. .122 .007 .384615 0.68 .02

fuel radii
rs(cl) rs(s)
0.  0.15

pellet radii
rs(cl) rs(s)
0.  0.005

grain diameter, grsk
5*1.0E-2

the following indices for variables to be plotted must be read in
the same order as done in the calculations. This means that k's
are read in descending order, the l's in ascending order.

read in k,l,file name for k,l results

Fig. A-1. Typical DART input file
Fig. A-1. continued
<table>
<thead>
<tr>
<th>Input No.</th>
<th>Name</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>ITLE</td>
<td>descriptive title</td>
</tr>
</tbody>
</table>
|          | IRSTAR | IRSTAR = 0: Normal execution  
|          |      | IRSTAR = 1: Problem restart; program reads restart dump from Unit 15 |
| 2        | DUMP1 | Defines Unit 15 for reading restart dump  
|          |      | (PC version only) |
|          | DUMP2 | Defines Unit 16 for writing restart dump  
|          |      | (PC version only) |
| 3        | GRS  | Initial amount of gas in fuel/cladding gap. |
|          | FL   | Fuel rod length (cm) |
|          | IGS  | IGS = 1,2,3: equation of state for Xe, Kr, or Ar |
|          | NF   | Total number of vertical sections in plate or axial sections in rod |
|          | LF   | Total number of horizontal sections in plate or radial rings in rod |
|          | KF   | Total number of radial rings in fuel particle; each ring has a K value (1 inner to KF outer) |
IDIS

IDIS = 0;
Crystalline fuel

IDIS = 1;
Amorphous fuel

NXI(I)

I = 1, 2, 3, 4:
NXI = 0: Don't calculate
dislocation.

NXI = 1: Calculate
bulk, dislocation.

face, and edge.

I

This card set provides the capability of
modifying any member in labelled COMMON/
PROG(250). Last card of this set must
have I = blank or zero. This card set is read
in subroutine ZRDWR.

GEOM

GEOM = 0: Plate

GEOM = 1: Rod

PRSOL

External pressure (PSI)

VFMO

Fuel volume fraction

VPMO

As-fabricated pore volume fraction

TMTP
Ratio of the bulk thickness to the plate thickness

CVFO

Cladding volume fraction
POROS Initial porosity in fuel particle

7 RS(cl), RS(s) Position of plate (rod) center and surface (cm)

8 RS(cl), Rs(s) Radius of fuel particle center and surface (cm)

9 GRSK Grain diameter (cm) of each K node

10 k l "name" Read in k, l, file name for k, l results

11 k l "name" Read in k, l, file name for specified distributions

12 l "name" Read in l, file name for l results

13 l "name" Read in l, file name for l distributions for each region type
“name” Read in file name for j results

**DELT** Time step (s)

**NPRINT** Printout option
- NPRINT = 1: No printout
- NPRINT = 2: Partial printout for axial totals and rod totals only
- NPRINT > 2: Full printout

**IREAD**
- IREAD = 0: No change operating conditions for this time step
- IREAD = 1: Fuel operating conditions to be updated for this time step; read in inputs #17-18

  IP
  - IP = 0: No action
  - IP = 1: Read in inputs #19-21

**IRSTAR**
- ISTAR < 0: Halt calculation, write restart dump on Unit 16, write summary printout
- ISTAR > 2: Read in new Prog Array values with same format as input #4

  ISTAR = other No action

**ITRAN**
- ITRAN = 0: Steady–state mode
- ITRAN ≠ 0: Transient Mode
**NOPT**

- **NOPT = 0:** No grain growth/grain boundary sweeping
- **NOPT = 2:** Theoretical grain growth law
- **NOPT = 3:** Empirical grain growth law

**NX0**

- **NX0 = 0:** No writes to data files
- **NX0 = 1:** Read in input #16

**16**

**NX1**

Write k, l results every NX1 time steps

**NX2**

Write specified k, l distributions every NX2 time steps

**NX3**

Write l results every NX3 time steps

**NX4**

Write specified l distributions every NX4 time steps

**NX5**

Write j results every NX5 time steps

If IREAD = 0 skip inputs #17-18

**17**

**TS(cl) TS(S)**

Temperatures at boundaries of regions

**18**

**POWER, POW**

Linear power in j sections (kW/ft)

If IP = 0, skip input #19-21

**19**

**TMAX**

The code will execute until the total time = TMAX
IPRINT Printout for every IPRINT time steps with
IWRITE NPRINT = IWRITE

IPOW IPOW = 0: Do not read in POW(J)
IPOW = 1: Read in POW(J)

20 TD(cl) TD(s) Temperatures TS(cl) and TS(s)) incremented by TD
during DELT

21 DPOW Power incremented by DPOW during DELT

If IPOW = 0, skip Input #22

22 POW Linear power in section J (kW/ft)

Repeat sequence starting with Input #15
Table B-1 lists the symbols and values of variables in COMMON/PROG/PROG(250), whereas Table B-2 lists the definitions of these variables.
Table B-1. Symbols and values of variables in COMMON/PROG/PROG(250)

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<td>1.0e12</td>
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<td>xk4(1)</td>
<td>4.25e4</td>
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<td>xk4(2)</td>
<td>3.5e4</td>
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<tr>
<td>prog(100)</td>
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<td>xk4c</td>
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<tr>
<td>zcon(1)</td>
<td>1.0e-3</td>
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<tr>
<td>zcon(2)</td>
<td>0.00</td>
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</table>
vda = 2.9e-26
vdrho = l.e9
vdb = 2.375e-8
vdqu = 131786.
vdql = 4.5
prog(110) = gc
gc = 8.5e-23
fexp = 1.d0

mod = unused
gemo = unused

prog(134-186) are unused in this version

prog(187) = rhodsl
rhodsl = 1.d9

prog(190) = epsj
epsj = 1.d12

ffdsle = 10.d0
fodslc = .31831d0
fogbdy = .63662d0
gbs2 = .5d0*1.43d-4
rm = 10.d0
tkcr = 2373.d0

fnn(1) = 1.d0
fnn(2) = 2.d-7
fnn(3) = 2.d-7
prog(200) = avf
avi = .1d0
bl = 6.d17
ei = .2d0
esf = .70d0
ev = .9d0
ev1 = 1.3d0
e3v = 1.3d0
e4v = .9d0
riv = 2.d-8
rsi = 2.d-8
prog(210) = rsm

rsm = 3.d-8
tmr = 1.5d0
xi = 1.0.d-6
xni = 5.d14
xnv = 5.d13
zb = 2.d0
grdx = 1.d-4
usr(1) = 1.5d0
usr(2) = 2.6d22
prog(220) = usr(3)
usr(3) = .625d0
usr(4) = 1.d-5
usr(5) = 3.d0
usr(6) = 4.d22
usr(7) = 1.5d0
sy0fp = 200.d0

tkdx = 1000.d0
dal0 = 42.d0
epsal = 6.d4

adp = 1.7d0
prog(230) = adpl
adpl = .5d0

tsw33 = .3333333d0
xalm = 0.d0
xpand = 1.d0
xicl = 0.d0

tamo = 723.d0
prog(236-250) unused
Table B-2. Definition of variables in COMMON/PROG/PROG(250)

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<td>Fraction of areal coverage of grain face by bubbles required for channel formation</td>
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<td>Volume associated with one molecule of fuel (cm³)</td>
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<td>CR1</td>
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<td>Activation energy for vacancy diffusion corresponding to DU1(1) above (cal)</td>
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<td>Activation energy for vacancy diffusion corresponding to DU1(2) above (cal)</td>
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<td>FFN</td>
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<td>PTPL</td>
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<td>Term</td>
<td>Description</td>
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<td>Preexponential in the expression for the vapor pressure of the fuel (dynes/cm²)</td>
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<td>Activation energy for surface diffusion (ergs/mole)</td>
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<td>Heat of transport for surface diffusion (ergs)</td>
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<td>QSURF</td>
<td>Activation energy for surface diffusion (cal)</td>
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<td>QVSTAR</td>
<td>Heat of transport for the volume diffusion mechanism (cal)</td>
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<td>RCV</td>
<td>Universal gas constant, R (cal/K)</td>
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<td>Average distance traveled by an atom ejected from a grain boundary bubble (cm)</td>
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<td>Re-solution constant (cm³)</td>
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<tr>
<td>RG</td>
<td>Gas constant (ergs/</td>
<td>gmol•K</td>
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<td>RHOL</td>
<td>Liquid density (g/cm³)</td>
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<td>RLAMS</td>
<td>Proportional to gas atom jump distance (cm)</td>
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<td>SBCF</td>
<td>Width of probability distribution for grain-face channel formation</td>
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<tr>
<td>SIG</td>
<td>Average collision diameter of fuel and Xe molecules (cm)</td>
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<td>Parameter for the modified hard-sphere equation of state</td>
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<td>Width of probability distribution for grain edge porosity interlinkage</td>
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<tr>
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<td>Parameter for the modified hard-sphere equation of state</td>
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<tr>
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<td>Twice THETA is the dihedral equilibrium angle that a gas bubble makes with the grain boundary</td>
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<td>Viscosity of liquid or liquidlike material (g/s•cm)</td>
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<td>WM1</td>
<td>Molecular weight of fuel</td>
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<tr>
<td>WM2</td>
<td>Molecular weight of Xe</td>
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<td>Maximum size of time step h used internally during steady state (s)</td>
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<td>Maximum size of time step h used internally during transient (s)</td>
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<td>XDL(3)</td>
<td>Maximum size of time step h used immediately after amorphization (s)</td>
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<td>XK1(1)</td>
<td>Nominal value of parameter in grain growth model, NOPT = 2</td>
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</tr>
<tr>
<td>230</td>
<td>ADPL</td>
<td>Parameter in expression for thermal diffusivity of aluminum</td>
</tr>
<tr>
<td>231</td>
<td>TSW33</td>
<td>Fractional density increase upon formation of aluminide</td>
</tr>
<tr>
<td>232</td>
<td>XALM</td>
<td>Unused</td>
</tr>
<tr>
<td>233</td>
<td>XPAND</td>
<td>If nonzero, phase boundaries within fuel particle move in response to fuel swelling</td>
</tr>
<tr>
<td>Page</td>
<td>Code</td>
<td>Description</td>
</tr>
<tr>
<td>------</td>
<td>------</td>
<td>-------------</td>
</tr>
<tr>
<td>234</td>
<td>XICL</td>
<td>Flag for different types of aluminum:</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$XICL = 0$: 1000-0 Al</td>
</tr>
<tr>
<td></td>
<td></td>
<td>$XICL = 1$: 6061-0 Al</td>
</tr>
<tr>
<td>235</td>
<td>TAMORF</td>
<td>Temperature above which the fuel cannot become amorphous</td>
</tr>
<tr>
<td>236-250</td>
<td>Unused</td>
<td>Unused</td>
</tr>
</tbody>
</table>
Appendix C: DART Output Description

The first part of DART output consists of a listing of the input file and a listing of the PROG array. Figure C-1 shows the remainder of a typical DART output file and Table C-1 lists definitions of these output quantities.
Fig. C-1. Typical DART output file
Fig. C-1. Continued
<table>
<thead>
<tr>
<th>Quantity</th>
<th>Description</th>
</tr>
</thead>
</table>
| NPRINT           | NPRINT = 1: No output  
= 2: Limited output  
> 2: Full output |
| AREA             | Surface area of region \((K,J)\) \((\text{cm}^2)\)                        |
| AVS              | Sum of AVSL, AVSF, and AVSE                                                |
| AVSL             | Fractional swelling in region \((L,K,J)\) due to gas atoms in the lattice |
| AVSF             | Fractional swelling in region \((L,K,J)\) due to gas atoms on the grain faces |
| AVSE             | Fractional swelling in region \((L,K,J)\) due to gas atoms on the grain edges |
| BDMODL(N)        | Diffusion coefficients of atoms \((N=1)\) and bubbles \((N>1)\) \((\text{cm}^2/\text{s})\) |
| BDSURF(N)        | Diffusion coefficients for bubble movement, based on surface diffusion \((\text{cm}^2/\text{s})\) |
| BETAB(N)         | Intragranular bubble nonequilibrium parameter                              |
| BULKFR           | Fraction of generated gas residing in the grain lattice                    |
| BULK REGION K    | Gas bubble concentration in each size class for bubbles in the grain lattice \((#/\text{cm}^3)\) |
| BUPL             | Fractional burnup                                                          |
| BVLK             | Swelling strain in section \((J,L)\) due to gas bubbles                   |
| BVMODL(N)        | Bubble velocity based on BDMODL(N) \((\text{cm/s})\)                      |
| BVS              | Swelling strain in region \((L,K,J)\) due to gas bubbles                  |
BVSJ  Swelling strain in section J due to gas bubbles
BVSL  Fractional gas bubble strain due to bubbles trapped in the lattice
BVSE  Fractional gas bubble strain due to bubbles trapped on grain edges
BVSF  Fractional gas bubble strain due to bubbles trapped on grain faces
BVVOL  Bubble velocity based on volume diffusion in a temperature gradient
CI  Fractional interstitial concentration in region \((L,K,J)\)
CORN REGION K  Gas bubble concentration in each size class for bubbles on the grain faces (#/cm\(^3\))
CV  Fractional vacancy concentration in region \((L,K,J)\)
CVF  Cladding volume fraction
DCIE  Fission-enhanced diffusion coefficient (cm\(^2\)/s)
DELT  Time step (s)
DTDT  Heating rate in region \((K,J)\) (K/s)
DTPJ  Fractional change in thickness of fuel plate in Section J
EDGE REGION K  Gas bubble concentration in each size class for bubbles on the grain edges (#/cm\(^3\))
EDGEFR  Fraction of generated gas residing on the grain edges
EGRE  Rate of gas migration from grain faces to edges due to grain face channel formation (s\(^{-1}\))
<table>
<thead>
<tr>
<th>Term</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>EPRF</td>
<td>Rate of gas atom release due to increased edge tunnel interconnection</td>
</tr>
<tr>
<td>ERR</td>
<td>Total fractional error in calculation</td>
</tr>
<tr>
<td>ERRJ</td>
<td>Fractional error in calculation in Section J</td>
</tr>
<tr>
<td>ERRK</td>
<td>Fractional error in calculation in Region (L,K,J)</td>
</tr>
<tr>
<td>ERRL</td>
<td>Fractional error in calculation in Section (J,L)</td>
</tr>
<tr>
<td>FACEFR</td>
<td>Fraction of generated gas residing on the grain faces</td>
</tr>
<tr>
<td>FBDE''</td>
<td>Fraction of grain face area per unit volume covered by bubbles</td>
</tr>
<tr>
<td>FDEN</td>
<td>Fission density (fissions/cm³)</td>
</tr>
<tr>
<td>FDNTS</td>
<td>Fission density at which $\text{U}_3\text{Si}_2$ enters the unstable part of the U-Si phase diagram</td>
</tr>
<tr>
<td>FDX</td>
<td>Fission density at which fuel in region will recrystallize</td>
</tr>
<tr>
<td>FGRJ</td>
<td>Fractional gas release from Section J</td>
</tr>
<tr>
<td>FGRK</td>
<td>Fractional gas release from Region (L,K,J)</td>
</tr>
<tr>
<td>FGRL</td>
<td>Fractional gas release from Section (J,L)</td>
</tr>
<tr>
<td>FGRT</td>
<td>Total fractional gas release</td>
</tr>
<tr>
<td>FLUX</td>
<td>Rate at which gas is diffusing to the grain faces (atoms/cm³/s)</td>
</tr>
<tr>
<td>GAMMA</td>
<td>Surface tension of fuel (dynes/cm)</td>
</tr>
<tr>
<td>GBS</td>
<td>Rate of intragranular gas release due to grain boundary sweeping mechanism (s⁻¹)</td>
</tr>
<tr>
<td>GOTT</td>
<td>Total quantity of released fission gas (moles)</td>
</tr>
</tbody>
</table>
GOUJ  Total quantity of released fission gas in Section J (moles)
GOUK  Total quantity of released fission gas in Section (J,L) (moles)
GOUT  Total quantity of released fission gas in Region (L,K,J) (moles)
GRD   Grain size (cm)
GSGEN Quantity of generated fission gas in Region (L,K,J) (moles)
GSGJ  Quantity of generated fission gas in Section J (moles)
GSGK  Quantity of generated fission gas in Section (J,L) (moles)
GSGT  Total quantity of generated fission gas (moles)
GSIN  Fission gas generation rate (atoms/s/cm$^3$)
H     Current time increment (s)
HNXT  Suggested value of next time increment (s)
IMX1  Total number of size classes considered during H in Region (L,K,J)
IMX2  Total number of equations solved during H in Region (L,K,J)
J     Axial section
K     Radial section of fuel particle
L     Linear section of fuel plate (annular region of rod)
LDMK  Phase of region (LDMK = 0: normal; LDMK = 6: amorphous)
NCDI  Number of size classes for dislocation bubbles
NCEI  Number of size classes for edge bubbles
NCFI  Number of size classes for face bubbles
PBKGBY  Biased flux of gas to the grain faces (s')

POROS  Average as-fabricated porosity in fuel particle in region (K,J)

PRF  Pore interlinkage probability fraction at end of current time step

PRFOLD  Pore interlinkage probability fraction during the previous time step.

PRSO  Hydrostatic pressure in region (L,K,J) (lbs/cm²)

PRSOL  Hydrostatic pressure on bubbles in section (J,L) (lbs/cm²)

PRSOO  Hydrostatic pressure in region (L,K,J) during previous time step (lbs/cm²)

RAD  Bubble radii (cm). Note: For grain faces and edges, RAD is the equivalent radius assuming a spherical shape, i.e., lenticular and ellipsoidal bubble geometries are used on grain faces and edges, respectively

RATIO  Fractional radius of Region (L,K,J)

RBD3  1/2 the interbubble spacing on dislocations

RBF3  1/2 the interbubble spacing on the faces

RBL3  1/2 the interbubble spacing in the lattice

RET  Retained quantity of fission gas in Region (L,K,J) (moles)

RETJ  Retained quantity of fission gas in Section J (moles)

RETK  Retained quantity of fission gas in Section (J,L) (moles)

RETT  Total quantity of retained fission gas (moles)

RGB  Quantity of retained gas in lattice (moles)
<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>RGE</td>
<td>Quantity of retained fission gas on edges (moles)</td>
</tr>
<tr>
<td>RGF</td>
<td>Quantity of retained fission gas on faces (moles)</td>
</tr>
<tr>
<td>RGGB</td>
<td>Fraction of retained gas that resides in lattice</td>
</tr>
<tr>
<td>RGGE</td>
<td>Fraction of retained gas that resides on grain edges</td>
</tr>
<tr>
<td>RGGF</td>
<td>Fraction of gas retained that resides on grain faces</td>
</tr>
<tr>
<td>RGGL</td>
<td>Fraction of gas retained that resides in lattice and on dislocations</td>
</tr>
<tr>
<td>RPIN</td>
<td>Fraction of retained intragranular fission gas that resides in bubbles</td>
</tr>
<tr>
<td>RRCON</td>
<td>Fractional release rate of fission gas</td>
</tr>
<tr>
<td>RRGBIP</td>
<td>Rate at which gas is arriving at the grain edges (s⁻¹)</td>
</tr>
<tr>
<td>RS(K,J), RS(K+1,J)</td>
<td>Radii of the two boundaries of Region (L,K,J) (cm)</td>
</tr>
<tr>
<td>SAVG(N)</td>
<td>Number of gas atoms/bubble in size class N: The last row is for the bubbles in the dead-end nodes</td>
</tr>
<tr>
<td>TFPV</td>
<td>Fission rate per unit volume in Region (L,K,J) (fissions/cm³/s)</td>
</tr>
<tr>
<td>TGRAD</td>
<td>Temperature gradient in Region (K,J) (K/cm)</td>
</tr>
<tr>
<td>TK</td>
<td>Average temperature in Region (L,K,J) (K)</td>
</tr>
<tr>
<td>TS(K,J), TS(K+1,J)</td>
<td>Temperatures of the two boundaries of Region (L,K,J) (K)</td>
</tr>
<tr>
<td>TSWLK</td>
<td>Total fission-product-induced swelling strain in Section (J,L)</td>
</tr>
<tr>
<td>VAM</td>
<td>Aluminum volume fraction</td>
</tr>
<tr>
<td>VFM</td>
<td>Fuel volume fraction</td>
</tr>
</tbody>
</table>

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VFMA  Fractional volume occupied by region of given phase

VOLTP  Fractional gas bubble strain due to bubbles trapped in dead-end nodes

VOLUME  Volume of the Region (L,K,J) (cm³)

VPM  As-fabricated pore volume fraction

WKPAR  Change in thermal conductivity of fuel particle due to irradiation-induced porosity (W/m/K)

XKDIS  Thermal conductivity of the dispersion in Section L (W/m/K)

XKDSJ  Thermal conductivity of the dispersion in Section J (W/m/K)

XKGXKU  Fractional change in thermal conductivity of fuel from as-fabricated value in Section L

XKUG  Thermal conductivity of fuel (W/m/K) in section L

XKUO  As-fabricated value of dispersion thermal conductivity (W/m/K) in Section L

XKU3SI2  Thermal conductivity of the fuel particle (W/m/K) in section L

XKXXKU  Fractional change in thermal conductivity of dispersion from as-fabricated value in Section L

References


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