Radiation re-solution of fission gas in non-oxide nuclear fuel

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Abstract

Renewed interest in fast nuclear reactors is creating a need for better understanding of fission gas bubble behavior in non-oxide fuels to support very long fuel lifetimes. Collisions between fission fragments and their subsequent cascades can knock fission gas atoms out of bubbles and back into the fuel lattice. We showed that these collisions can be treated as using the so-called “homogenous” atom-by-atom re-solution theory and calculated using the Binary Collision Approximation code 3DOT. The calculations showed that there is a decrease in the re-solution parameter as bubble radius increases until about 50 nm, at which the re-solution parameter stays nearly constant. Furthermore, our model shows ion cascades created in the fuel result in many more implanted fission gas atoms than collisions directly with fission fragments. This calculated re-solution parameter can be used to find a re-solution rate for future bubble simulations.

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1. Introduction

Recent investigations in fast reactor technology have focused on utilizing depleted uranium in non-oxide fuel forms for in-situ conversion and utilization, with many designs hoping to employ a 30 year fuel pin lifetime [1, 2]. For such
5 long fuel lifetimes, the highly energetic fission events will result in a nearly unrecognizable fuel form, both physically and chemically [3]. One in four fissions result in the production of a gaseous fission product that will diffuse through the fuel matrix. A portion of these atoms collect in bubbles within the grain or along the grain-boundaries. As burnup increases, the individual bubbles
10 along the grain boundaries will become interconnected and form a network of inter-granular bubbles. Once these bubbles reach an outside fuel surface, they will discharge their contents into the fuel plenum. To extend fuel lifetime, fuel pin gas accommodation or venting will be necessary to prevent cladding overpressurization [4]. Since many of the gaseous fission products are radioactive,
15 they must be properly contained to prevent an uncontrolled environmental release.

Accurate estimation of fission gas release is essential to the design and operation of a collection system. In the most simplest terms, the fission gas release can be calculated using a spherical grain model which solves for the grain and
20 grain boundary concentrations using empirical diffusivity values. Complicating this simple model is the tendency of the insoluble fission gas to collect and form bubbles within the fuel grain before reaching the grain boundary. In addition, highly energetic fission fragments can strike the intra-granular bubbles, resulting in re-resolution of gas atoms back into the fuel lattice. Many models account
25 for these different trapping and re-resolution behaviors by tuning the diffusivity [5, 6, 7, 8]. However, estimation of fission gas in its different physical forms may result in more accurate calculation of fission gas release [9].

The re-resolution event has been described as either a collisional atom-by-atom loss or through a complete destruction process (see Olander and Wong-
30 sawaeng [10] for a recent review). The latter theory first developed by Turnbull

[11], termed “heterogenous” re-solution by Olander and Wongsawaeng, assumes a bubble is destroyed if it lies within a destruction zone of approximately a nanometer around a given fission track. A second “homogenous” theory originally presented by Nelson [12] assumes that individual gas atoms are knocked
35 out of bubbles through direct collisions with fission fragments or from fuel cascades produced in the fuel. Many previous studies have looked at one or both of these theories in UO_2 [5, 9, 13, 14, 15, 16, 17]. In general, the homogenous theory tends to underestimate the re-solution rate in UO_2 , while success has been achieved with the heterogenous theory [9, 17, 18]. Although fewer stud-
40 ies have looked at re-solution in non-oxide fuels, a study by Ronchi and Elton showed the homogenous theory produces favorable results in uranium carbide (UC) fuels [17].

The ability of the heterogenous re-solution model to accurately estimate re-solution in oxide fuels, while homogenous re-solution seems more applicable to
45 uranium carbide fuel, lies in the inherent differences between the two materials; uranium carbide is bonded by a mix of covalent and metallic contributions [19], resulting in different energy transport properties such as higher thermal conductivity and diffusivity when compared to UO_2 . Fission fragments are well known to create displacement spikes in materials [20]. Following the lattice
50 disorder, a local temperature increase on the order of 2000°C occurs in UO_2 , along with a mechanical shock that moves through the lattice as a result of rapid thermal expansion [17, 21]. However, theoretical calculations have shown that considering the higher electrical conductivity and thermal diffusivity present in uranium carbide which permits rapid dispersal of energy, the temperature
55 increase is on the order of only 50°C [17]. As a result, the thermoelastic stress field caused by a thermal spike is nearly absent in UC [22, 23].

In light of the differences between UC and UO_2 , it is understandable that the bubble destruction model has seen success in oxide fuels, while the atom-by-atom knockout microscopic model is applicable to carbide fuels [17]. Because
60 of this, the typically used, albeit computational expensive, Molecular Dynamics (MD) fission spike models of determining re-solution can be avoided in favor of

Binary Collision Approximation (BCA) models.

In his original 1969 formulation, Nelson estimated the re-solution rate of a 5 nm xenon gas bubble in UO_2 by assuming Rutherford potential for fission
65 fragment collisions and a hard-sphere potential for all other collisions, with no electronic losses [12]. An atom was assumed to be implanted back into the fuel if a gas atom located within a critical distance of 1 nm from the surface of the bubble was struck by an ion and transferred a minimum implantation energy $E_{min} = 300$ eV [12]. The critical distance limit assumed that all centrally
70 located fission gas atoms would suffer a large angle collision before reaching the bubble surface, while atoms close to the bubble surface result in a re-solution event if struck with sufficient energy. Ronchi and Elton extended the calculation by allowing E_{min} , as well as the radius of the bubble, to be a variable parameter of the calculation in oxide and carbide fuels [17]. Ronchi and Elton utilized the
75 critical distance criterion for re-solution as well, ignoring the centrally located atoms in the bubble. However, due to the larger bubble sizes in their study, the critical distance was not held constant, but rather allowed to increase in order to compensate for the lower atomic densities present in larger bubbles.

While re-solution in oxide fuels has been studied experimentally, the lack of
80 specific experiments to measure the re-solution parameter in uranium carbide makes direct verification difficult [17]. Many UC irradiations focused on bubble populations as a function of temperature and burnup [24, 25, 26, 27, 28]. Through the use of rate-equation type models, it may be possible to correctly simulate the bi-modal behavior that exists in UC fuel irradiated at high tem-
85 perature [29].

An important link in such a rate-equation model is the bubble loss term, thus motivating the current work to develop a radius dependent re-solution parameter for use in fission gas bubble simulations. By using BCA to calculate the trajectory of fission fragments and their subsequent cascades, the fraction of
90 atoms that escaped the bubble and became implanted in the surrounding fuel was tracked, resulting in a re-solution parameter that can be used to calculate the total re-solution rate. We will show that the re-solution parameter de-

creases as a function of radius up to a threshold. In addition, we will show that by accounting for electronic losses and through replacement of the hard-sphere
95 potential with the more realistic Ziegler-Biersack-Littmark (ZBL) universal potential, knocked uranium atoms have a much greater role in implanting gas atoms than previously thought.

2. Methodology

The BCA code 3DOT [30] was used for all calculations in the current work.
100 3DOT is based on Schwen’s 3DTrim [31] which utilizes the previously published TRIM algorithm [32] to track ion cascades in non-Cartesian geometry. The TRIM algorithm utilizes the ZBL universal potential to model the interactions between moving ions and stationary samples, and calculates the electronic stopping power by scaling proton stopping powers using the Brandt-Kitagawa theory
105 [32, 33]. Due to the nature of TRIM calculations, each ion interacts with an undamaged, 0 K amorphous target.

Each 3DOT simulation model consisted of a fuel cube with an implanted sphere of xenon. Owing to the small computation expense of BCA and the wide spread of bubble sizes present in uranium carbide [19], the simulated bubble radii
110 ranged from 0.5 nm to 500 nm with periodic boundary conditions enforced on all box sides. As the current study was focused on intra-granular bubbles, grain boundary effects were not considered and the theoretical density of 13.63 g/cm³ was assumed for uranium carbide. Fission fragments were randomly created based on the probability distribution functions of typical fission fragment mass
115 and energies.

For these calculations, a fission gas atom was considered implanted if it exited the bubble surface with an implantation energy greater than E_{min} . The value of $E_{min} = 300$ eV first utilized by Nelson has been implemented in many re-resolution studies [12, 17, 18]. More recently, a study aimed at determining the
120 implantation energy in UO₂ fuels determined that while re-resolution did occur for atoms with implantation energies less than the 300 eV, the original implantation

energy of 300 eV resulted in a 85% probability of re-solution [34]. In light of this, the value of $E_{min} = 300$ eV will be utilized unless otherwise specified, although model sensitivity to this value will be explored.

125 The total re-solution rate at which atoms are knocked back into the fuel can be calculated by,

$$R [\text{atom}/(\text{s} \cdot \text{m}^3)] = \int \dot{F} b(r) m(r) \rho(r) dr, \quad (1)$$

where r is the bubble radius, $\dot{F}$ is the fission rate, b is the re-solution parameter, m is the number of atoms in a bubble, and ρ is the bubble concentration distribution function,

$$N [\text{bub}/\text{m}^3] = \int \rho(r) dr. \quad (2)$$

130 Here, N is the total concentration of bubbles in the sample.

In stress free solids, the number of atoms in a bubble m is generally calculated using the Van der Waals equation of state (EOS):

$$m = \frac{4}{3} \pi r^3 (B + kTr/2\gamma)^{-1} \quad (3)$$

where $\gamma = 1$ N/m is the surface energy of uranium carbide [35], k is Boltmann's constant, T is temperature, and $B = 8.5 \times 10^{-29}$ m³/atom [20]. However, the high
 135 temperature and stress involved with very small bubbles in nuclear fuel results in an underestimation of atomic density, thus the EOS values calculated by Ronchi were utilized at small bubble radii [36]. Although more recent evaluations show that the atomic density may actually be higher in very small bubbles [37], a smooth transition from Ronchi's data for small bubble sizes to values calculated
 140 using Equation 3 is utilized to calculate the atom density in the bubble due to the large spread of bubble radii, giving the "Combined" model types, as displayed in Figure 1.

Considering the many combinations of bubble radii and box sizes, any dependence on simulation volume must be removed. Due to the periodic boundary
 145 conditions, the approximately 6 μm fission fragment path will wrap around the model many times. Due to the relatively low density within the bubble, as the porosity increases, the total fission fragment path will also increase. In order

Figure 1: Atomic densities calculated from different EOS models.

to avoid a bubble concentration dependent path length, comparative studies of various bubble and box sizes showed that the artificial lengthening of the fission
150 fragment path was minimized when the cube length was at least 10 times the bubble radius. In this way, a value for b can be calculated independent of the bubble concentration.

2.1. Applicability of BCA

The ability of 3DOT to quickly analyze ion trajectories lies in the basic BCA
155 simplification in which each collision is modeled as a single two-body collision. While this approximation is physically appropriate for high ion energies (typically above 1 keV), multi-body collisions tend to occur at lower ion energies. Several publications have attempted to quantify the limits of BCA with limited success [38, 39, 40, 41].

160 The error introduced by BCA must be quantified in order to justify its use within this study. Fortunately, the use of a threshold implantation energy allows all ions below E_{min} to be ignored. Above this limit, the error introduced by ignoring multi-body collisions can be estimated by calculating the maximum deviation that can occur from the next nearest-neighbor atom. If the angular
165 and energy difference from the otherwise ignored atom has minimal effect on

the re-resolution rate, then the use of BCA is appropriate in this study for ions down to E_{min} .

In general, the kinematics of two body collisions can be described by the angle of deflection of the ion, θ . The energy transfer T can then be calculated

170 as,

$$T = \Lambda E_0 \sin^2(\theta/2), \quad (4)$$

where $\Lambda = 4m_1m_2/(m_1 + m_2)^2$, and E_0 is the initial ion energy. In 3DOT, the value $\sin^2(\theta/2)$ is calculated using the ZBL potential with the ion and target atomic attributes, and the impact parameter p . As with all potentials, the smaller the impact parameter, the larger the angular deflection. Using Equation 4, large angle deflections correspond to high energy transfer. The greatest effect a second body can have on an ion, and thus the smallest impact parameter, is exactly between two atoms. The deviation caused by a target atom at this minimum impact parameter will estimate the angular deviation that is ignored by the BCA approximation in the worst case scenario.

180 In general, the fission gas escape process can be separated into two events. First, a fission gas atom must be hit by either a fission fragment or by a fuel atom that has been knocked out of its lattice site by a fission fragment. Due to the random nature of fission fragment creation in 3DOT, any error introduced to the fission fragment scatter angle can be ignored as long as all fission fragments are treated similarly. The same is also true for lattice atom (uranium and carbon) collisions. However, since the energy of knocked fission gases needs to be explicitly tracked, fission fragment and lattice ion energies must be correctly tracked for all ion energies above E_{min} . Uranium carbide has a simple cubic NaCl crystal structure with a lattice parameter of roughly 0.5 nm, resulting in $p_{min} = 0.125$ nm as an ion travels between a uranium and carbon atom. Due to the Λ factor included in the energy transfer equation, uranium-uranium collisions result in the highest energy transfer. Using the minimum impact parameter, the maximum energy transferred in a uranium-uranium collision is 60 eV for all initial ion energies. This value quickly diminishes as the impact

parameter increases, reducing to less than 3 eV when the impact parameter is 0.2 nm. In the worst possible case, a lattice atom with energy 300 eV will overestimate the ion energy after a collision by 20%. However, the probability of such an event is small enough that BCA accurately represents fission fragment and lattice collisions for the purposes of this work.

The second event that must occur to create an implanted atom is the transport of a fission gas atom from the interior to the surface of the bubble. As opposed to the fuel lattice, both fission gas ion energy transfer and angular deflection are both important to track, as a knocked fission gas atom can receive a large-angle deflection very near the bubble surface. In the amorphous bubble region, the distance between fission gas atoms in the bubble d can be approximated by,

$$d = 2 p_{min} = 2 (3/4\pi m)^{1/3}. \quad (5)$$

Using the Combined EOS described previously, the density in a 1 nm bubble at 2000 K is 15.3 atoms/nm³. Since the minimum impact parameter occurs directly between two atoms, $p_{min} = 0.25$ nm. At this large of an impact parameter, the direction of the ion in a representative Xe-Xe collision deviates by only 2° with an initial ion energy of 300 eV. The ion energy must be reduced below 10 eV to result in a deviation of greater than 30°. In addition, such small deflections result in negligible energy transfer. Since these deviations occur during the most conservative atomic densities and smallest impact parameters, reduction of collisions within the bubble to single collisions was deemed appropriate for this work.

3. Results

Figure 2 shows the re-resolution parameter b as a function of radius r for different EOS models, where b represents the number of escaped atoms per bubble atoms for a single fission and single bubble. A quick decrease initially occurred, reducing b nearly 60% as the bubble radius increases from 1 to 50 nm, beyond which the re-resolution parameter became nearly constant. Since b was

calculated on a per bubble atom basis, it represents the average probability of any given bubble atom to be implanted. As the bubble radius increases, interior atoms have further to travel before becoming implanted, resulting in the quick decrease in b as a function of radius. However, as r becomes larger than 10 nm, the atomic density exponentially decreases as a function of radius (Figure 1), boosting the probability of a struck interior atom reaching the surface and flattening b as a function of radius. If the bubble sizes increase past the radii of interest present here, the low atomic density will eventually serve to create a positive slope in the re-resolution parameter at very large radii.

Figure 2: Calculated b for several atomic density calculation methods.

Figure 2 also includes the re-resolution parameter using different EOS methods: combined at 1000 K, 1500 K, and 2000 K, and van der Waals at 1500 K. In general, b was inversely proportional to the atomic density, producing fewer implanted ions at higher atomic densities.

As discussed previously, there is some uncertainty on the value of E_{min} . Figure 3 displays b for various values of E_{min} at 1500 K. Previous studies have shown that E_{min} may be less than 300 eV [34]. By reducing the assumed E_{min} to 150 eV, the re-resolution parameter only increases by 30%, without much variation in the shape of the curve.

Figure 3: Calculated b for various E_{min} thresholds.

A gas atom can be knocked out of the bubble after first being struck by either a fission fragment or indirectly through a fuel cascade. Figure 4 displays the fraction of implanted gas atoms that were a result of either a fuel cascade or solely through a direct fission fragment hit in a 5 nm bubble at 1500 K. Roughly 90% of all implanted ions were a result of a cascade started within the fuel, showing the overall importance of fuel cascades over direct fission fragment collisions.

As ions propagate through the material, they produce additional “daughter” ions by knocking atoms from their lattice site. Figure 5 displays the probability of each type of “parent” as a function of bubble radius. For nearly all bubble radii, the direct fission fragment contribution remained near 10% due to the low cross-section of small bubbles and low interaction probabilities for low density, large radii bubbles. Due to their small mass and Λ factor, the relative importance of carbon atoms was insignificant. For very small bubble sizes, the majority of all collisions were a result of uranium atoms directly knocking out fission gas atoms. The increase in fission gas parents indicates that as the bubble size enlarged, a knock-on effect occurred, resulting in implanted atoms different than the original struck gas atoms.

Figure 4: Probability of a direct fission fragment implantation or fuel cascade implantation.

As shown in Figure 4, the importance of fission fragment collisions were relatively minor compared with the importance of fuel cascades. However, it can be expected that the highly energetic fission fragments create daughter ions with relatively high energies, thus resulting in more energetic and more deeply implanted atoms. This phenomenon can be shown by plotting the re-resolution parameter in a 1500 K 5 nm bubble as a function of E_{min} , (Figure 6). For low E_{min} energies, fuel cascades have a much higher importance in the total re-resolution parameter than fission fragments, similar to what was displayed in Figure 5. However at a crossover energy of about 40 keV, fission fragment interactions produced more implanted atoms than fuel cascades.

4. Discussion and Conclusions

When comparing the current work to the previous calculations, two results seem to conflict. The first is that for a bubble radius of 5 nm, we found the re-resolution parameter to be $1.4 \cdot 10^{-25}$ atoms/(fns $\cdot$ m³), an order of magnitude less than the previously calculated value of $b = 3 \cdot 10^{-24}$ atoms/(fns $\cdot$ m³) [17, 12]. In addition, the previous re-resolution parameter vs. E_{min} results showed the cascade/fission fragment importance cross-over occurring at 5 keV, while

Figure 5: Parent fractions as a function of bubble radius.

our calculations show a cross-over at 50 keV. The reasons for these differences are rooted in differences between the models used in each study and warrant discussion.

By tallying energy losses in a 3DOT simulation, we found the amount of energy dissipated due to electronic losses accounted for about 90% of the original fission fragment energy. In light of this, it can be expected that by ignoring these losses, the fission fragment range, and thus b , will increase by an order of magnitude. This was verified by running 3DOT simulations without accounting for electronic losses in which we calculated the re-solution parameter for a 5 nm bubble at 1500 K to be $b = 4.8 \cdot 10^{-24}$ atoms/(fsn·m³), within 50% of the previously calculated value [17].

One of the largest improvements over the previous studies is the use of the ZBL potential for all atoms and energies, as opposed to the Rutherford potential for fission fragment collisions, and the hard-sphere potential for all other collisions. The Rutherford potential is an adequate representation of high energy ion collisions, and in fact is utilized in 3DOT at high ion energies [32]. Conversely, the hard-sphere approximation is adequate for very low ion energies. However, at intermediate energies, neither approximation is appropriate [42].

Figure 6: Re-resolution in a 5 nm bubble due to fission fragment and fuel cascades as a function of E_{min} .

The hard-sphere potential calculates the scattering angle for use in Equation 4 from the geometry of the problem, thus each scatter is independent of the ion's energy. This results in a much higher probability of high angle collisions and ultimately an underestimation of an ion's range. When applied to lattice atoms, the hard-sphere potential ensures that an entering ion will only penetrate a short distance into the bubble. Likewise, gas atoms far from the bubble surface have a low probability of re-resolution due to an enhanced probability of large-angle scatter events. With the more physical ZBL potential, the scattering cross-section is inversely proportional to the ion's energy, thus uranium atoms are allowed to penetrate to more realistic depths. In addition, all atoms in the bubble become "available" for re-resolution, albeit with a frequency less likely for atoms near the center of the bubble. Since the ZBL potential is well approximated by the Rutherford potential, similar behavior is not reproduced in the highly energetic fission fragments that were originally treated with a purely Coulombic potential. All of this resulted in a higher probability of the less energetic lattice cascades, shifting the fuel cascade contribution to b to higher E_{min} values in Figure 6, and increasing the cross-over point to 50 keV.

One final note about the previous studies must be addressed; one of the most

interesting results from Ronchi and Elton was a positive slope in the re-resolution parameter at high radii and high E_{min} [17]. It should be noted that the value plotted is actually the combination of the product of the re-resolution parameter and critical distance, thus the positive slope is heightened by an increasing critical distance as a function of radius. Although similar phenomenon can be achieved with the results from 3DOT, they were not nearly as drastic without the inclusion of the critical distance.

In conclusion, due to the relatively high energy transfer material properties in uranium carbide, fission gas re-resolution can be modeled using the homogeneous, atom-by-atom loss model. We found a re-resolution parameter that was an order of magnitude lower than previous studies due to the inclusion of electronic ion energy losses in this study. A decrease in the re-resolution parameter as a function of radius occurred for low radii, with a nearly constant re-resolution parameter for radii above 50 nm. The BCA approximation allowed the computationally cheap analysis of many different types of bubbles, and it was shown that the fundamental BCA assumption is appropriate for use in the simulations presented here. Through comparative studies on the re-resolution parameter for various values of implantation energy and atomic density in the bubble, we found that while the re-resolution parameter did change, the overall shape did not. The re-resolution parameter calculated here can be used in rate-equation type simulations to model fission gas bubble behavior, and ultimately fission gas release.

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