Modeling of the integrity of ZrN-coated U-Mo/Al dispersion fuel during fabrication

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ABSTRACT

After the promising results of the SELENIUM test, ZrN-coated UMo/Al dispersion fuel has gained attention and has received central focus for the next tests such as the EMPIRE and SAMPER FIDELIS. The purpose of the coating is chiefly to protect the UMo from interdiffusion with the Al. Fuel performance is, therefore, dependent upon the integrity of coating during plate rolling fabrication and irradiation. A FEM model was developed to assess the integrity of the coating. This paper reports the first part: simulation for the rolling stage. The second part, simulation for the irradiation stage, is a subject of a future study.

1. INTRODUCTION

Since interaction layer (IL) growth has been one of the challenges in the UMo fuel qualification in world-wide, there have been many methods to suppress IL growth. One of them was Si addition into Al matrix that contains UMo dispersion. It was an effective remedy for IL suppression until intermediate burnup range, but IL formation was still observed in the high burnup range above \sim 70% U²³⁵.

A technique for surface modification for UMo fuel kernel has been recently proposed to prevent IL formation at UMo and Al interface by a thin coating layer as a diffusion barrier [\[1\]\[2\].](#page-8-0) Candidate materials as a surface coating are Si and ZrN. It was shown that they indeed could play a significant role to reduce IL formation effectively.

However, it was also observed IL growth still proceeded on the surface of UMo fuel kernels where the coating layer was not intact by crack formation. As the thickness of coating layer is

 \sim 1 µm for ZrN and \sim 0.6 µm for Si [\[2\],](#page-8-1) the coating layer is vulnerable to any compressive force exerted during plate rolling fabrication process. In this regard, it is necessary to investigate whether or how those coating layers on UMo fuel kernels are possibly fractured during fabrication and furthermore during irradiation period.

In this study, the plate rolling process is simulated to evaluate the integrity of ZrN coating layers after fuel plate fabrication with rolling process by using finite element method(FEM).

2. ROLLING SIMULATION

Rolling is one of metal forming processes to transform preformed shapes into a form suitable for further processing. UMo/Al dispersion fuel plate is typically produced by both hot and cold rolling. The plate is passed through a gap between two rollers with typical range of the reduction ratio from 10 to 30% per each pass.

In the rolling process, a dimensional change in the thickness direction is most significant since other directions are rather constrained. The thickness changes of fuel plate during rolling step are summarized in Table. 1

Table 1 Summary of dimensional changes during rolling process utilized in FEA simulation.

[Fig. 1](#page-2-0) shows schematics showing plate fabrication sequences: plate assembling, plate rolling, and finalization. Typically, two Al alloy cover plates are welded in a picture frame. They cover the meat compact. This assembly passes through rollers according to pre-determined fabrication parameters including rotation velocity, roller size, and draft size. After rolling, the formed plate assembly undergoes finalization process for obtaining final product dimensions.

Fig. 1 Schematics of fuel plate fabrication by a rolling method.

The overall rolling process can be summarized in the following steps:

- Preheating step: A plate assembly, which is composed of two Al cladding covers welded to the top and bottom surface of a picture frame, is pre-heated in a temperature of 500°C for 50 minutes.
- Hot-rolling step: The heated plate is passed into the gap between two rollers with reduction ratio of 30% per pass. After each pass, the plate is re-heated for 10 minutes at 500°C to improve formability. Total number of hot-rolling pass is four.
- Cold-rolling step: After hot rolling, cold rolling is performed with adjustment of rotating speed, and the gap between rollers. The cold-rolling pass can be performed up to two tim es in maximum.

Both preheating step and hot-rolling step are considered for finite element analysis in this study.

3. FINITE ELEMENT MODELING

A reduced-size plate was modeled due to the complexity of the geometry in case of using a full-size plate. However, the dimensions used for the finite element analysis are sufficient to simulate the mechanical effects on the ZrN coating layer with several symmetric boundary conditions. A quarter-sized model is shown in [Fig. 2.](#page-3-0)

Fig. 2 A schematic of finite element modelling in the rolling simulation.

Two steps including the preheating step and hot-rolling step are implemented in the finite element analysis. In the preheating step, it is assumed that fuel plate is thermally steady-state for 50 minutes.

A constant angular velocity of 1 revolution per second (6.28 rad/sec) was applied to the roller. It corresponds to a roller surface speed of 0.2 m/sec. Since rolling is normally performed at a relatively low speed, it is natural to assume that static analysis is the proper modeling approach. Thus, as inertia effects are not significant at this speed, so the response is quasi-static. A quasistatic implicit method is employed for the rolling step.

A surface-to-surface contact condition is applied between the roller surface and the plate surfaces with a friction coefficient of 0.3, as it is the most important mechanism by which the plate is pulled through the rolling stand.

Symmetric conditions were applied in the width and thickness directions, so only a single pass rolling on the plate top surface was considered.

3.2. MATERIAL PROPERTIES

Mechanical properties used in the FEM simulation are summarized in [Table 2.](#page-4-0) Only elastic response is considered for the UMo due to the fact that UMo has higher rigidity than Al. Both elasticity and plasticity are applied to Al alloy cladding (AA-5154) and matrix (AA-1060) with strain hardening coefficients of 0.23 and 0.133, respectively. Other properties are also used for the thermal stress calculation.

For mechanical properties of ZrN, it is known that its properties are dependent on fabrication method, and particularly on the coating layer thickness. Since no data are available for this thinfilm sized coating layer, its mechanical properties in the bulk size are used in the simulation. Since the thin-film sized ZrN is highly likely to have much higher mechanical strength due to very fine grain size, the use of mechanical properties of bulk sized ZrN could be justifiable as a conservative approach.

Failure of ZrN coating layer was assumed to be the initiation of crack formation, at 2% plastic strain with the direct crack stress of 587 MPa [5]. The failure of the coating layer was then determined by checking whether the total plastic strain from the simulation results exceeded 2% plastic strain.

Table 2 Summary of material properties used in the simulation.

Failure of ZrN coating layer was assumed to be the initiation of crack formation, at 2% plastic strain with the direct crack stress of 587 MPa [\[5\].](#page-8-4) The failure of the coating layer was then assessed by evaluating whether the total plastic strain from the simulation results exceeded 2% plastic strain.

4. PRELIMINARY RESULTS

4.1. Post pre-heating step results

[Fig. 3](#page-5-0) shows a contour for the Von Mises stress exerted on ZrN coating layer during a preheating step at 500°C. A Higher magnitude of stress was obtained from ZrN coating layers near to the clad-matrix interfaces since heat flux flows into the fuel meat region from the Al cladding, which causes a larger extent of the difference in thermal expansions between Al matrix, UMo fuel particle, and ZrN coating layer.

Fig. 3 A contour of Von Mises stress for ZrN coating layers.

Some ZrN coating layers undergo yielding by the stress higher than its yield strength (see [Fig.](#page-5-1) [4\)](#page-5-1). A stress exceeding the yield strength of ZrN is an indication of a brittle fracture. Hence, a finite element with yielding can be interpreted as a fracture in the coating layer.

4.2. Post hot-rolling step results

[Fig. 5](#page-6-0) shows a contour of Von Mises stress and total true strain of ZrN coating layer after hotrolling process. The magnitude of the von Mises stress is lower than its yield strength and fracture strength. In addition, the total true strain is calculated to be lower than the failure strain, suggesting that most of the ZrN layers during the hot-rolling step maintain mechanical integrity.

(b) Total true strain

Fig. 5 Contour for (a) Von Mises stress and (b) total true strain on ZrN coating layer after fourtime passed.

[Fig. 6](#page-7-0) shows contours of the Von Mises stress and effective plastic strain for Al cladding and Al matrix region. Plastic flows of both Al cladding and matrix, particularly in the Al cladding region, are likely to play a significant role in mitigating stress exerted on ZrN coating layers. Thus, no more damage and fracture are expected to form during hot-rolling step.

(b) Equivalent plastic strain

Fig. 6 Contours showing the Von Mises stress and equivalent plastic strain for Al cladding and Al matrix regions.

5. SUMMARY

A finite element simulation by using ABAQUS was performed for hot-rolling fabrication to assess the integrity of ZrN coating layers on UMo fuel particles. Two fabrication steps including preheating step and hot-rolling step with four passes were considered. Some ZrN coating layers were predicted to be failed by yielding during pre-heating step due to the differences in thermal expansion of UMo, Al, and ZrN. However, no significant damage and fracture for ZrN coating layer were predicted because of the high plasticity of Al cladding and Al matrix. Thus, it can be concluded that the ZrN coating layers lost their integrity observed from the SELENIUM test [\[7\]\[8\]](#page-8-5) occurred during irradiation by fuel swelling induced stress.

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