Effect of the difference in the distribution of crystallographic orientation on the irradiationinduced deformation of Zr-2.5wt%Nb material

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1. Introduction

A pressure tube used in CANDU (Canada Deutrerium Uranium) reactor is the one of the most important structural component in the fuel system. The integrity of the tube is the main concern in the points of safety and efficiency of the reactor. Unfortunately, the harsh operation condition with high neutron flux and high temperature leads unwanted deformation in the dimension of the tube, for example, expansion and elongation. So, predicting the dimension change is necessary for the reactor.

Texture, which describes the distribution of the crystal orientations in a material, is a well-known microstructure parameter affecting the pressure tube deformation [1]. Crystal plasticity based deformation model of single crystal and texture information can be applied to the pressure tube deformation [1]. In order to explicitly separate the effect of texture from the other parameters affecting the deformation, the crystal plasticity based modeling method is a proper approach.

In the study, the effect of the difference in the distribution of crystal orientations on the tube deformation was analyzed using crystal plasticity finite element method (CPFEM) with some texture information having slightly different distributions.

2. Methods and Results

In this section some of the equations used to characterize the texture and predict the tube deformation are described. The brief results are shown as well.

2.1 Kearns Factor

In many studies, Kearns factor is used to simply express the crystal orientation distribution in hexagonal close-packed structure material [2]. The following equation display how to calculate the factor.

$$F_i = \sum V_i \cos^2 \theta$$

where F_i , V_i and θ are Kearns factor along `i` direction (`i` = axial, radial and transverse direction in the tube), the volume fraction of the (002) basal fiber and an angle with the fiber and the `i` direction, respectively. Since the factor indicates the fraction, three factors along three main directions necessarily sum to one. Through the factors, the texture of the tube can be quantitatively characterized with only three numbers.

Fig. 1 shows the pole figure of (002) basal plane on the transverse plane. Base on the figure, 0.629, 0.340 and 0.031 of Kearns factors along transverse, radial and axial directions were obtained, respectively.



Fig. 1. Pole figure of (002) basal plane on the transverse plane where 'x', 'y' and 'z' axes indicates axial, radial and transverse, respectively.

2.2 CPFEM

Crystal plasticity theory is applied into finite element software (ABAQUS) through user-subroutine 'UMAT'. The main deformation mechanisms in the pressure tube under operation are thermal and irradiation creep. Two mechanisms are assumed to independently contribute to the total irradiation deformation. The deformation rate of single crystal having the mechanisms is defined by,

$$\dot{\varepsilon}_{ij} = \sum_{s} \dot{\gamma}_{0}^{s} \left(\frac{m^{s}:\sigma}{\tau^{s}}\right)^{n} m_{ij}^{s} + K_{ijkl}\sigma_{kl}$$

The first term in the right side is the constitutive equation about thermal creep and the other is about irradiation creep. All parameters used in the model had been optimized using the measured data from CANDU reactor and then fixed except the texture information when the deformation was predicted.

2.3 Texture

For our analysis, some texture information having same Kearns factors to the values from the tube but some different profile in the intensity from the radial direction to the transverse direction was generated using MATLAB with a free-software MTEX. Fig. 2 shows the three profiles obtained from the tube (the first graph) and the generation process (the second and third graphs).



Fig. 2. Intensity profiles (left) along the line from the radial direction to the transverse direction as shown right pole figure. Top is of the tube and middle and bottom are of the generation process.

2.4 Tube Expansion

Fig. 3 shows the expansion strain along the tube calculated using the tube texture (left) and the generated tube texture (right). Since a finite number of crystal orientation was considered in the calculation, difference choice from the same texture can lead some variation in the results, however, their difference is insignificant when the same texture is used as seen in fig. 3 (a). On the other hand, the calculated strain values are quite different if the intensity distribution along the line from the radial to the transverse changes as found in fig. 3 (b).

The clear difference found in fig. 3 implies even if Kearns' factors are almost same the deformation trend can show significant diversion by changing the specific distribution of orientation.



Fig. 3. Calculated tube expansion strains using randomly generated orientations from (a) the tube and (b) the generate texture information.

3. Conclusions

In order to analyze the effect of the difference in the distribution of crystal orientations on the tube deformation, crystal plasticity finite element method (CPFEM) and some texture information having slightly different distributions were used. Through the calculation, we found that the difference in the profile of texture intensity introduces significant difference in the deformation trend in the tube even though whole textures show the same Kearns factors.

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