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Modeling of sink-induced irradiation growth of single-crystal and polycrystal zirconiums in nuclear reactors

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ABSTRACT

The objective of this study is irradiation growth modeling of polycrystal zirconium using the advanced mean-field rate theory (MFRT) and growth equation. Since the 1960s, irradiation growth of zirconium has been among the most important phenomena in nuclear reactors. However, there is no general irradiation growth model that can explain changes in both the microstructure morphology and growth strain in polycrystal zirconium owing to lack of knowledge of the relevant atomistic information and MFRT. Although two groups have developed a single-crystal zirconium irradiation growth model, a general polycrystal zirconium model has not been developed. In this study, therefore, the defect flux was calculated using the MFRT, and the dislocation loop density was calculated from the defect flux. Moreover, the bias factor for each sink (dislocation lines, loops, and grain boundaries) was adopted in the MFRT. In addition, dislocation line and grain boundary effects were examined in polycrystal zirconiums. Finally, irradiation growth equation was established and growth strain was calculated using the average strain factor and anisotropy factor considering grain-interaction. For single-crystal zirconium and cold-worked polycrystal zirconium, irradiation growth strain results show good agreement with the experimental results. For annealed polycrystal zirconium, the results deviate from the experimental results.

1. Introduction

Zirconium and its alloys are widely used as nuclear fuel cladding and guide tubes in commercial and research reactors because of their excellent radiation and corrosion resistance. However, despite these excellent properties, irradiation growth occurs. Irradiation growth is volume-conservative distortion without applied stress. It is distinguished from other radiation-induced dimensional changes such as swelling and creep. Radiation-induced swelling is isotropic volume expansion without any applied stress, whereas radiation-enhanced creep is volume-conservative distortion due to applied stress. Zirconium, hafnium, and titanium are representative materials that exhibit irradiation growth. Therefore, the in-pile behavior of zirconium has to be verified; hence, zirconium alloys have been demonstrated by many theoretical and experimental methods since the 1960s.

Traditionally, radiation-induced phenomenon such as swelling, creep, and growth are simulated using the mean-field rate theory (MFRT). The defect concentration and sink strength and density are calculated using the MFRT. In the early 1980s, much theoretical research on irradiation growth was based on the MFRT [1–3]. However, in early studies of the MFRT, this application was limited to the region of low displacements per atom (dpa) because of limited computation performance. Moreover, the MFRT could not possibly explain changes in the irradiation growth rate with temperature because there was no fundamental understanding of irradiation phenomenon. Therefore, irradiation growth modeling failed to precisely predict zirconium irradiation growth. However, at the end of the 1980s, these problems were solved by the development of two concepts. First, Woo suggested the diffusion anisotropy difference (DAD) concept, which explains that irradiation growth is caused by the difference between the diffusion coefficients of the <*a*> and <*c*> axes [4,5]. Second, Holt et al. [6] showed that the production bias model (PBM) effects this difference. The PBM concept, which is based on computer simulation science, assumes different fractions of interstitial and vacancy

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clusters. In addition, with the development of computers, the calculation region for irradiation growth could be expanded to hundreds of dpa [7].

With progress in the MFRT, irradiation growth was calculated independently for single crystals by two groups, Christien et al. [8] and Golubov et al. [7]. Both of the calculation results show good agreement with measured single-crystal irradiation growth. Christien et al. used the cluster dynamics model (CDM) of point defects to calculate the growth. In this model, it was assumed that only point defects are mobile, and all the clustering defects are immobile. Although neutron-induced defects are not the only point defects, electron irradiation generates only point defects. Therefore, this model is quite reasonable for electron irradiation. However, Christien work has some argument in the modeling assumption. First, the diffusion coefficient used in their model was much smaller (10^{-1} order) than the computer-simulated value [9]. Second, the defect concentration was assumed to be homogenous in the matrix; hence, the interstitial defect flux is much higher than the vacancy defect flux anywhere. Therefore, only an interstitial dislocation loop could survive in the prism plane in the framework. In contrast, Golubov et al. [7] used the PBM to calculate the growth strain. The concept of the PBM is opposite to that of the CDM. Specifically, interstitial clusters are mobile defects in the PBM but not in the CDM. Therefore, in the PBM framework, interstitial clusters could be the most important influence on the growth modeling result. However, Golubov et al. [7] neglected the effect of defect recombination. Therefore, the work of both groups has certain limitations. The irradiation growth rate of cold-worked polycrystal zirconium was calculated in a wide temperature range [6]. However, this model did not explain the irradiation growth of annealed polycrystal and single-crystal zirconium because dislocation line, loop, and grain boundary effects are harder to predict than those of cold-worked polycrystal zirconium.

Therefore, there is no general prediction model of irradiation growth that could explain zirconium from single crystals to polycrystals, although prediction modeling of single-crystal zirconium growth and cold-worked polycrystal zirconium has been done using the MFRT and growth equation. Therefore, this paper focuses on theoretical modeling of single-crystal and annealed and cold-worked polycrystal zirconium irradiation growth, which could fully explain the microstructure and growth strain. To predict the growth of various types of zirconium, a simplified assumption was developed that point defects evolve directly from sinks such as dislocation loops, dislocation lines, and grain boundaries.

2. Methodology

2.1. Irradiation growth mechanisms

To model irradiation growth of zirconium, several basic mechanisms should be defined. First, the sink characteristics are simply defined by the results of experimental work because the characteristics of sinks have been identified as the most fundamental reason for irradiation growth of zirconium by an experiment at Northern Research Laboratories of United Kingdom Atomic Energy Authority [10–15]. Next, the effects of sinks on irradiation growth of zirconium are established by considering the sink characteristics. Finally, in order to describe polycrystal irradiation growth, the effect of grain interaction was briefly reviewed.

2.1.1. Characteristics of sinks

In single-crystal zirconium, unlike the polycrystal case, grain boundaries are not considered [10,11]. Therefore, dislocation lines and loops are the major sinks causing irradiation growth. Dislocation loops are either <*a*> or <*c*> dislocation loops, which are perpendicular to the corresponding axis. Experimental results have confirmed that all <*a*> and <*c*> dislocation loops have a uniform direction [16–19]. Specifically, <*a*> dislocation loops have a Burgers vector $\vec{b} = 1/3 <1\,1\,2\,0>$, which is parallel to the *a* axis and lies in the prismatic plane $(10\bar{1}0)$. Moreover, these types of loops are observed to coexist as vacancy and interstitial types in the prism plane. In contrast, <*c*> dislocation loops lie in the (0 0 0 1) plane, and the Burgers vector is $\vec{b} = 1/2 <0\,0\,0\,1>$ or $\vec{b} = 1/6 <2\,0\,\bar{2}\,3>$ along the *c* axis [20]. Further, <*a*> dislocation loops are generated immediately after irradiation, whereas <*c*> dislocation loops appear after several dpa.

In polycrystal zirconium, dislocation loops and lines are generally considered to be main sinks, and grain boundaries are also considered to be main sinks [12–15]. However, the sink characteristics of grain boundaries are hard to establish experimentally owing to their three-dimensional shapes. Therefore, several different models of the sink strength of grain boundaries are considered in the MFRT. (Physically, the sink strength determines the defect reaction rate with the sink at a given defect diffusivity and concentration.) Among these models, that derived by Brailsford and Bullough [21] considers the sink strength of grain boundaries when the dislocation density is sufficiently high compared with that of any other sink. (This is explained further in section 3.1.) MacEwen and Carpenter [2] used Brailsford and Bullough's grain boundary model [21] because it was assumed that both annealed and cold-worked polycrystal zirconium have a high number of dislocation loops and high line density. However, MacEwen and Carpenter calculated irradiation growth of zirconium only at the beginning of the few-dpa region, and their results are inconsistent with experimental results owing to the lack of information in the experimental database and lack of atomistic constants. Therefore, Brailsford and Bullough's sink model of grain boundaries [21] is used in this model with the advanced MFRT and the latest constant. The sinks in hexagonal close-packed (hcp) zirconium are shown schematically in Fig. 1. The shapes and locations of dislocation loops, dislocation lines, and a grain boundary are sketched.

2.1.2. Effect of sinks on irradiation growth of zirconium

In dislocation line and loop-induced irradiation growth, defect reactions with dislocation lines and loops are the driving force. In the first stage, an irradiation defect is developed by the <*a*> dislocation lines and loops because they are interstitial bias sinks, as interstitials diffuse more rapidly than vacancies. This phenomenon could be expressed as a defect flux given by a diffusion coefficient ($D_{v\ or\ i}$) and a defect concentration ($C_{v\ or\ i}$). This concept is derived from the defect accumulation rate. Because the reaction rate with sinks is proportional to a given defect sink density, the defect flux is the defect accumulation rate at unit sink density. This concept is well established in the Brailsford and Bullough's work [21]; i.e., $D_iC_i >> D_vC_v$, where $D_i >> D_v$, and $C_v = C_i$ in dislocation lines and loops. Therefore, irradiation growth occurs in the <*a*> direction because <*a*> dislocation lines and loops have a Burgers vector of $\vec{b} = 1/3 <1\,1\,2\,0>$. In a single crystal zirconium, this initiation of irradiation growth, which is caused by the dislocation loop growth, occurrs in 0 ~ 1 dpa regime.

Next, in the middle stage, the <*a*> dislocation and loop densities are saturated because many of the interstitial defects are consumed by <*a*> dislocation loops. In this situation, <*c*> dislocation loops could be formed on the basal plane because the vacancy concentration is increasing; i.e., $D_iC_i = D_vC_v$, where $D_i >> D_v$, *and* $C_v >> C_i$. Because of the saturation of <a> dislocation loop in this stage, the strain of irradiation growth could be negligible in 1 ~ 4 dpa regime.

In the last stage, the <*c*> dislocation loops have consumed the vacancy defects in the basal plane. Therefore, the <*a*> dislocation lines and loops could absorb the interstitial defects, and the