INTRODUCTION

Irradiation of uranium-based nuclear fuel (UO₂, UC, UN) generates fission products and interstitial impurities. Among radiation-induced point defects, noble gases (krypton and xenon) stand out. They are notable for a low solubility in nuclear fuel. Therefore, gaseous fission products (GFPs) diffuse toward internal drains and the outer surface of the products. If intergranular pores serve as internal drains, GFPs reduce or even completely eliminate the Laplace pressure on the pore surface. This is accompanied by the diffusion migration of radiation-induced vacancies into the pore. The boundary of the pore moves, and its volume increases. Macroscopically, this process shows up as the gaseous swelling of nuclear fuel. When neighboring pores merge, the volume of a new pore will be larger than the total volume of individual pores.

Merging of pores along grain boundaries in a polycrystal results in the formation of extended intergranular channels through which fission products and interstitial impurities escape. The physical model of this process is as follows. First, cylindrical cavities arise near triple joints of grain boundaries (linear effect) due to grain-boundary sliding slowdown. Noble gases diffuse toward these cavities and reduce the Laplace pressure. After all GFPs are completely eliminated, the gases produce a radial pressure on the surface of the cavity. Circumferential tensile stresses arise near the cylindrical cavity, which wedge apart adjacent grain boundaries and facilitates cracking. If the circumferential stresses do not cause grain-boundary embrittlement of the material, the diffusion-controlled growth of pore nuclei takes place owing to a radiation-induced vacancy flow. Such is a qualitative pattern of formation of channels along grain boundaries through which fission products and interstitial impurities escape during nuclear fuel burnout.

A grain boundary in a nanodimensional polycrystal (Fig. 1) represents a finite-size polygonal wall of edge dislocations. It is bounded by triple joints on two sides. Wedge disclinations of opposite sign (disclination dipole) may serve as an elastic model of these joints. A finite-size polygonal wall of edge dislocations does not have a long-range stress field. The stress fields of individual dislocations cancel each other, so that the total...
stress exponentially decays along the normal to the grain boundary (according to the linear theory of elasticity). In the absence of the long-range stress field, the diffusion flow of radiation-induced point defects is due to their concentration gradient. Wedge disclinations (the elastic model of a grain-boundary triple joint) possess a long-range stress field. As a result, radiation-induced point defects migrate toward the triple joints of grain boundaries with a different dilatation. Interstitials diffuse toward the area of tensile stresses; vacancies, toward the area of compression stresses.

In this work, we mathematically simulate the GFP diffusion in the cylindrical cavity. GFPs arise near the triple joints of grain boundaries in nuclear fuel due to grain-boundary sliding slowdown. The article is constructed as follows. In Section 1, the elastic models of the triple joints of grain boundaries (the joints represent wedge disclinations of opposite sign) are considered. Section 2 is devoted to the GFP diffusion in the cylindrical cavity with regard to the first invariant of the wedge disclination stress tensor. Section 3 considers the diffusion kinetics of GFPs in the steady-state approximation. Simple analytical expressions for the Laplace pressure on the surface of the cylindrical cavity as a function of the wedge disclination stress field are derived. Analytical data for the diffusion kinetics of GFPs arising under nuclear fuel irradiation touch upon swelling of the fuel and the formation of channels through which fission products and interstitial impurities migrate along grain boundaries.

1. ELASTIC MODELS FOR TRIPLE JOINTS OF GRAIN BOUNDARIES

It is necessary to use the first invariant of the stress tensor of a wedge disclination for quantitative description of diffusion processes. This structural defect simulates the stress field of a triple joint under load. Analytically, the first invariant of the stress tensor logarithmically varies with the radial coordinate up to insignificant constants [1, 2],

\[
\sigma_{II} = -\frac{\mu\omega(1 + \nu)}{2\pi(1 - \nu)} \left(1 + 2\text{ln}\frac{r}{R}\right) , \quad r_0 \leq r \leq R . \quad (1)
\]

Here, \(\mu\) is the shear modulus; \(\nu\) is Poisson’s ratio; \(\omega\) is the Frank vector magnitude (in radians); and \(r_0\) and \(R\) are, respectively, the inner and outer radii of the wedge disclination environment. At \(\omega < 0\) (disclination with a negative dilatation), \(\sigma_{II} < 0\) on the inner surface of the disclination and \(\sigma_{II} > 0\) on the outer one. If \(\omega > 0\) (disclination with a positive dilatation), \(\sigma_{II}\) changes sign. Characteristic size \(r_0\) equals several interatomic distances, and \(R\) is half the mean distance between the triple joints of grain boundaries. Below, the value of \(\sigma_{II}\) for a free (not entering into a polygonal wall) edge dislocation is given for comparison.

![Graph: Reduced values of \(\sigma_{II}\) for the positive-dilatation wedge disclination, \(\sigma_{II} = \frac{2\pi(1 - \nu)}{\mu\omega(1 + \nu)}\), and edge dislocation, \(\sigma_{II} = \frac{\mu b}{1 - \nu}\), vs. the dimensionless radius at \(\frac{r}{R} = \frac{b}{R} = 0.01\).]

\(\sigma_{II} = \frac{\mu b(1 + \nu)}{\pi(1 - \nu)} \frac{\sin\theta}{r} , \quad r_0 \leq r \leq R , \quad 0 \leq \theta \leq 2\pi , \quad (2)\)

where \(r\) and \(\theta\) are polar coordinates and \(b\) is the modulus of the Burgers vector. The remaining parameters are designated as before. Quantity \(r_0\) describes the core of the edge dislocation (several interatomic distances), and \(R\) is half the mean distance between edge dislocations, which depends on their scalar density. Figure 2 plots dimensional quantities \(\sigma_{II}\) given by (1) and (2) versus the dimensionless radius at \(\omega > 0\) and \(\theta = 3\pi/2\). It is distinctly seen that these structural imperfections have long-range stress fields unlike edge dislocations entering into the polygonal wall, all other things being the same. Therefore, during fuel burnout, the fission products and interstitial impurities migrate largely toward the triple joints of grain boundaries and then are transferred through them.

The elastic energy of a wedge disclination indefinitely grows with the outer radius. Therefore, dislocation loops appear in the system. The dilatation fields are somewhat separated in space, which decreases arising stresses and keeps the material intact. Here, an analogy with an edge dislocation arises for which the fields of tensile and compression stresses are also close to each other (the separation is no more than several interatomic distances).

The triple joints of grain boundaries are concentrators of thermal stresses due to nuclear fuel irradiation. This is because the yield stresses of adjacent grains depend on the crystallographic direction. A wedge disclination serves as the elastic model of such stress concentrators. When grain-boundary sliding slows down, a cylindrical cavity arises near triple joints. Such is one