

IRRADIATION GROWTH IN ZIRCONIUM AT LOW TEMPERATURES BY DIRECT ATHERMAL DEPOSITION OF VACANCIES AT EXTENDED SINKS

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ABSTRACT

Irradiation growth is a dimensional change at constant volume experienced by anisotropic materials such as Zr alloys when exposed to neutron irradiation. Growth rates at 350 K, although smaller than at 550 K, are significant, and models based on migration of point defects have difficulty rationalizing its characteristics. We propose an irradiation growth mechanism based on the direct athermal deposition of point defects onto extended sinks. Self-interstitial atoms are deposited preferentially on crystallographically aligned sinks, either because of the cascade anisotropy in the Zr hcp structure, or because of their highly anisotropic diffusion through the lattice. The model is non-saturating, and the strain rate is linearly proportional to the flux as observed. Preliminary calculations show cascades are anisotropic, which can contribute to the observed growth strains.

1. Introduction

Irradiation growth of zirconium alloys has now been extensively studied both experimentally and theoretically. The salient characteristics of the long term growth of Zr alloy polycrystals are [1, 2, 3]: (i) expansion along directions containing a high proportion of **a**-axes, (ii) contraction along directions containing a high proportion of **c**-axes, (iii) an increase in the early growth rate with increasing density of the original dislocation network, (iv) the growth rate in materials with a low initial network dislocation density increases with fluence as the population of **c**-component defects (dislocations/loops) grows, and (v) the growth rate is linear in displacement damage rate at temperatures down to 330K.

There seems to be a consensus that at high temperatures (where vacancies are mobile) growth can be accounted for using a combination of :

a) the traditional rate theory description of growth and swelling originally developed by Bullough and co-workers [4], but where the driving force is the “diffusional anisotropy difference” (DAD) between vacancies and self-interstitial atoms (SIAs) as proposed by Woo and Gosele [5,6]. This theory seems to adequately explain growth at “normal reactor operating temperatures” (470-620 K).

b) the “production bias” theory developed by Woo and co-workers [7-9], in which different proportions of vacancy and interstitial “primary clusters” are formed in the cascades caused by neutron damage and these clusters are immobile, and therefore are only accessible to mobile sinks (dislocations via climb and glide). This theory appears to adequately explain the strong temperature dependence of growth at higher temperatures, associating that with the “evaporation” of the primary vacancy clusters.

Growth at lower temperatures is a different matter. Early results for cold-worked material irradiated at 330-350 K demonstrates the same shrinkage along directions containing a high proportion *c*-axes as at high temperatures [10] showing that true growth is occurring (approximating constant volume), and subsequent data at 330K indicated that, as at higher temperatures the steady state growth rate is linearly proportional to the displacement damage rate [2]. In annealed material the growth rate quickly saturates (unless there are significant built-in intergranular constraints [11]) and no further change in dimensions occurs (to fluences up many 10's of displacements per atom (dpa)).

In annealed material, the *a*-loop structure is barely visible by TEM (loops < 5nm). X-ray line broadening indicates saturation in the dislocation density after about 5 dpa. No *c*-component loops form in annealed material to fluences equivalent to ~ 40 dpa. Typically, the *a*-loop structure in cold-worked material irradiated at 330K is similar to that in annealed material, i.e. a high density of sub-5 nm loops, which appears to saturate quickly.

The major issue in explaining the growth in this temperature range is the disposition of the vacancies. With the rate theory/DAD formulation for growth, the sensitivity of the growth rate to displacement damage rate depends upon whether the point defect kinetics are “sink controlled” or “recombination controlled”. In the former case, the growth rate is linearly dependent on the displacement damage rate, while in the latter case the growth rate is proportional to the square root of flux. The transition from sink-controlled behaviour to recombination-controlled behaviour depends upon the vacancy mobility. Early attempts to model growth at low temperatures [2] assumed “facile” vacancy migration to be occurring in zirconium, with a much lower activation energy than would be expected based on melting point, and atomic size considerations [12]. Hood and co-workers [13,14] subsequently showed that the observations of low self-diffusion activation energies (attributed to “facile” vacancy migration) are an extrinsic effect associated with the presence, in solution, of Fe, which is hypothesized to form a fast diffusing binary complex with the vacancy [15]. Superficially, this effect would be expected to be infinitesimal at 333-353 K because of the low solubility of Fe. Irradiation is known to redistribute iron and it is possible that Fe solubility is enhanced under irradiation and this could explain the apparent mobility of vacancies in the HVEM.[16]

A study of growth of pure zirconium under proton irradiation at 350K [17] showed the growth rate, and the sensitivity of growth rate to flux to be independent of Fe concentration for concentrations of 5 and 64 ppm by weight (8 and 107 ppm atomic), the growth rate being linearly dependent on damage rate. Some Fe was transported to the surface of the (50 μ thick) specimens of both materials during the experiment indicating some interaction of Fe with the radiation-produced point defects. However, the total strain in the material with 5 ppm Fe during the experiment was >0.002. Even assuming that growth is 100% efficient (all of the vacancies actually causing measurable strain),

each Fe atom would have to account for the transport of > 250 vacancies to sinks in order to explain the linear growth rate sensitivity. During the experiment each Fe atom would have to travel about half the mean distance between sinks ($\sim 5 \times 10^{-8} \text{m}$) 250 times during the duration of the experiment ($1.33 \times 10^6 \text{s}$). This corresponds to a diffusion coefficient of $4.7 \times 10^{-19} \text{m}^2 \text{s}^{-1}$, 8-9 orders of magnitude faster than expected, based on extrapolation of high temperature data for diffusion of Fe in Zr [18].

Woo [3] is able to replicate most of the low temperature observations with a combination of the DAD driven rate theory and the production bias theory. Vacancies are immobile, but accumulate at sinks that are mobile. The displacement damage rate dependence was not reported, but the process is stated to be recombination dominated, and the calculated rate drops substantially ($\sim 5 \times$) with reduced temperature indicating a substantial increase in the vacancy concentration and reaction rate of SIAs with vacancies. Hence it seems likely that the predicted sensitivity of growth rate to displacement damage rate would be sub-linear and an alternative mechanism to explain the growth appears to be necessary.

In this paper, we will consider an alternative to the mechanisms proposed to date – direct deposition on existing network dislocations of point defect produced close to the initial knock-on event (a net vacancy deposition) combined with the escape of SIA's from the vicinity of the initial knock-on event by replacement collision sequences (RCS's). Net segregation of vacancies and SIA's to different sinks is attributed to the anisotropic diffusion of SIA's (thought to be ~ 20 times faster in the basal plane than in the *c*-direction at these temperatures [3,19]), or, alternatively to anisotropy in the number and length of RCS's which we will demonstrate using MARLOWE. We will compare the magnitude of the strains produced by such a mechanism with the observed strains.

2. Conditions for feasibility of athermal growth mechanism

Any new model must account for the work previously done. In addition, if we are to seek an alternative mechanism to rationalize irradiation growth at low temperature, then this mechanism must meet certain criteria:

(i) because the growth strains increase at an approximately steady rate up to very irradiation high doses the mechanism must operate at steady state (cannot be a transient mechanism operating only for a short time). This means that vacancies and SIAs must be eliminated at equal rates within the microstructure.

(ii) because the growth strains keep increasing with dose, the mechanism must be non-saturating, i.e. it cannot rely on microstructural sinks whose sink strength depends on dose.

(iii) the mechanism must provide a source of anisotropy, that is, the vacancies and SIAs must partition to crystallographically distinct sinks in the microstructure.

(iv) the order of magnitude of the calculated and observed strains must correspond.

As mentioned above, the main concern at low temperature is that the vacancy mobility is thought to be too low to provide a flux of vacancies to sinks to offset flux the SIAs to alternate sinks. In this paper, we propose that the direct interaction of the vacancy-rich cores of cascades with fixed network dislocations could result in the net deposition of vacancies. This mechanism we term a direct deposition or "DD". The source of the anisotropy then comes from the behavior of the SIAs, which are ejected from the core during the cascade, either thermally (as in the usual rate theory approach) or by an athermal mechanism. The anisotropy would arise from the highly anisotropic diffusion of the SIAs or from anisotropic creation of replacement collision sequences (RCS) which could also interact directly with sinks. The next section considers first the

viability of the DD mechanism for Zr alloys and then the anisotropic nature of RCS creation.

3. Calculations

The mechanism proposed here involves the interaction of a displacement cascade with the existing microstructure, originating either from the initial fabrication and processing of the material or from irradiation induced processes. In Zr alloys in addition to these irradiation-induced dislocation loops we have a pre-existing microstructure of cold-work dislocations and grain boundaries. All of these features represent microstructural sinks that can absorb the point defects (vacancies and SIAs) created by irradiation, if these migrate thermally to them.

If, as assumed here, the temperature is too low for long-range migration of vacancies to sinks, then the vacancies have to be deposited directly into the sinks through a cascade-dislocation interaction. The average energy of the atoms in a typical cascade is very high in the first few picoseconds after the PKA impact, and during that time the bulk temperature is less important. As the cascade cools down, thermal processes start to become important. It has been shown previously that in Zr alloys when a cascade interacts with a loop, the loop is reformed with few additional defects created [17]. This is because the size of the cascade is comparable to that of the dislocation loop and the loop essentially “ceases to exist” during the high temperature phase of the cascade. By contrast, a network dislocation line extends past the periphery of the cascade, so this provides a “memory” at the edge of the cascade that can orient defect deposition when the cascade cools. A similar process can occur at grain boundaries. We now perform calculations to determine whether direct deposition can indeed provide an adequate vacancy flux to sinks necessary to explain the observed growth.

3.1 Direct Deposition of Vacancies at Dislocations

We will consider the growth of 25% cold-worked and stress-relieved Zircaloy-2 which exhibits a growth rate of about $3 \times 10^{-29} \text{ n}^{-1} \cdot \text{m}^2$, or $1.2 \times 10^{-4} \text{ dpa}^{-1}$ during neutron irradiation at 350K [20]. We assume a network dislocation density of $\rho_d = 3 \times 10^{14} \text{ m}^{-2}$, and a cascade with a radius r_c of 4 nm. The probability that the center of such a cascade will impinge on a network dislocation is the volume fraction of material within a radius r_c of a dislocation, or

$$P_d = \pi r_c^2 \rho_d \quad (1)$$

Neutron irradiation creates a range of recoils, and the number of displacements depends on the recoil energy. The atoms that are displaced from their lattice positions can (i) recombine with a vacancy, thus annealing the damage, (ii) combine with other displaced atoms to form interstitial clusters or (iii) remain as isolated point defects. The relative importance of the three possibilities changes with recoil energy. It has been shown previously [19] that the fraction of isolated defects (or freely-migrating defects) can influence microstructural evolution under irradiation. We take a typical recoil energy of 20 keV, and use the NRT model with a threshold displacement energy of 40 eV to calculate displacements [23] obtaining

$$V_{NRT} = \frac{0.8 \times 20000}{2 \times 40} = 200 \quad (2)$$

Of these 200 displacements only about 48 survive immediate recombination according to Wooding [16]. Of these, 70% are in defect clusters [21], and are assumed not to be available. Thus 30% or 16 displacements (8% of the NRT displacements) are in

the form of individual defects. The corresponding SIAs are assumed to escape the core of the cascade, and the corresponding vacancies are assumed to be available for net direct deposition. Thus the volume shrinkage strain rate due to vacancy absorption is $(-1.5 \times 10^{-2} \times 0.08 = -1.2 \times 10^{-3} \text{ dpa}^{-1})$. There is an equivalent volume strain due to the SIAs which can reach sinks by thermal diffusion or by anisotropic DD.

Some fraction of the dislocations, (say 20%) have a **c**-component burgers vector, so the vacancy deposition causes a strain in the **c** direction of $-2.4 \times 10^{-4} \text{ dpa}^{-1}$. Assuming that the population of **a**-type dislocations is isotropically distributed, the remaining strain is isotropic in the basal plane, $-4.8 \times 10^{-4} \text{ dpa}^{-1}$ in each direction.

3.2 Direct deposition of vacancies at grain boundaries

Grain boundaries can also serve as sinks for point defects. Clearly, their influence in point defect absorption is greater in small grain materials. We can calculate the strain rate for vacancy deposition at grain boundaries in a similar manner to the way we calculated the deposition at dislocations. The probability that a cascade core of radius of r_c will impinge on the boundary of a grain of radius r , is the volume fraction of a layer at the grain boundary of thickness r_c i.e.,

$$P_b = \frac{(4\pi r^2)r_c}{4/3(\pi r^3)} = 3 r_c/r \quad (3)$$

For the approximately equiaxed grains of diameter $6 \times 10^{-6} \text{ m}$, reported for the 25% cold-worked Zircaloy-2 in question, and a cascade core radius of $4 \times 10^{-9} \text{ m}$, the probability is 4×10^{-3} and the volume strain rate due to vacancy deposition is $(4 \times 10^{-3} \times 0.08 = -3.2 \times 10^{-4} \text{ dpa}^{-1})$. There is an equivalent positive volume strain for the SIA. Because the grains are approximately equiaxed, the volume strain due to the direct deposition of vacancies is $-1.1 \times 10^{-4} \text{ dpa}^{-1}$ in all directions.

3.3 Self-interstitial atom absorption at sinks

The probability of direct deposition of SIAs escaping the core of the cascade on extended sinks will depend on the sink orientation because of the anisotropic nature of the cascades as shown in Section 3.5. Direct deposition will occur if the volume traced by an RCS impinges on an extended sink. In the general case (ignoring anisotropy), the probability of direct deposition of the individual SIA is much lower than that for vacancies because the effective volume ($5 \times 10^{-28} \text{ m}^3$ for an RCS displacing 5 atoms) is more than two orders of magnitude less than that of a cascade ($2.7 \times 10^{-25} \text{ m}^3$).

Most of the SIA's then must migrate through the lattice to deposit at sinks. This migration is extremely anisotropic (about 20 times faster in the basal plane than in the **c** direction at 350K [3,19]). According to the DAD model used at high temperature, the SIAs thus reach sinks that are perpendicular to the basal plane (e.g. **a**-type loops and **a**-type edge dislocations) more easily than those parallel to it, mainly causing expansion in the directions within the basal plane.

We can make an estimate of the maximum (upper bound) strain rate in the basal plane due to segregation of SIAs to **a**-type loops and dislocations. This is $\frac{1}{2}$ (two equivalent directions perpendicular to the **c** direction) of the volume strain from Section 3.1 ($1.2 \times 10^{-3} \text{ dpa}^{-1}$) plus $\frac{1}{2}$ of the volume strain from Section 3.2 ($3.2 \times 10^{-4} \text{ dpa}^{-1}$) for a total of $7.6 \times 10^{-4} \text{ dpa}^{-1}$. This is partially offset by the strain rates due to DD of vacancies on dislocations ($-4.8 \times 10^{-4} \text{ dpa}^{-1}$, from section 3.1) and on grain boundaries (-1.1×10^{-4}

dpa⁻¹, from section 3.2) leaving a net strain rate of 1.7×10^{-4} dpa⁻¹ in the basal plane (vs. -3.5×10^{-4} dpa⁻¹ along the **c**-axis from the direct deposition of vacancies).

3.4. Strains in a Polycrystal

In a textured polycrystal the strains must be averaged over all orientations of crystals. To do this rigorously a self-consistent polycrystalline model is needed. An approximation can be made using the “Kearns” factors[25], F_d , the resolved fraction of **c** axes in the “d” direction of the polycrystal. For the material in question $F_L = 0.06$, $F_T = 0.49$ and $F_R = 0.45$. According to this approximation:

$$\epsilon_d = \epsilon_a(1 - F_d) + \epsilon_c F_d \quad (4)$$

Where: ϵ_d is the strain in the “d” direction of the polycrystal, ϵ_a is the strain in the **a** direction of the crystal, and ϵ_c is the strain in the **c** direction of the crystal

To a first approximation, the strain rates in the material in question are then:

Axial $\sim 1.38 \times 10^{-4}$ dpa⁻¹, transverse $\sim -0.85 \times 10^{-4}$ dpa⁻¹, radial $\sim -0.64 \times 10^{-4}$ dpa⁻¹.

The approximate agreement with experimental values where $\epsilon_L = 1.2 \times 10^{-4}$ dpa⁻¹, and $\epsilon_T = 0.64 \times 10^{-4}$ dpa⁻¹ is certainly fortuitous in view of the many simplifying assumptions made, but it does indicate that the DD mechanism warrants further examination.

3.5. MARLOWE Calculations

MARLOWE is a computer code that simulates the development of collision cascades using binary collision (BCA) approximation in single crystal, polycrystalline, and amorphous targets. It is able to identify and characterize point defects created in the material by energetic particles. The method of calculation is based on the evaluation of elastic scattering integral using the selected pair potential for each binary collision [23]. The Molière potential with a screening parameter of 0.0862972 \AA is used throughout the study. Moving atoms may undergo a number of collisions which is limited by the maximum impact parameter assigned by user. Inelastic energy losses are included in calculations assuming that inelastic stopping cross section is proportional to the velocity of the moving atom.

The linearity of replacement collision sequences is monitored with a parameter which is the cosine of deflection angle. If a specified deflection angle (1.46 degrees in our case) is exceeded, the linear collision sequence is terminated. Calculations were performed for a range of initial projectile directions, as defined by the two angles; theta, polar angle measured from the z axis (parallel to 0001), and phi, azimuthal angle measured from the x-axis (parallel to 1010). These angles are selected between 0 to 90 degrees with 10 degrees increments. For a given phi-theta pair, to obtain good statistics, the angles defining the initial direction of primary particle are changed within a range of ± 0.015 degrees. Simulations are performed for 1000 cases for each theta and phi angle couple. Simulations were performed at initial energies of 5, 10, 20 keV. Hence, 3 energy cases, 100 angle combinations for each energy, and 1000 randomly selected angles for each combination, total 300,000 simulations were performed. Information about RCS's are retrieved from MARLOWE outputs and processed separately.

It is a general observation that most of RCS's are aligned along $\langle 1120 \rangle$, $\langle 0001 \rangle$, and $\langle 1100 \rangle$ directions, for all initial particle direction and energies. RCS's along other directions are very rare, i.e., less than one in thousand. Along these crystallographic directions, the average RCS length is longer for the $\langle 1120 \rangle$ and $\langle 1100 \rangle$ directions:

approximately 4.19 atoms as compared to 3.26 along the $\langle c \rangle$ direction (for RCS's greater than three atoms). The maximum length of the RCS is significantly longer RCS's along $\langle 1120 \rangle$ and $\langle 1100 \rangle$ directions as compared to RCS's along the $\langle 0001 \rangle$ direction (12-15 atoms for $\langle 1120 \rangle$ and at most 5-6 atoms for $\langle 0001 \rangle$). However, the averages are similar since most of the RCS's are only three or four atoms long. The difference between the two directions is more pronounced when we compare the numbers of RCS's along $\langle 1120 \rangle$ and $\langle 1100 \rangle$ directions to those along $\langle 0001 \rangle$, as shown in table 1.

Table 1: Number of RCS and total number of atoms in RCS averaged over all theta-phi combinations

E (keV)	Average Number of RCS			Av. Number of Atoms in RCS		
	$\langle 1120 \rangle$	$\langle 1100 \rangle$	$\langle 0001 \rangle$	$\langle 1120 \rangle$	$\langle 1100 \rangle$	$\langle 0001 \rangle$
5 keV	1.55	0.74	0.23	6.5	3.15	0.77
10 keV	2.86	1.46	0.36	12.0	6.18	1.18
20 keV	5.36	2.84	0.68	22.3	11.8	2.19

The number of RCS's along the $\langle 1120 \rangle$ direction are roughly double that along the $\langle 1100 \rangle$ direction. The number of RCS's along the axial direction $\langle c \rangle$ is much smaller than along either of these directions. This observation clearly shows that the propagation of RCS's are concentrated on basal plane of crystals. Table 1 also shows the product of the average length by the number to give the total number of atoms involved.

Calculations are performed with the binding energy of 3.052 eV which was experimentally determined for Zr [24]. There are other reported values of binding energy for zirconium; 4.633 eV [25], and 2.45 eV [26]. Hou et al. [27] point out that the binding energy is a critical parameter determining RCS characteristics by binary collision approximation. They compared the results of BCA simulations to more realistic molecular dynamics simulations finding that BCA simulations underestimate RCS's. To compensate they then defined a lower binding energy value for atoms already displaced and sitting in interstitial sites. When a lower binding energy, 0.5 eV, is employed in our calculations the RCS's are extended significantly, and the displacement cascades become more anisotropic.

4. Conclusions

We have presented a mechanism for irradiation growth in Zr alloys at low temperature based on the direct deposition of vacancies in cascades and on the anisotropic distribution of SIAs to oriented sinks. The main conclusions are:

1. The direct depositions of vacancies in extended sinks (dislocations and grain boundaries) allows vacancies to reach sinks athermally, potentially removing the previous discrepancy between theory and experiment.
2. The SIAs created in the cascade can interact thermally with the sink microstructure according to a classical DAD model to give the observed strains. However, MARLOWE simulations show that the cascades in Zr are anisotropic with greater length directions normal to $\langle 0001 \rangle$, which can contribute to the observed growth.

More work needs to be performed to discern the interaction of cascades with extended defects of different types using molecular dynamics. However the present work highlights the importance of understanding the details of the damage production process

beyond the amount of damage in dpa. It shows that even temporary effects such as cascade shape (lasting only picoseconds) can significantly affect material evolution under irradiation.

5. References

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