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Application of generalized deformation theory to irradiation creep of fcc and bcc stainless steels

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Abstract

The physical framework employed for most of the current irradiation creep models of cubic polycrystalline materials is a single crystal with a dislocation system consisting of three orthogonal Burgers vectors. The irradiation creep models based on this crystal system can be broken into two categories, one where irradiation creep occurs by dislocation climb alone, and the other where irradiation creep occurs by a combination of dislocation climb and glide. Often, irradiation creep is presumed to proceed by dislocation climb alone at low applied stresses, but by a combination of dislocation climb and glide at higher applied stresses. However, the rules for generalized deformation, as applied to dislocation climb, determine if a polycrystal is capable of deformation by dislocation climb alone. The current work analyzes generalized deformation by dislocation climb of fcc and bcc stainless steel crystals. Some implications for irradiation creep of polycrystalline fcc and bcc stainless steels are discussed.

1. Introduction

Until recently, nearly all models of irradiation creep of polycrystalline cubic crystals were based on a single simple cubic (SC) crystal with a dislocation system consisting of three orthogonal Burgers vectors [1–10]. In some instances, the dislocations were considered to be faulted cases, while in other instances, the dislocations were considered to be network dislocations. Fig. 1(a) shows the typical orientation of faulted loops, and Fig. 1(b) shows the typical orientation of network edge dislocations. In at least one instance, screw dislocations were also included with network dislocations [5]. For either the faulted loops or the network edge dislocations, there are three unique Burgers vectors. For an applied stress containing only uniaxial components along any of the principal axes, these models can be used to describe irradiation creep by dislocation climb. Implicit in these models is the idea that irradiation creep of cubic materials is either due to dislocation climb alone or is very strongly dominated by dislocation climb.

In recent years, there have been several researchers who have performed theoretical studies of irradiation creep of fcc crystals and polycrystals using the dislocation system observed in fcc metals [11,12]. These researchers arrived at several interesting conclusions. Wolfer [11] showed that deformation by climb of faulted loops of a single fcc crystal is not possible when a uniaxial stress is applied along any of the ⟨1 0 0⟩ axes. Later, Adams [12] showed that only a transient amount of creep deformation is possible for irradiation creep of fcc polycrystalline materials by dislocation climb of faulted loops.

The current work further explores the theory of irradiation creep of polycrystalline materials by dislocation climb when using the real dislocation system rather than a simplified dislocation system. The study focuses on fcc and bcc stainless steels but has applicability to other fcc and bcc crystal systems. In examining irradiation creep of fcc materials using the actual dislocation system, both Wolfer and Adams [11,12] used analytical methods to arrive at their conclusions. The current work explores the nature of irradiation creep by dislocation

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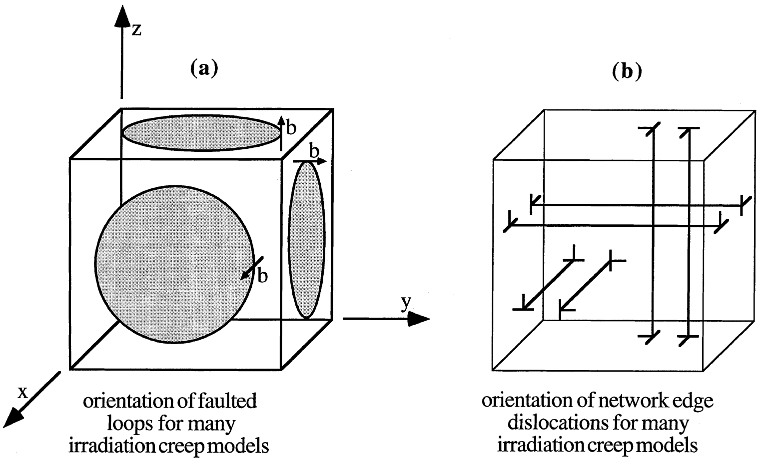

Fig. 1. Orientation of dislocations used in many irradiation creep models of fcc and bcc materials [1–10]: (a) shows the orientation of faulted loops; while (b) shows the orientation of network edge dislocations. In either scenario, there are three unique Burgers vectors which point along the principal axes.

climb using the von Mises [13–15] rules for generalized deformation.

2. Theory

von Mises has shown that for generalized deformation to occur in a crystal, there must be five linearly independent deformation modes present in a crystal [13–15]. Generalized deformation means that a crystal can be arbitrarily deformed with the constraint that volume be conserved. If a polycrystalline material is to be deformed either plastically or through volume conservative mass redistribution (irradiation creep in absence of swelling), the constituent grains must be capable of generalized deformation. von Mises applied his result only to deformation by dislocation slip, but generalized deformation theory can also be applied to the study deformation by dislocation climb.

For arbitrary deformation of a crystal, all the components of the deformation tensor are non-zero. If a crystal is to be capable of generalized deformation, the deformation tensor must contain exactly five independent components. Each of the three shear strain components must be independent,[1] and any two of the principal strains may be independent. The third principal strain is related to the two independent principal strains by

$$\varepsilon_{11} + \varepsilon_{22} + \varepsilon_{33} = 0. \tag{1}$$

If there are to be five independent components of the deformation tensor, then there must be five linearly independent modes of deformation in the crystal [13]. Both dislocation slip and dislocation climb are viable modes of deformation.

If generalized deformation is to occur by dislocation climb, then there must be five linearly independent climb systems. For deformation by dislocation slip, each slip system is uniquely determined by the Burgers vector of the dislocation and its slip plane. However, because deformation by dislocation climb occurs in the direction of the edge component of the Burgers vector, and because the edge component of a dislocation is not, in general, uniquely associated with any particular slip plane, the direction of deformation by dislocation climb is independent of the dislocation slip plane and is only dependent on the direction of the edge component of the dislocation. Since the amount of climb is only due to the movement of dislocations in the direction normal to the vector defining the edge component, deformation by dislocation climb is also independent of the specific trajectory of the dislocation.

For fcc crystals and then for bcc crystals, generalized deformation by dislocation climb of the following systems of dislocations will be considered:

- faulted loops;
- network dislocations;
- faulted loops and network dislocations together.

Since generalized deformation is possible only when a set of five linearly independent deformation modes exists, the task is to search for sets of five linearly independent deformation modes among the possible deformation modes. Because deformation by dislocation climb occurs in the direction of the edge component of the Burgers vector, a set of climb deformation modes will be linearly independent if the edge component of each Burgers vector in the set cannot be described by a

[1] Recall that $\varepsilon_{12} = \varepsilon_{21}$, $\varepsilon_{13} = \varepsilon_{31}$, and $\varepsilon_{23} = \varepsilon_{32}$.

linear combination of the other edge Burgers vectors in the set. Thus, it is possible to search for sets of five linearly independent deformation modes by searching for sets of five linearly independent edge Burgers vectors. A straightforward technique, employed here, is to examine all the sets of five edge Burgers vectors among the possible edge Burgers vectors and determine the sets which contain five linearly independent edge Burgers vectors. The method is analogous to that presented in Chapter 9 of Ref. [13]. Due to the required brevity of this paper, only the result of each analysis is presented. The study is limited to those dislocations which have been observed or thought to be present in fcc and bcc stainless steels.

2.1. Generalized deformation by dislocation climb in fcc stainless steel crystals

Consider generalized deformation by climb of $a/3\langle 1\ 1\ 1\rangle$ faulted loops in an fcc crystal. There are four possible faulted loop orientations, and so there are four unique but not necessarily linearly independent deformation modes for climb of faulted loops in an fcc crystal. With this information, one can immediately understand whether generalized deformation is possible by climb of faulted loops in an fcc crystal. Since there are only four deformation modes, and five are required for generalized deformation, generalized deformation obviously cannot occur by climb of $a/3\langle 1\ 1\ 1\rangle$ faulted loops in an fcc crystal. Using an analytical method, Adams [12] previously arrived at this conclusion.

Next, consider generalized deformation by climb of network dislocations in an fcc crystal. Since climb of $a/6\langle 1\ 1\ 2\rangle$ type extended dislocations in fcc materials is not possible because of the resultant high fault energy, these dislocations are not considered here. This leaves the six $a/2\langle 1\ 1\ 0\rangle$ Burgers vectors which describe perfect dislocations. So, there are six unique, but not necessarily linearly independent modes of deformation by dislocation climb. The task now is to search for sets of five linearly independent Burgers vectors among the six possible Burgers vectors. It was determined that there are zero sets of five linearly independent Burgers vectors.[2] Thus, generalized deformation is not possible by climb of $a/2\langle 1\ 1\ 0\rangle$ perfect network dislocations in fcc materials.

Now consider generalized deformation of an fcc crystal by the combined climb of $a/3\langle 1\ 1\ 1\rangle$ faulted loops and $a/2\langle 1\ 1\ 0\rangle$ perfect dislocations. The task is to search for sets of five linearly independent Burgers vectors among the ten possible Burgers vectors. It was determined that there are 60 ways to choose five linearly independent Burgers vectors. Thus, generalized deformation is possible by the combined climb of $a/3\langle 1\ 1\ 1\rangle$ faulted loops and $a/2\langle 1\ 1\ 0\rangle$ perfect dislocations.[3]

2.2. Generalized deformation by dislocation climb in bcc stainless steel crystals

In his numerous studies of irradiated ferritic and ferritic–martensitic steels, Gelles [16] has not observed faulted loops in these materials. Bullough et al. [17] have discussed the possibility that faulted loops might form on $\{1\,1\,0\}$ planes. Bullough et al. suggested that because these faulted loops have a high stacking fault energy, the faulted loops quickly unfault by a shear mechanism to form either $a/2\langle 1\ 1\ 1\rangle$ or $a\langle 1\,0\,0\rangle$ dislocation loops. Thus, if faulted loops form in bcc stainless steels, these loops would contribute very little deformation in the $\langle 1\ 1\ 0\rangle$ directions. If it is assumed that these faulted loops do form, the analysis to determine the number of sets of five linearly independent deformation modes for $a\langle 1\ 1\ 0\rangle$ faulted loops in bcc materials is identical to that for the analysis of $a/2\langle 1\ 1\ 0\rangle$ perfect dislocations in fcc materials, where it was determined that there are zero sets of five linearly independent deformation modes. Thus, generalized deformation cannot occur by climb of $a\langle 1\ 1\ 0\rangle$ faulted loops in bcc materials.

In bcc crystals, the most common network dislocation is the $a/2\langle 1\ 1\ 1\rangle$ dislocation [13]. By analogy with the previous case of climb of $a/3\langle 1\ 1\ 1\rangle$ faulted loops in fcc materials, there are zero sets of five linearly independent deformation systems for climb of edge dislocations with $a/2\langle 1\ 1\ 1\rangle$ Burgers vectors in bcc crystals. Gelles [16], however, has observed $a\langle 1\ 0\ 0\rangle$ dislocations in irradiated ferritic and ferritic-martensitic steels. Thus, we must determine if there are any sets of five linearly independent deformation modes for climb of both $a/2\langle 1\ 1\ 1\rangle$ and $a\langle 1\ 0\ 0\rangle$ edge dislocations. It was determined that there are zero sets of five linearly independent Burgers vectors when choosing among $a/2\langle 1\ 1\ 1\rangle$ and $a\langle 1\ 0\ 0\rangle$ Burgers vectors.[4] As a result, generalized deformation is not possible by climb of these dislocations in bcc materials.

If faulted loops were to form in bcc stainless steels, the combined climb of $a\langle 1\ 1\ 0\rangle$ faulted loops, $a/2\langle 1\ 1\ 1\rangle$ perfect dislocations, and $a\langle 1\ 0\ 0\rangle$ perfect dislocations could be considered. Again by analogy with the analysis of the combined climb of $a/3\langle 1\ 1\ 1\rangle$ faulted loops and

[2] At best, there are three sets of four linearly independent deformation modes.

[3] If there are multiple sets of five linearly independent deformation modes, then the set which is unhindered and best aligned to provided the required deformation will be activated.

[4] There are zero sets of four linearly independent deformation modes, and there are 29 sets of three linearly independent deformation modes.

$a/2\langle 1\,1\,0\rangle$ perfect dislocations in fcc materials, generalized deformation is possible by the combined climb of $a\langle 1\,1\,0\rangle$ faulted loops, $a/2\langle 1\,1\,1\rangle$ perfect dislocations, and $a\langle 1\,0\,0\rangle$ perfect dislocations.

3. Discussion

For irradiation creep to occur in a polycrystalline material, each grain must be capable of generalized deformation. The required linearly independent deformation modes can come from any of the possible deformation mechanisms which include but are not limited to elasticity, dislocation slip, dislocation climb, and grain boundary migration. Because of the production of point defects during irradiation and the stress-induced interaction between point defects and dislocations, deformation by dislocation climb is likely to be the favored deformation mechanism. In fact, irradiation creep of cubic materials at low stresses has long been assumed to occur by dislocation climb alone. However, in light of the analysis of generalized deformation by dislocation climb, it appears that even though dislocation climb is the favored deformation mechanism, irradiation creep may not be due entirely to dislocation climb, even at low applied stresses. If generalized deformation is not possible by dislocation climb alone, then some other deformation mechanism would be necessary to provide the linearly independent deformation modes that are not supplied by dislocation climb.

In the case of fcc stainless steels, generalized deformation by dislocation climb is possible if both faulted loops and perfect network dislocations are present. However, many theories for irradiation creep, such as the stress-induced preferential nucleation (SIPN) theory, consider only the formation and growth of faulted loops as the mechanism for irradiation creep [9,10,18,19]. From this study of generalized deformation, irradiation creep evidently cannot occur by a SIPN process alone. If deformation is to proceed by dislocation climb, then both faulted loops and network dislocations must participate. While there are theories for irradiation creep which presume the presence of both faulted loops and network dislocations [20,21], these theories include both faulted loops and network dislocations for the sake of completeness and not from a necessity to satisfy the rules for generalized deformation.

Since faulted loops have not been observed in bcc stainless steels, there appears to be an insufficient number of climb deformation modes for generalized deformation to occur by dislocation climb in bcc stainless steels. Thus, when irradiation creep occurs in bcc stainless steels, another deformation mechanism must be acting along with the climb of the network dislocations. However, for selected orientations of a grain with respect to the applied stress, there are fewer than five imposed strains, and in these grains, climb alone can provide the necessary deformation.

While the von Mises approach provides a method to determine if generalized deformation is possible using a given set of deformation modes, the approach is not quantitative. If a given set of deformation modes does not allow for generalized deformation, the von Mises approach does not predict the amount of deformation required by additional deformation modes if generalized deformation is to proceed. If only a very small amount of additional deformation is required, then elasticity may be able to provide enough accommodation. If the required additional deformation is large, then some other deformation mechanism capable of providing a large amount of deformation, would be necessary. Either dislocation glide or grain boundary migration are capable of providing large amounts of deformation.

4. Summary and conclusions

For irradiation creep to occur in a polycrystalline material, each grain in the material must be capable of generalized deformation. A von Mises style analysis of generalized deformation has shown that in both fcc and bcc materials, generalized deformation cannot occur either by climb of faulted loops alone or by climb of perfect dislocations alone. Generalized deformation can, however, occur by the combined climb of both faulted loops and perfect dislocations. In fcc stainless steels, both faulted loops and perfect dislocations are often present at the same time, suggesting that generalized deformation is possible by the combined climb of faulted loops and perfect dislocations. However, faulted loops have not been observed in bcc stainless steels, suggesting that generalized deformation cannot occur in bcc stainless steels by the climb of dislocations that have been observed in bcc stainless steels.

From this analysis of generalized deformation by dislocation climb, several new insights into irradiation creep have been obtained. For both bcc and fcc materials, if irradiation creep is to proceed by climb of dislocations, then both faulted loops and network dislocations must climb. Hence, a SIPN mechanism for nucleation of faulted loops cannot alone account for irradiation creep in fcc materials. If irradiation creep at low applied stresses is to occur by dislocation climb alone, as most theories for irradiation creep of fcc steels predict, then network dislocations must also climb. Since faulted loops have not been observed bcc stainless steels, the current work suggests that other deformation mechanisms are acting along with dislocation climb in bcc stainless steels. Elasticity is one possible additional deformation mechanism, but it is more likely that the additional deformation is provided either by dislocation glide or by grain boundary migration. In conclusion, the simple dislocation systems that have in the past been used to study irradiation creep theory do not fully describe the irradiation creep phenomenon.

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