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Micromechanics of dislocation channeling in intergranular stress corrosion crack nucleation

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ABSTRACT

While driven by a combination of stress, a susceptible microstructure and an aggressive environment, the mechanistic origin of stress corrosion cracking remains poorly understood. The emergence of localized deformation as a key process in SCC has resulted in considerable experiment and simulation studies. The effectiveness of irradiation in localizing deformation into dislocation channels has provided a tool for studying the interaction between channels and grain boundaries. Experiment and simulation have shown that normal stress can be in excess of twice the applied stress and that cracking correlates well with the high normal stress. Shear stresses in the channel can add an additional component to the normal stress at the channel-boundary intersection. While the exact role of localized deformation in stress corrosion cracking is not yet full understood, it is known that the degree of localized deformation correlates well with SCC susceptibility. Further, both experiments and simulations indicate that cracks preferentially nucleate in grain boundaries that are perpendicular to the loading direction, are non-special high angle boundaries, are not oriented for easy deformation under the applied load, and are effective barriers to slip transmission. This paper will review recent progress in understanding the behavior of localized deformation and the impact on stress corrosion cracking.

1. Introduction

A mechanistic basis for understanding the phenomenon of intergranular stress corrosion cracking (IGSCC) continues to prove to be a difficult and elusive journey. The difficulty stems, in part, from the rather unique and multi-component environment required for IGSCC to occur: a susceptible microstructure, imposition of a tensile stress, and an aggressive environment. The task is further complicated by the fact that there does not exist precise definitions or quantitative descriptions for how each of these components affects cracking. It has also become evident, that a statement of the *initial conditions* (microstructure, stress, environment) may be insufficient to explain the processes contributing to SCC. Rather the evolution of the deformation microstructure of the material may play an important, but as yet, unrecognized role. One of those processes contributing to the evolving microstructure is the deformation state of the strained sample. Stress concentration also plays a key role in the IGSCC process and also evolves with time and deformation. Crack growth is affected by factors that influence the buildup of the required stress concentration, such as planarity of slip, stacking fault energy, SFE, as well as dislocation and interface structure. Sadananda and Vasudevan [1] define a chemical stress concentration factor for a given material/environment system as the ratio of failure stress with and without the damaging chemical environment. They point out that this chemical stress concentration factor is coupled with the mechanical stress concentration factor. In general, environmental factors can enhance crack tip ductility by reducing the energy for dislocation nucleation and glide, and also reduce cohesive energy for cleavage. The interplay between these two opposing factors is important in a complete model that can account for cracking in aqueous environments [1].

Application of stress above the yield strength produces a dislocation microstructure that can vary depending on the alloy composition and microstructure. In particular, it was noted some time ago, that SCC depends on the degree of slip planarity in austenitic stainless steels. Swann [2] conducted a study on the effect of SFE on slip behavior of a series of Fe–18Cr–x Ni alloys where $8 < x < 23$. They showed that for the 8% Ni alloy, slip was entirely planar and as x increased above 13%, cross-slip became progressively more apparent. By 20% Ni, there was no evidence of planar slip and the deformation microstructure consisted of a web of dislocation tangles, evident of wavy slip in a high SFE material. Thompson and Bernstein [3] found that increasing SFE correlates

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well with increased reduction in area and decreased SCC susceptibility of similar alloys. These early data highlighted the importance of the localization of deformation in the SCC process. This importance has gained even more visibility lately as irradiation assisted stress corrosion cracking (IASCC) has emerged as a prime failure mode for light water reactor core components. Straining of irradiated alloys results in very heterogeneous deformation, and a significant enhancement of IASCC susceptibility. The connection between localized deformation and IGSCC has become the subject of intense investigation.

This paper examines the role of localized deformation in the nucleation of intergranular stress corrosion cracks. As localized deformation is most pronounced in irradiated microstructures, the emphasis will be on irradiated materials, though the concepts apply to the unirradiated condition as well. Following a brief summary of evidence supporting the linkage between localized deformation and SCC, the mechanisms by which grain boundary channels can affect deformation is discussed. The role of stress, both normal and shear, in dislocation channeling-driven IGSCC is discussed next. Approaches to model the effect of stress on grain boundary cracking are discussed next, followed by a treatment of the role of the environment in the IGSCC process.

2. Localized deformation and IGSCC

Irradiation is one of the most effective ways to induce localized deformation in metals. Straining of irradiated metals results in the formation of dislocation channels in which most or all of the deformation is contained. Further, irradiated austenitic alloys have been found to be highly susceptible to stress corrosion cracking, giving rise to a process termed irradiation assisted stress corrosion cracking (IASCC). The occurrence of a high degree of susceptibility to SCC in microstructures that exhibit intense localized deformation has focused much attention on the role of dislocation channels. Numerous studies have been conducted linking dislocation channels to IGSCC in neutron-irradiated steels [4–7]. However, evidence also suggests that a cold worked structure can also induce cracking via localized deformation [8], and that the material need not be a steel [9]. In fact, Fournier et al. [10] showed that localized deformation induced by fatigue of a precipitation-hardened alloy, when subjected to subsequent straining in high temperature water, underwent IGSCC in a similar manner as an irradiated alloy. Thus, the role of localized deformation in IGSCC is generic.

In the last 10 years, much progress has been made in understanding localized deformation and how it can induce IGSCC, though a clear cause-and-effect has yet to be established. The picture that is emerging from experimental studies is that deformation channel-grain boundary interaction leads to the initiation of intergranular stress corrosion cracks. Various processes can occur when a dislocation channel interacts with a grain boundary; (1) slip transfer to a neighboring grain, (2) cross-slip within the same grain, (3) absorption of dislocations by the grain boundary followed by grain boundary sliding, and (4) pile-up of dislocations at the grain boundary. Slip transfer has been observed to occur if the slip planes of the adjacent grains are within some misorientation, resulting in little local changes at the grain boundary. Fig. 1 shows some examples of slip transfer across the grain boundary of irradiated stainless steel strained in an inert environment [11,12]. Slip transfer can result in the formation of a step in the grain boundary. Nishioka et al. [13], Sauzay et al. [14], and Jiao and Was [11] have all observed steps in grain boundaries caused by the interaction with a dislocation channel. Fig. 2 shows examples of steps at dislocation channel-grain boundary intersections. As measurements indicate that the number of dislocations in a channel can be very large (>100), the step at the boundary can be several tens of nm in size. This step, or localized displacement of the grain boundary, could lead to cracking of an oxide film if the process were to occur on a boundary that intersected the surface of a sample. Dislocation channels are very prominent on the sample surface and the height of the channel is directly proportional to the amount of slip in the channel. Channels can account for nearly all of the plastic deformation in a sample and the strain in a channel can reach 100%.

The length scale at which the IGSCC phenomenon is observed is typically macroscopic but it is determined by the presence of chemical impurities in the region near the tip of the crack, at the nanometer and atomic scale. Atomistic scale simulations are required in order to understand the effects of chemical impurities on the crack tip, where the important processes occur that determine the brittle or ductile nature of the material. Ideally, this should include a quantum mechanical description of the system, including ions and electrons. A complete modeling strategy for the problem should then consist of: (i) quantum–mechanical level, (ii) molecular dynamics with forces derived from effective interatomic potentials at the scale of 100 nm, (iii) dislocation dynamics at the micron scale, and (iv) continuum elasticity [15]. There has been great progress in the bridging of length scales [16] and in understanding length and time scale effects [17]. Studies of stress corrosion cracking can now be undertaken at the atomistic level [18]. The following sections will review recent experimental data and modeling and simulation results on the role of localized plastic deformation in stress corrosion cracking.

2.1. Role of dislocation channels

The importance of dislocation channels in IASCC is highlighted in Fig. 3, which shows a correlation between the weighted average height of channels intersecting the surface with the degree of IG cracking measured as the crack length per unit area on the sample surface [19]. Samples were strained in simulated boiling water reactor (BWR) normal water chemistry (NWC – 288 °C, 200 ppb oxygen, <0.2 μS/cm conductivity) at a rate of $3 \times 10^{-7}\ s^{-1}$. The data shows that for channel heights below about 300 nm, no cracking was observed. Above about 340 nm, all samples cracked, and there is a narrow region between 300 and 340 nm in which there are mixed results. The correlation between cracking and weighted average channel height is stronger than that with other key variables linked to IASCC, such as yield stress, grain boundary chromium level or stacking fault energy. The importance of this data is that it was constructed from seven high-purity Fe–Cr–Ni alloys with stacking fault energies that vary from 15 to 61 mJ/m^2, irradiation doses of 1 or 5 dpa and strains of 1% or 3%. Regardless of the alloy, SFE, dose or strain, the weighted average channel height governed cracking.

The role of localized deformation on cracking is believed to be due to one of two processes or their combination; grain boundary deformation and high local stresses. The large amount of strain in the channel can result in either a wedge-type crack due to the pile-up of dislocations at the channel-boundary intersection, or the dislocations can be incorporated into the boundary. Dislocation incorporation into the grain boundary does indeed lead to wedge-type cracks. Fig. 4 shows the formation of small voids or cracks (grain boundary channel cracks – GBCs) at the intersection of dislocation channels and the grain boundary. These occur independent of the environment. However, they do not lead to the growth of IG cracks at temperatures around 288 °C in Ar. They also do not easily develop into an intergranular crack in high temperature water [20]. Thus, while providing a means to open the grain boundary, these crack nuclei do not easily propagate.

If the dislocations-boundary interaction results in a component of the product dislocation that is mobile in the grain boundary,