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The effect of grain boundary yield and disconnections on grain boundary fracture strength

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ABSTRACT

During high-temperature interfacial strain, e.g., creep or sintering, grain boundaries will sample non-equilibrium states associated with the non-equilibrium disconnections that mediate strain. This work tests the hypothesis that those non-equilibrium states should affect the mechanical properties of the grain boundary. High-temperature bicrystal tensile strain experiments performed on Sc-doped ZrO₂ as a function of strain rate enable the observation of fracture before and after grain boundary yield. Yielded boundaries exhibit a median fracture strength $\approx$ 50 % lower than those that did not yield. Molecular dynamics simulations performed on boundaries with and without interstitial-type disconnection loops indicate that the presence of those loops reduce the failure stress.

Engineering the structure, chemistry, and distributions of interfaces provides potential strategies for tuning the mechanical properties of polycrystals [1–7]. So-called grain boundary (GB) engineering, wherein the grain boundary character distribution is modified, has been demonstrated as a particularly effective method, since grain boundaries of different structure have different properties. Atomic simulations also indicate that grain boundaries of the same macroscopic character, but distinct atomic structure will exhibit different properties. Classical steady-state models for processes like grain growth, creep, sintering, and related grain boundary processes typically assume grain boundaries rapidly relax towards equilibrium structures and effectively retain low-energy structures during associated kinetic processes. There is, however, a growing appreciation for the role of disconnection nucleation in affecting interfacial transport kinetics [8,9]. For example, disconnection nucleation kinetics capture many trends observed within the literature for grain growth [10]. Recent experiments and theory also suggest that disconnection nucleation kinetics describe densification during sintering well [11]. Disconnection nucleation kinetics also predict the non-Newtonian grain boundary creep response well [12]. The analyses of sintering and creep suggests that the local driving forces associated with nucleating climb-mediating disconnections may be much higher than the average driving forces, i.e., applied stress or

average sintering stress. As a result, their concentrations may be relatively low, even within the Newtonian grain boundary creep regime, i.e. Coble creep. In this context, the nucleation of high energy disconnections must be facilitated by evolved stress concentrations that push regions of the material, such as triple junctions, far from equilibrium.

Disconnections can be equilibrium structures that exist to minimize misfit strain energy or non-equilibrium features that nucleate and migrate to dissipate energy, analogous to lattice dislocations [13]. Several recent papers characterizing *in situ* grain boundary migration under applied stresses at room temperature with atomic resolution demonstrate the importance of disconnection nucleation and motion in mediating combined grain boundary migration and strain [14–20]. For interfacial strain, disconnection motion via climb and/or glide is geometrically necessary. The analysis of bicrystal and polycrystalline grain boundary creep data in oxides suggest that the disconnection nucleation stress is a significant fraction of the lattice dislocation nucleation stress [12,21]. Such non-equilibrium disconnections should, therefore, exhibit large energies. Measurements of dihedral angle evolution during *in situ* sintering and creep, indeed, indicate that the relative interfacial energy increases at the onset of interfacial yield, which is associated with disconnection nucleation [11]. Significant changes in grain boundary structure and energy should influence their physical

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properties. It was, for example, shown that grain boundary phase transitions, or complexion transitions, can dramatically affect the fracture strength of interfaces [22]. The existence of non-equilibrium disconnections will be transient as they nucleate, for example, at one triple line and annihilate at another. In the process, they will mediate a strain of $\epsilon \sim \vec{b}/d$, where $\vec{b}$ is the Burger's vector and d is grain size [23]. The non-equilibrium disconnection concentration will depend on the stress and temperature under which the material is processed, as well as the microstructure. Processing conditions could, thus, represent an under-appreciated method for tuning the physical properties of grain boundaries and, by extension, polycrystals, via their non-equilibrium disconnection content.

This study aims to test the hypothesis that grain boundary yield influences the subsequent fracture strength of grain boundaries. The idea that grain boundaries with non-equilibrium structures should exhibit distinct fracture strengths is intuitive. Classical models for processes like sintering and creep, however, inherently assume that grain boundary structures remain near equilibrium configurations. Thus, little reason existed to expect that the properties of a boundary of a specific crystallographic character should have properties sensitive to processing history. Indeed, the authors are not aware of any prior knowledge base that predicts or supports such a hypothesis, which motivates the current work. Furthermore, capturing known transient non-equilibrium grain boundary states *ex situ* and testing their mechanical properties presents numerous experimental challenges associated with capturing boundaries in known transient states and comparing them to equivalent reference states. Instead, this work seeks to measure the yield, maximum, and fracture strengths associated with different failure modes. Depending on temperature and strain rate, oxide grain boundaries will either yield and creep under steady-state conditions, yield and then fracture if diffusional transport is not sufficiently facile, or exhibit only brittle fracture at relatively high loading rates. Rate-dependent measurements enable comparison of the fracture strength before and after grain boundary yield, particularly at rates where the competing failure pathways are both active.

In prior work, grain boundary yield and fracture was observed during tensile creep of ZrO₂ bicrystals [24]. These experiments contained some initial indications that yield could affect the fracture strength of the samples, however, such analysis was outside of the scope of that work and not presented. Furthermore, these experiments did not emphasize capturing both types of fracture response at a single

temperature with good statistics. Ignoring temperature as a potential variable, it is possible to compare all the data from that work with reasonable statistics. Fig. 1 shows an example data set highlighting the experimental test and the results re-analyzed from that work. The data show the brittle fracture strength along with a series of observations of fracture after yield, which occurred at lower average stresses. The activation volume for grain boundary yield is temperature-dependent and the relative preference for yield versus brittle fracture is temperature-dependent, so it would be ideal to make a similar comparison at a single temperature. Since a more brittle fracture was observed at lower temperatures and more yielding was observed at higher temperatures, the effects of temperature cannot be conclusively decoupled from the fracture strength results in this analysis.

In this paper, a series of rate-dependent tensile creep experiments are performed at a single intermediate temperature to observe fracture occurring prior to yield and fracture occurring after yield. This provides an initial assessment as to the influence of non-equilibrium climb-mediated disconnections in affecting grain boundary mechanical properties. Molecular dynamics simulations also probe the fracture response of fluorite bicrystal geometries with and without disconnection loops in order to understand how their presence influences fracture.

Two pieces of 10 % Sc-doped ZrO₂ were prepared via mechanical polishing, see reference [25] for sample synthesis and the Supporting Information for additional details. One was prepared in a needle shape and the other as a thin wedge, both with edge thicknesses on the order of several μm . The needle shaped sample was mounted on the moveable indenter portion of a Bruker PI-95 nanomechanical TEM holder, while the thin wedge was placed on the fixed sample portion of the holder. These materials were heated *in situ* inside a highly modified JEOL 2100 LaB₆ transmission electron microscope (TEM) using localized IR laser heating – see Ref. [24] for details regarding the testing geometry. Sample temperature was calibrated based on lattice parameter expansion measured between room temperature and the melting temperature of the specimen. A temperature was selected that enabled the observation of both purely brittle fracture and yield before fracture to occur consistently within the range of accessible displacement rates. This temperature $T \approx 1650$ K was low relative to prior experiments that were performed at $T > 1700$ K. Samples were brought into contact *in situ* and allowed to sinter for several minutes. Grain boundary diffusivities measured *in situ* from these bicrystals indicate that the time constant for diffusion across the grain boundary should be ≈ 5 –10 s. The boundary should be able to sinter and equilibrate on a similar timescale. The grain

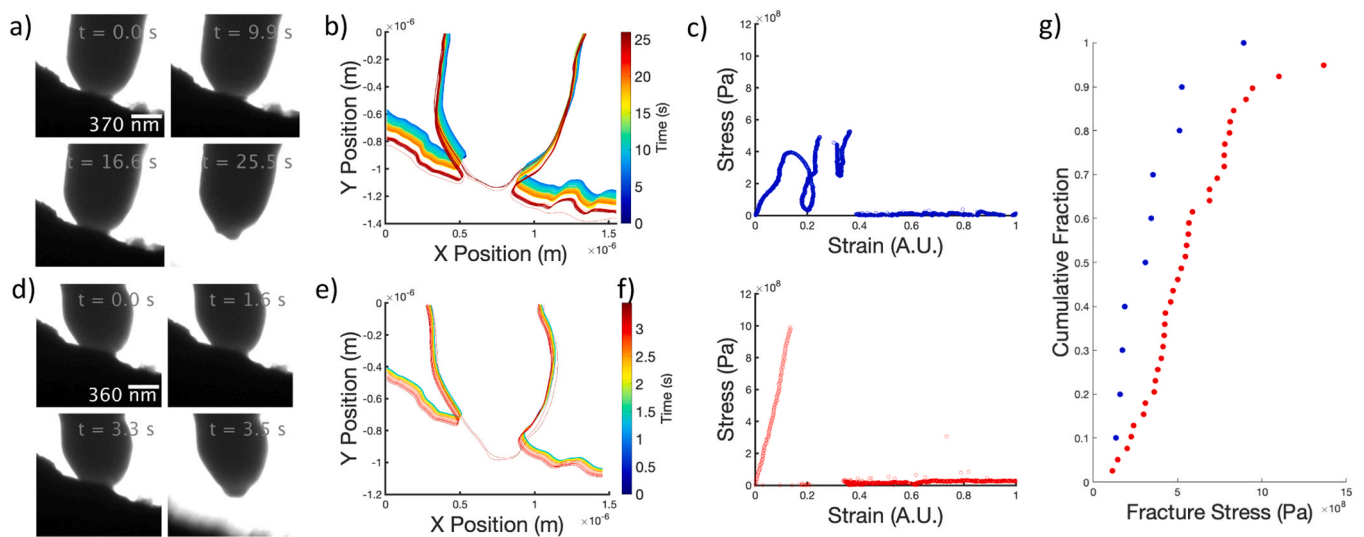


Fig. 1. Example ZrO₂ bicrystal tensile test data including (a,d) time-lapse images of the test, (b,e) the profile of the test geometry at each time image, and (c,f) the stress-strain response. The data in (g) show the cumulative distribution of fracture stresses measured when the sample yielded before fracture (blue) and when brittle fracture occurred without yielding (red).

boundaries were then loaded in tension. The grain boundary width is measured just prior to fracture and a circular cross-section is assumed to calculate the stress from the load. The assumption of a circular contact may introduce some error; however, averaging over multiple tests should provide a reasonable average value. The zero-load value is based on the load after fracture.

Fig. 2 shows example stress-strain curves for Sc-doped ZrO_2 loaded in tension at 1 nm s^{-1} , 2 nm s^{-1} , 7 nm s^{-1} , and 50 nm s^{-1} at $\approx 1650 \text{ K}$. Almost all tests were performed at the same asperity contact in approximately the same location as can be seen in Fig. 2. Additional stress-strain curves are provided in Figure S4 and corresponding image sequences are shown in Figures S2 and S3. At the highest loading rate, the grain boundaries exhibit brittle fracture with little or no evidence of yield prior to fracture. At lower loading rates, the onset of yield is observed prior to grain boundary fracture and the fracture occurs at lower stresses than the purely brittle fracture. The type of yield observed with a corresponding load drop indicates the nucleation of strain mediating defects. If such defects pre-existed the response would be continuous following a response dictated by an underlying stress-strain rate response, such as predicted by, for example, the Coble creep model [26] or other continuous models [23]. The importance of disconnections in mediating grain boundary motion and plasticity has been observed at high resolution [14–16,20], but it is not yet possible to perform similar high-resolution experiments with corresponding quantitative load-displacement data at high temperatures. Indeed, prior analysis of bicrystal GB yield in ZrO_2 [12,24] was consistent with Arrhenius nucleation kinetics and produced an activation enthalpy, activation volumes, and activation volume thermal expansion comparable to values expected for dislocation nucleation. The nucleation of climb mediated disconnection nucleation should exhibit activation constants comparable to dislocation nucleation. Furthermore, these constants were used to parameterize analytical models for disconnection nucleation rate limited polycrystalline creep and predict macroscopic response well without invoking fitting parameters, supporting the validity of the hypothesis that GB yield results from disconnection nucleation.

Reducing the loading rate further allows the bicrystal to creep to higher strains prior to grain boundary fracture. The associated fracture strength is even further reduced. At the lowest loading rates the sample creeps continuously at stresses on the order of 10^8 Pa and does not fracture. Fig. 2 shows an example loading at 2 nm s^{-1} where the sample fractures after some strain, but other samples loaded at the same rate did

not fracture at similar strains. Tests performed at 7 nm s^{-1} produced both types of characteristic response, both brittle fracture and yielding prior to fracture. Under this condition, the fracture strength of the unyielded and yielded grain boundaries may be compared directly without significant influence of strain rate effects. The same trend holds, that grain boundary fracture strength prior to yield exceeds the value after yield. Fig. 2 highlights the geometric changes in the surface profile observed at each frame of the imaging data. Strain of the interface is observed, but there are no clear correlations with the onset of yielding and load oscillations in the stress-strain response.

The data obtained at 1650 K only is shown in supporting data S7. The data from Fig. 1 measured between 1877 K and 2371 K produce fracture strengths both before and after yield that are 17 % and 18 % higher than the data at 1650 K . The Pearson coefficients are both > 0.98 indicating distributions of similar shape. This could suggest some temperature dependence to the fracture strength or possibly differences in the degree to which the grain boundaries initial equilibrated. Currently, there are few theoretical models that would account for the temperature dependence of brittle bicrystal grain boundary fracture. The same trend, nevertheless, holds wherein yielding prior to fracture clearly reduces the median fracture stress, in this case by $\approx 50 \%$ and 56% for the lower and higher temperature data, respectively. Since the influence of yield on fracture stress is approximately the same in each case, Fig. 3 plots all

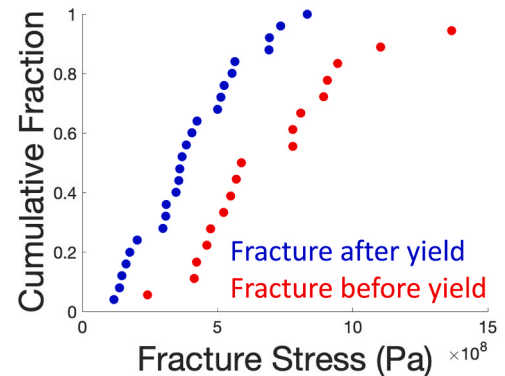


Fig. 3. The cumulative distribution of fracture stresses measured when the sample yielded before fracture (blue) and when brittle fracture occurred without yielding (red). This plot contains data from all temperatures, the data isolated from $T \approx 1650 \text{ K}$ can be seen in Fig. S7.

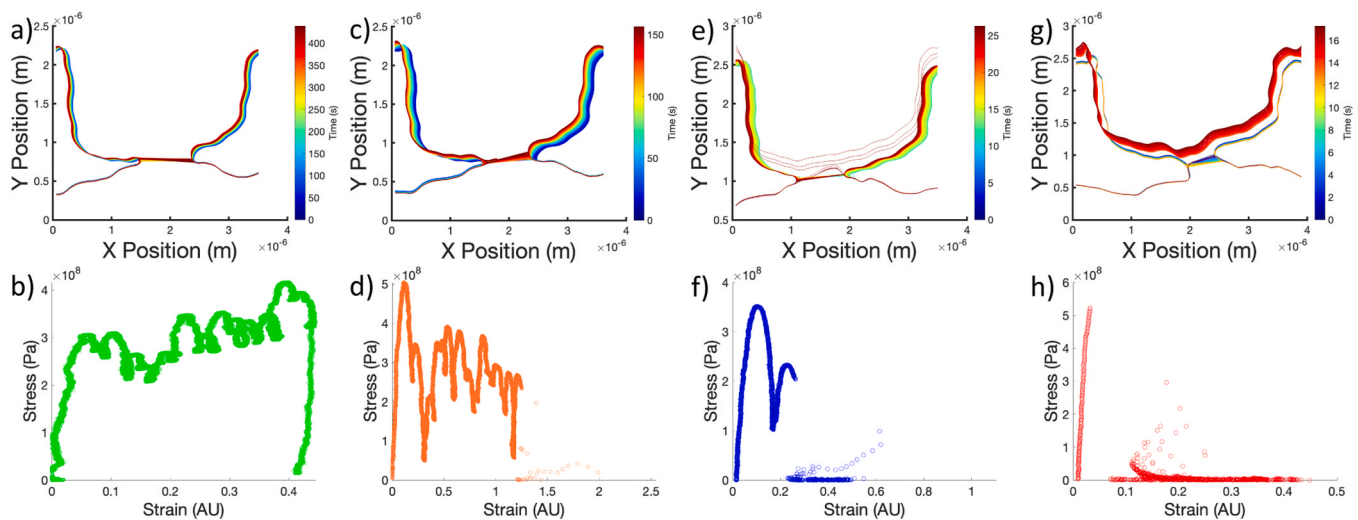


Fig. 2. Time-lapse surface profiles extracted from image sequences and associated stress-strain curves for bicrystal tensile tests performed at (a-b) 1 nm s^{-1} , (c-d) 2 nm s^{-1} , (e-f) 7 nm s^{-1} , (g-h) and 50 nm s^{-1} at $\approx 1650 \text{ K}$. Note, the approximate grain boundary position is indicated based on connections between points of local maximum surface curvature, but may not indicate the precise position of the grain boundary and are shown here as a guide.

the data together as cumulative distributions for the brittle grain boundary fracture stress distribution in the range of 1650 K to 2371 K. It can be seen in Fig. 2 that steady-state creep response may almost be achieved at the lowest loading rate of 1 nm s^{-1} , although the large oscillations in stress suggest the system may still be in the non-Newtonian response regime.

Disconnection nucleation during *in situ* TEM based straining has been imaged at high-resolution [16]. The instrumentation that allows for such experiments are either not designed for measurement of load or are not suitable for use at ultra-high temperatures. It is hypothesized that grain boundary yield occurs with the onset of disconnection plasticity that has been shown to mediate grain boundary deformation [16], analogous to lattice dislocations mediating lattice plasticity. Direct observation at the temperatures used in this work is not currently possible. The second hypothesis is that the presence of non-equilibrium grain boundary disconnections causes the reduction in grain boundary strength. To test this hypothesis, molecular dynamics simulations are performed on grain boundaries with and without disconnections formed by introducing an interstitial loop into the grain boundary. A variety of disconnections can form at a given grain boundary, at various concentrations, and degrees of complexity. This portion of the work seeks to evaluate the basic hypothesis that non-equilibrium disconnections can measurably affect the fracture stress.

A symmetrical tilt UO_2 grain boundary ($\Sigma 9$ with a rotation axis of (110)) was generated for atomistic simulations with a rotation angle equal to half the misorientation angle (38.94°). ZrO_2 potentials can exhibit stress-dependent phase transitions that complicate the analysis. UO_2 [27] was selected as a surrogate due to its structural similarity to cubic ZrO_2 , but the phenomenology is anticipated to be general to ceramic grain boundaries exhibiting brittle fracture. Molecular dynamics simulations cannot capture processes relevant to the experimental strain rates, dynamic grain boundary structures, or loading conditions relevant to the experiments. Instead, this work seeks to identify how the presence of an interstitial-type dislocation loop in the grain boundary plane influences the fracture stress of the boundary. This dislocation loop very approximately simulates the formation of a climb mediating disconnection that would form at the onset of grain boundary yield. The experiments suggest that yield displacement is associated with more than a single Burgers vector and such defects likely nucleate heterogeneously from the surface triple lines and these defects can exhibit a range of Burgers vectors defined by the displacement shift complete lattice [28]. Nevertheless, these simulations are intended to test whether the presence of a non-equilibrium disconnection alone can

directly impact the fracture strength of the boundary, the magnitude of the effect, and a potential source of the effect.

A grain boundary was equilibrated via the γ -surface within a simulation box size was $186 \text{ \AA} \times 196 \text{ \AA} \times 139 \text{ \AA}$ in the x, y and z directions, respectively. Details of the simulation set-up are provided in the [supporting information](#). A dislocation loop was generated within the boundary by introducing a $15.1 \text{ \AA}$ radius disk of atoms with positions replicating the grain boundary structure. Following this step, the structure was energy minimized, equilibrated, and energy minimized again using a series of different energy minimization routines at zero pressure. To represent a stress concentrator that would exist in the microstructure and provide an initiation site for failure, some of the grain boundary structures with a dislocation loop also contained a notch. The notches were created by introducing a $50 \text{ \AA}$ lenticular void at the grain boundary, while maintaining stoichiometry. Samples were strained normal to the grain boundary plane by straining 0.001 and holding for 30 ps and iterating this process until a maximum strain of 0.05 was achieved.

Fig. 4 shows a plot of the modeling stress-strain results. It highlights the effect of a single dislocation loop on the failure stress of grain boundaries with or without a notch. The presence of this disconnection results in a reduction in the failure stress and failure strain in each case. This interstitial loop represents the type of defect that could mediate diffusion-dependent grain boundary tensile creep. It is important to note that creep is not observed in the simulation results. In each case, the dislocation loop reduces the failure strength of the boundary. Fig. 4b highlights how the position of the loop relative to the notch also influences the failure stress. When the edge of the loop is displaced toward the notch, the failure strength decreases presumably due to interactions between the elastic field of the disconnection and the stress at the notch tip. Corresponding renderings of the atomic positions at different strains are shown in Figure S8. Real specimens are unlikely to nucleate disconnections homogeneously, but their stress fields are likely to interact with surface triple junctions elastically. The experiments suggest that multiple disconnections likely nucleate during yielding as the displacement response exceeds a single Burgers vector. This could drive pile-up of the disconnections that may exacerbate such elastic effects. The reduction in strength due to the presence of the dislocation loop in the simulation is $\approx 9\%$. Similar results were obtained with an alternative interatomic potential [29], results of which are shown in Figure S9. The calculations support the general hypothesis that the formation of climb-mediating disconnections during creep influence the failure strength of the grain boundaries and may account for the reduction in

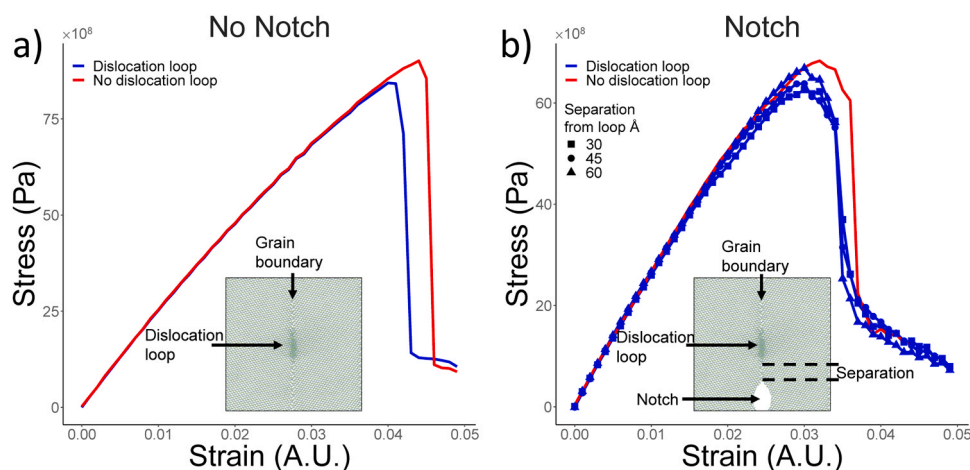


Fig. 4. Modeling predictions of stress-strain in fluorite structures described by a UO_2 potential, mimicking the cubic ZrO_2 system. The color outlines whether the grain boundary contained a dislocation loop or not, while the shapes represent the distance from the edge of the dislocation loop to the notch tip. Insets show top-down views of the simulation setup. The green and blue spheres represent the uranium and oxygen atoms, respectively. Note that structures containing a notch were multiplied by a scaling factor to account for some of the missing grain boundary to make them comparable to the structures without a notch.

failure stress induced by prior grain boundary yielding. The comparison here is intended to be qualitative and helps answer the question as to whether the presence of non-equilibrium disconnections at grain boundaries can affect their fracture strength. The grain boundary structure evolved during straining, however, is likely to be substantially more complex than the simulated structure. The interactions between multiple disconnections should further affect the strength in ways not predicted by our simulation of a single loop. The simulated cracks tend to evolve in parallel across the boundary, while it might be anticipated from experiments that cracks begin at one region and then propagate across the interface [30]. The difference in fracture mode might also, in part, account for the discrepancy in the magnitude of the effect. The simulations suggest that the cracks tend to open more at regions furthest from the interstitial loop at the interface, which is reasonable since the loop region should be under relative compression versus regions outside of the loop.

Arrhenius kinetics predict that disconnection nucleation will be more facile at higher temperatures and stresses. This may lead to different concentrations of these defects being present for materials processed at different temperatures, but also different levels of residual stresses being stable at different temperatures. The relative effects of these two factors are not trivial to predict, but it is anticipated that different processing schemes may result in nominally identical continuum scale microstructures having different mechanical properties.

This work has focused on mechanical properties; however, other physical properties are anticipated to be sensitive to the presence of non-equilibrium grain boundary disconnections. For example, it has been suggested that interfacial dislocations affect thermal conductivity across them [31]. Similarly, other processes involving scattering from defects, like electrical conduction, could be influenced by non-equilibrium disconnection content [32]. Corrosion is influenced by the presence of dislocations and qualitatively correlates with grain boundary energy; thus the presence of non-equilibrium disconnections could impact interfacial corrosion [33]. Understanding the distributions of non-equilibrium disconnections and how to control them may, therefore, provide a useful route towards controlling materials properties and the distribution of materials properties within a microstructure.

1. Conclusions

The experiments in this work indicate that the interfacial yield during tensile creep leads to a reduction in grain boundary fracture strength. The effect is hypothesized to derive from the presence of climb-mediated disconnections in grain boundaries that have undergone yield and are in the process of creeping. Molecular dynamics simulations demonstrate that the presence of non-equilibrium disconnections reduce the failure strength of the grain boundary, which supports the experimental hypothesis.

CRediT authorship contribution statement

Michael W.D. Cooper: Writing – review & editing, Project administration. **David A. Andersson:** Writing – review & editing, Project administration. **Khalid Hattar:** Writing – review & editing, Supervision, Funding acquisition. **Isaac Martinez:** Formal analysis. **Conor O.T. Galvin:** Writing – review & editing, Methodology, Investigation, Formal analysis. **Shen J. Dillon:** Writing – review & editing, Writing – original draft, Visualization, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis. **Ryan M. Schoell:** Writing – review & editing, Investigation.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.jeurceramsoc.2025.117680.

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