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INVESTIGATION OF THE ROLE OF MICROSTRUCTURAL INHOMOGENIETY IN DIFFUSIONAL CREEP: A MESOSCOPIC SIMULATION STUDY

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ABSTRACT

Superplastic deformation has been observed in a large number of metals, alloys and ceramics at elevated temperatures resulting in remarkably high amount of strains ranging from several hundred to several thousand percent. An extensive study of this phenomenon has suggested a direct influence of grain boundaries on the mechanical properties of the material [1]. The mass flow in the system during high-temperature deformation is governed by diffusion along grain boundaries (GB) under the conditions of moderate stress and temperature (Coble Creep) [2]. Microstructural attributes of a system like grain size distribution, inhomogeniety, grain boundary diffusivity also have a considerable effect on the stress-distribution in the system and thus the Coble creep. The presence of inhomogeniety results in stress-concentrations at grain-boundaries, which, in turn, affects the strain rate during creep. [3-6]

In this study, we use mesoscopic simulations to investigate characteristics of the deformation mechanism of grain-boundary diffusion creep in a polycrystalline material. The stress distribution along the grain boundaries in a polycrystalline solid under externally applied stress is determined and the mechanism of how topological inhomogeneities introduce stress concentrations is investigated. Microstructures with inhomogeneities of various sizes and distributions are considered and their effect on the stress distribution and creep rate is quantified.

Fig. 1 shows a microstructure consisting of 459 regular uniform sized grains, and one equiaxed larger grain in the middle. The uniform sized grains consist of 429 regular hexagonal grains and 30 smaller four or five-sided grains bordering the central large grain. The larger grain has an area about 66.46 times larger that the area of a hexagonal grain, A_h, and it accounts for about 13.5% of the total area of the simulation system. The accompanying graphs show the stress distributions along five distinct GB paths. Four paths are perpendicular to the straining direction and one is parallel to the applied stress. The stress distribution along

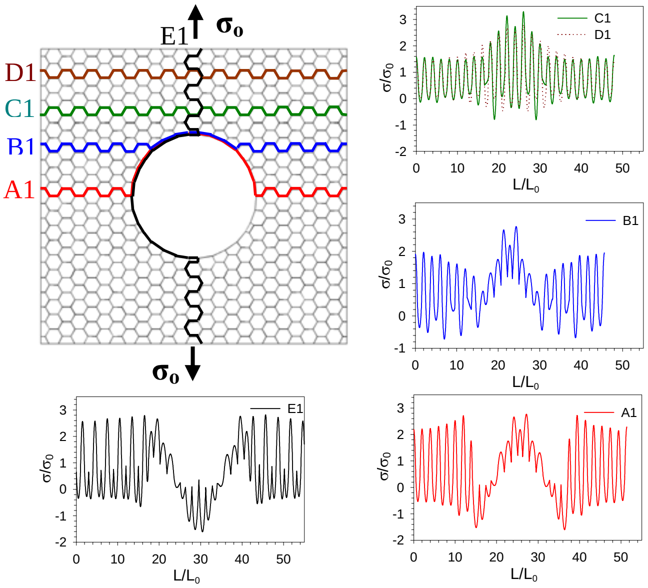

Fig 1: Microstructure with one large grain in the middle (A_{large}/A_{hex} = 66.5) subjected to the uniaxial tensile stress σ_0. The stress profiles are shown for the five distinct highlighted paths.

By comparing these five stress distributions we can observe the following details: i) the amplitudes of the stress distributions along the median paths A1, B1 and E1 that intersect the larger grain are larger than the amplitude along the paths C1 and D1 which do not touch the larger grain ii) the compressive stresses along paths C1 and D1 are significantly smaller and act on significantly fewer GBs than along the paths A1, B1 and E1 iii) the normal stress distributions converge to the characteristic periodic distribution of the normal stress in a uniform regular structure [7] (characterized by a maximum stress that is twice the value of the externally applied stress, σ_0) faster along the paths A1, B1 and E1 than along paths C1 and D1 and iv) the maximum normal stress in the microstructure, $\sigma_n = 3.25\ \sigma_0$, is found along path C1 at the center of a GB located about one grain diameter away from the surface of the large grain. The presence of smaller grains contribute directly to the lowering of stress concentration on the surface of the larger grain.

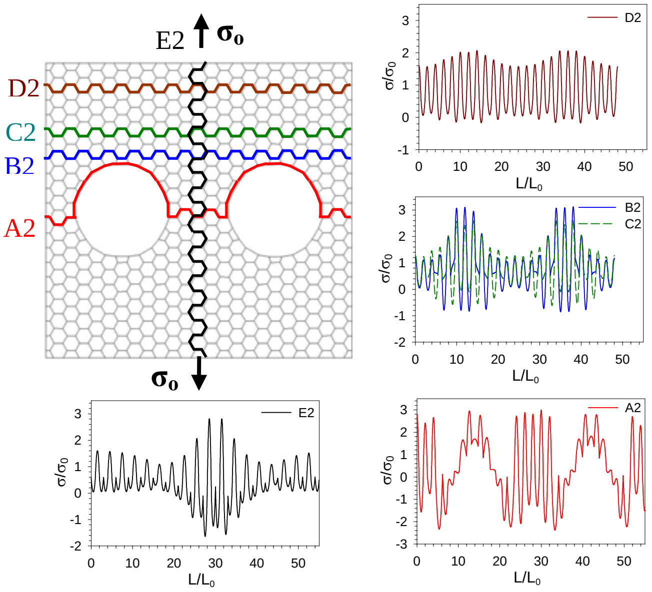

Fig 2: Microstructure with two large grains in the middle (A_{large}/A_{hex} = 34.3) subjected to the uniaxial tensile stress σ_0. The stress profiles are shown for the five distinct highlighted paths.

It is well-known that apart from the size of the inhomogeniety, its distribution in the system also affects the stress-distribution. Thus to study this effect, we investigated the same microstructure with larger grain broken up in two, three and four grains respectively. Fig. 2 shows the microstructure in the presence of two larger grains located close to the center of the system. Each of the two larger grains has an area of about 34.1 A_h, and their combined area is about 15% of the total system area. The accompanying graphs show the stress distributions along five distinct GB paths. Similar to the system in Fig. 1, the amplitude of the normal stress is larger along the median path A2. Moreover for this system, the maximum normal stress located along a GB on path B2 is only slightly larger than the stress at the tip of one of the larger grains (A2) and it is smaller than the maximum stress found in Fig. 1.

The creep deformation in the presence of a cluster of three large grains (Fig. 3(a)) was also investigated. Fig. 3(b) shows the normalized strain rates for four such non-uniform microstructures plotted against the strain rate for the regular homogeneous micrustructure [7]. The area of one large grain, A_l in the non-uniform microstructure is: 4.0; 6.1; 8.1 and 16.1 times larger than the area of a hexagonal grain A_h. Interestingly Fig. 3(b) shows that the presence of the inhomogeneity removes the singularity in the strain rate and the peak value of the strain rate has an amplitude that depends on area of the inhomogeneity.

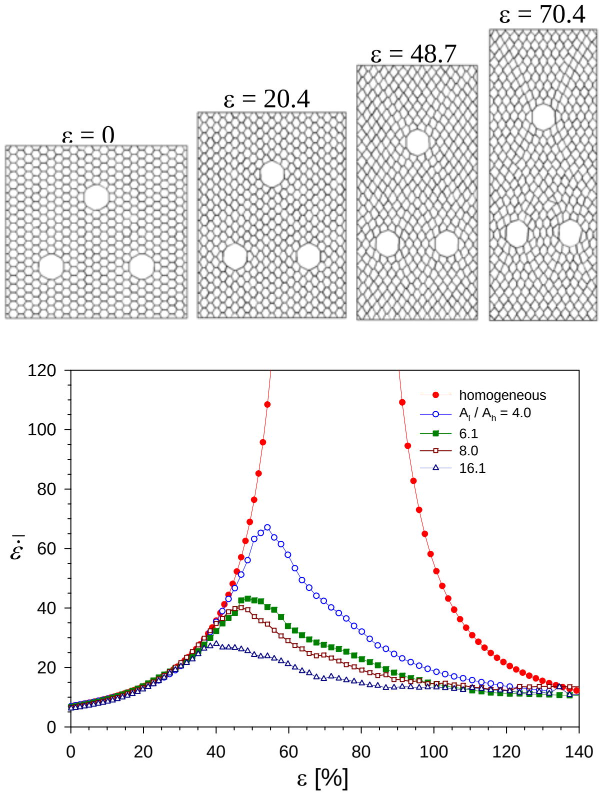

Fig 3. a) Snapshots during evolution of a microstructure with three larger grains (A/A_h =8.0). b) Strain rate vs. strain for the homogeneous regular hexagonal structure and four non-uniform microstructures each containing a similar three larger-grains cluster.

The larger the relative area A_l/A_h of the inhomogeneity the smaller the peak value in the strain rate. Moreover, the peak position is also shifted towards lower values of the strain.

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