ICMEd Summer School Mechanics Module

Summer 2017 García/Aagesen/Thornton

Computational Methods in MS&E

Mechanics Module Problem

In some polycrystalline metals, the mechanical properties of the grain boundaries can be considerably different from the bulk crystals within grain interior. For example, hydrogen diffusion, enhanced along the grain boundaries, leads to higher hydrogen concentration in the grain boundary regions. Therefore, observable elastic properties of polycrystalline materials are not those of the single crystal but of the composite consisting of crystalline regions and grain boundary regions. In this problem you will use a finite element calculation to (1) determine the effective properties of such a material based on its microstructure and (2) identify microstructural features that can more likely lead to failure or plastic deformation.



This image is a schematic representation of a polycrystalline material; the colored regions represent grains and the white regions represent the grain boundaries. (Hint: you can select the grains by first selecting the grain boundary phase then using the Invert tool in OOF2.) You can assume that both the grains and grain boundaries have isotropic mechanical properties as given below:

Grains: E = 300 GPa, *ν*= 0.3

Grain boundaries: E = 100 GPa, *ν*= 0.3

Sample size: 100 μm × 100 μm

1. Perform a finite element simulation to determine the effective modulus of the system. This can be done by applying a strain of 1.0% in the vertical direction (in the figure), finding the average stress, and finding the effective modulus using *σ*=*Eeff ε.* Start with 15 x\_elements x 15 y\_elements; your final mesh should have 7,000-10,000 elements. (Hint: The value for the strain given above should be used to set up the externally applied displacement.)

2. Prove that your results are mesh independent.

3. Visualization of the trace of the stress tensor provides insight into the fracture behavior of the material.

1. Define in your own words what the trace of the stress tensor is and how it relates to the fracture behavior of materials.
2. Plot the trace of the stress tensor over the computational domain.
3. Is the trace of the stress tensor larger in the bulk or in the grain boundary? Provide a possible explanation for the observed behavior.
4. Determine the point at which failure is most likely to occur. Can you correlate it with a microstructural feature?

4. Visualization of the von Mises stress provides insight into the plastic deformation behavior of the material.

1. Define in your own words what the von Mises stress is and how it relates to the plastic behavior of materials.
2. Plot the “deviator” stress over the computational domain. This quantity is the magnitude of the deviatoric part of the stress tensor, and is equivalent to the von Mises stress to a constant factor.
3. Is the deviator larger in the bulk or in the grain boundary? Provide a possible explanation for the observed behavior.
4. If the yield stress of the bulk and the grain boundaries are the same, where would you expect plastic deformation to occur?