27-750

Mid-term number 2

Released Apr. 22nd, 2016

Due Apr. 24th at 11:59 p.m.

10+15+10+25+15+10+20+20=125

Q1. [10] One of the tests to verify that a grain growth code is working correctly is to simulate the shrinkage of a single, isolated grain. If the mobility of the boundary of the grain is *M* and its energy is *E*, derive the rate of change of its area, *dA/dt* and show that this is constant.

A. The answer is as follows. Recall that the velocity of the boundary is given by
dr/dt = v = ME\kappa = ME/R.

Also, dA/dt = d(πR2)/dt = 2πR \* dR/dt

Therefore we combine to get:

dA/dt = 2πR \* ME/R = 2πME

Q2. [15] Aluminum has an average grain boundary energy of 0.5 J.m-2, shear modulus 27 GPa, Burgers vector 0.28 nm. For a grain size of 20 µm, estimate the dislocation density that would balance out the curvature driving force. Only two significant figures are expected.

A. [from slide xx in the 301 lecture notes]

Estimate of driving force, E, for rex:

Energy per unit length of dislocation ≈ Gb2

Thus energy/volume, E ≈ Gb2

Typical cold worked dislocation density,  = 1015.m-2

E.g.,
for Al, G = 27 GPa, b =0.28 nm, E ≈ 2 J.m-3 ( = 2MPa)

Estimate the curvature driving force as \gamma/R = 0.5/2.10-5 = 250 kPa.

Balance the two and get  = 250,000 / 27.109 / (0.28.10-9)2 = 1014 m-2.

Would be more interesting to convert to stress and estimate how much strain…

Q3. [10 points]

You have learned that the number of equivalent descriptions of the misorientation of a grain boundary in cubic materials is 1,152. A) For grain boundaries in tetragonal materials, how many equivalent descriptions are there? B) How many equivalents are there if you describe the orientations as active rotations (i.e. an active rotation of each crystal from the reference position to their orientation)?

Answer

a) The number is the order of the crystal symmetry, *8*, squared and multiplied by two for the switching symmetry, so the total is *8\*8\*2=128*.

b) The symmetry operators are combined together in between, so to speak, the two orientations so, since they are drawn from a group, only one set of operators applies. Switching symmetry still applies. Therefore the total = *8\*2=16*.

Q4. [25]

a) You have measured the orientations of two adjacent grains in a sample of (bcc) iron which, in Euler angles, turn out to be {0, 90, 45} and {0, 51.1, 45}. What is the misorientation across the boundary? Where does the misorientation axis lie relative to the sample axes? Hint: try plotting a {110} pole figure if you would like a quick, intuitive answer.

b) If the boundary plane normal is parallel to the sample Z axis, what is the tilt/twist character of the boundary?

c) If the boundary plane normal is parallel to the sample X axis, what is the tilt/twist character of the boundary?

d) Which CSL type does this boundary correspond to?

e) You should be able to find information on the variation in grain boundary energy for this misorientation type in bcc metals. Which of the grain boundary normals identified in b) and c) above is high energy, and which is low energy? Hint: you should be able to find such a paper with an MSE professor as a co-author.

A.

a) These two orientations happen to lie in the alpha fiber, so they share a common <110> // RD. Therefore, by inspection, the disorientation is 38.9°<110> and the common <110> is parallel to the X axis.

b) Pure tilt, based on above remarks.

c) Pure twist, based on above remarks.

d) sigma-9

e) Referring to the paper by Sutatch on bcc GB energies, the twist boundary, (c), is low energy and the tilt boundary, (b), is high.

Q5. [15]

Assume that slip occurs on {111} planes and in <110> directions.

(a) For a tensile axis located inside the 001-101-111 standard stereographic triangle, what are the indices of the active slip direction and active slip plane normal?

Direction: [uvw] = [0 1 1]; Plane: (hkl) = (1 -1 1).

b) Compute the coordinates of the point (tensile axis position) that gives a Schmid factor exactly equal to 0.5. Compute this for the point that falls in the 001-101-111 standard stereographic triangle. You may give a numerical answer (to 4 significant figures) or leave it in the form of surds.

A. The solution to this is to recognize that the angle between the TA and both the slip direction and the slip normal must be 45°. Therefore one can write that [uvw]•[0 1 1]/√2=1/√2, and [uvw]•[1 -1 1]/√3=1/√2. The first equation gives *v = 1-w*. Knowing the u2=1-v2-w2, we get u2=1-(1-2w+w2)-w2 or u2=2(w+w2). Adding the first to the second (knocks out v) gives u = (√3/√2 + 1) - 2w. Combining together, we get:

[uvw] = [ 1/√6 , (0.5 – 1/√6) , (0.5 + 1/√6)], or, [ 0.408, 0.092, 0.908]

Check that it’s a unit vector:

[ 1/√6 , (0.5 – 1/√6) , (0.5 + 1/√6)]2 = 1/6 + 0.25 +1/6 -1/√6 + 0.25 + 1/6 + 1/√6 = 0.5 + 3/6 = 1.

Proof: take dot products with 1/√2[0, 1, 1] and with 1/√3( 1, -1, 1) to check that the direction cosines are both 1/√2.

cos(\phi) = 1/√2 {0.5 – 1/√6 + 0.5 + 1/√6} = 1/√2

cos(\lambda) = 1/√3 [ 1/√6 - (0.5 – 1/√6) + (0.5 + 1/√6)] = 1/√3 {3/√6} = 3/(√3\*6)} = √3/√6 = √3/(√3\*√2) = 1/√2. Q.E.D.

Also valid: [ 28√2, √2, 14 ] (normalized to be a unit vector).

Q6. [10]

Explain how abnormal growth in subgrain networks can account for dependence of the (primary) recrystallized grain size in metals as a function of strain, above about 20 %. Include a description of why the grain size is insensitive to the annealing temperature, even though the rate of recrystallization increases with temperature via an Arrhenius expression. Explain which grain boundary property explains the latter point.

A. Subgrain networks have a characteristic spread in orientation. The spread is an increasing function of prior plastic strain. This spread leads to a certain number density of subgrains with high angle boundaries that are much more mobile than GBs in the general network. On annealing, AGG occurs. The resulting large subgrains appear as “nuclei” of recrystallization. Therefore the number density of abnormal subgrains determines the density of recrystallized grains, therefore the grain size. Obviously GB mobility depends on temperature via an Arrhenius term, which explains the T dependence of the recrystallization rate.

Q7. [20]

a) Convert (3 1 1)[1 0 -3] to:
Euler angles,
Transformation matrix,
Rodrigues vector, and
Unit quaternion (with cosine term in 4th position).

A. Eulers: -84.26° 72.45° 71.56°

Matrix:

|  |  |  |
| --- | --- | --- |
| 0.316227766 | -0.286038777 | 0.904534034 |
| 0 | 0.953462589 | 0.301511345 |
| -0.948683298 | -0.095346259 | 0.301511345 |

Rod.: 0.1543 -0.7208 -0.1112

Quat.: 0.1237 -0.5779 -0.0892 0.8017

b) Consider a rotation matrix that describes a 180° rotation about some arbitrary axis, [u,v,w]. How can one extract the axis from this matrix? Hint: write out the matrix for this case and consider how you can use one of the rows.

A. Here is the matrix, for which sin**=0, cos** = -1. Take, e.g., the first row. First extract *u = √{(a11+1)/2}*. Then obtain *v=a12/2u* and *w=a13/*2u.



Q8. [20 points]

(i) [5] Starting with the values provided in the notes for C11, C12 & C44 for sodium chloride (NaCl), show that you can obtain the stated values for E100 and E111.

(ii) [5] Write down a formula for the Young’s modulus as a function of direction between [110] and [001], where the angle is zero at [110] and 90° at [001]. Hint: consider how to write the direction cosines in terms of a single angle.

(iii) [5] Plot the modulus over this same range of directions.

(iv) [5] Repeat for Pb, plot the result on the same graph at the NaCl result and comment on the difference(s) between the two results.

Answers:

(i) To do this, one must first compute the values of s11, s12, and s44 from the values of stiffness coefficients (for NaCl). Then one can compute E100 and E111 to check. I got 4.358 for E100, which checked out.

(ii) The key to devising the formula is to recognize that we need to express the direction cosines in terms of a single angle. This is equivalent to writing the three direction cosines as parametric equations i.e. each one is a function of a single angle. The angle that we care about is the anti-clockwise rotation about [1,-1,0], starting at [1,1,0], which we will call theta. The three direction cosines can be (almost) written down by inspection.

Alpha\_1 = cosine(theta) \* sine(45°) = 1/√2 \* cosine(theta)

Alpha\_2 = cosine(theta) \* sine(45°) = 1/√2 \* cosine(theta)

Alpha\_3 = sine(theta)

Then we use the formula provided for the variation in the modulus.



1./{E(theta)} = 1/E100– 3\* { 1/E100 - 1/E111} {0.25\*cosine4(theta) +
 sine2(theta)\*cosine2(theta)}

(iii) See plot below



(iv) The Na and Pb plots should both show strong anisotropy but the stiffest direction will be 111 for Pb (blue line) and 100 for NaCl (red line).