**Solution Manual for Integrated Computational Materials Engineering (ICME) for Metals**

**Chapter 1 Homeworks/Exercises**

* 1. Historically the different disciplines (mechanics, materials, physics, and mathematics) have claimed that they have been examining multiscale aspects for years now. Write a summary comparing and contrasting the different perspectives and elucidate weaknesses of the disciplines not interacting.
  2. Explain how multiscale materials modeling can be a subset of Integrated Computational Materials Engineering (ICME) and also how (ICME) can be a subset of multiscale materials modeling.
  3. How is ICME different from computational materials engineering?
  4. Write a summary comparing and contrasting hierarchical versus concurrent multiscale modeling methods in terms of efficacy, the time it takes to get good solutions, and practicalities related to solving an engineering problem.
  5. In terms of solving a practical engineering problem using the ICME tools, explain why downscaling needs to occur before upscaling.
  6. Explain the benefits of employing design optimization methods over the standard design methodology. List the costs for either methodology.
  7. Once there is more than one objective, explain why an engineer (intelligent agent outside of the numerical system) is required in the decision making process. For example, one can use the example of a Pareto diagram as a starting point.
  8. In designing for the life cycle of a structural component, explain why there could be a different product design versus the case when the manufacturing steps are included in designing the component.
  9. Imagine a finite element simulation of an automotive component that is supposed to crush and absorb the energy under a crash situation. Now imagine that two different simulations were performed: one with the microstructural details like the grain sizes, particles sizes, etc. and the other has homogeneous materials. What would be the expected differences in the results of the simulations?
  10. Why is the notion of uncertainty and experimental validation important in ICME and multiscale materials modeling?

**Chapter 2**

2.1Given the following stress tensor in units of MPa: find the first three invariants of the stress, the deviatoric stress tensor, the first three deviatoric stress invariants, the stress triaxiality, the von Mises stress, and the principal stresses.



2.2 Given a deformation tensor, find the Green and Almansi strain tensors, the associated strain invariants, the associated von Mises strain for each strain tensor, and the principle strains. Here vx is the velocity in the x-direction and can be assumed to be 0.2 cm/sec; t is the time of interest and can be assumed in this problem to be 3 minutes; h is the height of the specimen being tested and can be assumed to be 2 cm; vy is the velocity in the y-direction and can be assumed to be .05 cm/sec; and L is the length in the x-direction which can be assumed to be 2 cm.



2.3 When incorporating damage and failure into a finite element analysis, the comment of loss of mass conservation is sometimes argued. Starting from kinematics where the deformation gradient is defined by the multiplicative decomposition into elastic, plastic, and volumetric components, prove that one can get an equivalence with the damage (pore volume fraction) when compared to the conservation of mass within a continuum element. This illustrates that mass conservation is not violated.

2.4 For the data given for 7075-T651 aluminum, find the Bauschinger Stress Parameter (BSP=fy-ry/fy, where “fy” means forward yield and “ry” means reverse yield) and reverse yield values for a forward strain level up to 5% for the two following cases: (a) when the ratio of kinematic hardening to isotropic hardening is 10% and (b) when the ratio of kinematic hardening to isotropic hardening is 90%. Assume that there is no difference between tension and compression.

2.5 For model calibration code, use data and plasticity-damage “DMG” model in the [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu) website. DMG can be found at “Macroscale” and the A356 aluminum alloy experimental data can be found at “Experimental Data.” Plot a stress-strain comparison of the model and experiments.

2.6 a one element finite element simulation of A356 aluminum undergoing tension using the finite element code Calculix with the input deck using the plasticity-damage (DMG) model at the website: https://icme.hpc.msstate.edu. At this website, go to “Macroscale” and look for the one element input deck. Plot a stress-strain comparison of the model and experiments.

2.7 Conduct a finite element simulation of A356 aluminum undergoing tension for the notch tensile specimen using the finite element code Calculix with the input deck using the plasticity-damage (DMG) model at the website: https://icme.hpc.msstate.edu/. At this website, go to “Macroscale” and look for the one element input deck. Plot a comparison the load-displacement curve of the model with experimental data using the load and displacements at the loading boundary.

2.8 Conduct a model calibration of A356 aluminum alloy with a strain-life curve for fatigue using the MultiStage Fatigue (MSF) model at the website: https://icme.hpc.msstate.edu. The MSF model at this website can be found at “Macroscale.” Plot a comparison the strain-life curve of the model with experimental data.

**Chapter 3**

3.1 Prove that another form of the plastic spin that can be used with , which is given by .

3.2 Using the [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), run a single crystal aluminum in compression: show the stress-strain curve and the associated crystal orientation change versus strain.

3.3 Using the [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), run a single crystal aluminum in tension: show the stress-strain curve and the associated crystal orientation change versus strain.

3.4 Using the [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), run a single crystal aluminum in simple shear: show the stress-strain curve and the associated crystal orientation change versus strain.

3.5 Using the [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), run a polycrystalline aluminum in compression:

a. plot the the stress-strain curve,

b. plot the associated crystal orientation change versus strain,

c. show the various yield surfaces as a function of five strain levels,

d. plot the Orientation Distribution Function as a function of strain,

e. plot the kinematic hardening (yield surface center) as a function of strain,

f. plot the isotropic hardening (yield surface radius) as a function of strain.

3.6 Using the [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), run a polycrystalline magnesium in compression:

a. plot the the stress-strain curve,

b. plot the associated crystal orientation change versus strain,

c. show the various yield surfaces as a function of five strain levels,

d. plot the Orientation Distribution Function as a function of strain,

e. plot the kinematic hardening (yield surface center) as a function of strain,

f. plot the isotropic hardening (yield surface radius) as a function of strain.

3.7 Using the [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), run a polycrystalline aluminum in tension:

a. plot the the stress-strain curve,

b. plot the associated crystal orientation change versus strain,

c. show the various yield surfaces as a function of five strain levels,

d. plot the Orientation Distribution Function as a function of strain,

e. plot the kinematic hardening (yield surface center) as a function of strain,

f. plot the isotropic hardening (yield surface radius) as a function of strain.

**Chapter 4**

4.1 How does the presence of dislocations in metals affect their yield strength and the flow stress later during deformation?

4.2 Define the difference between a positive and a negative edge dislocation. Clarify this in terms of the description of a dislocation at the continuum level and the corresponding atomic level.

4.3 Describe the difference between a junction and a jog. Under which conditions do each form and what is their effect on the flow stress of metals.

4.4 Using the dislocation dynamics code (can be accessed from “Microscale” link found under <https://icme.hpc.msstate.edu/mediawiki/index.php/Main_Page>), create a simulation box for copper so that the (111) plane is parallel to the x-y plane. Create a Frank-Read source with Burgers vector a/2[011] and size 20 nm. Determine the shear stress xz necessary to activate the source. Use free surface dislocation boundary conditions.

4.5 Start with the same setup created for problem 4.3 but now used rigid boundary conditions. How does the change in boundary conditions affect the source operation.

**Chapter 5**

5.1. Using [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), calculate the equilibrium fcc lattice parameter, cohesive energy, and the bulk modulus for aluminum.

5.2. Using [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), generate an fcc aluminum structure along [100], [010] and [001] direction orientations.

5.3. From the previous structure calculate the (100) surface energy for aluminum.

5.4. Using [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), calculate (110) and (111) surface energies for an fcc aluminum.

5.5. Using [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), perform a uniaxial tension in single crystal in fcc aluminum along [100] at 300 K. Calculate the slope of the curve (Young’s Modulus), yield stress and strain. What is the flow stress value for your simulation? Compare/contrast your values with experimental observations.

5.6. Perform Problem 5.5 again at 500 K, what is the difference? Why?

5.7. Perform Problem 5.5 again at different strain rate, what is the difference? Why?

5.8. Using [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), calculate generalized stacking fault energy curve for an fcc aluminum.

5.9. Take the sample that you generated at Problem 5.2 and equilibriate that 300 K for 200 ps. Check if your pressure and temperatures are equilibriated. Calculate the Diffusivity from your simulation.

5.10. Repeat the Problem 5.7 for up to 1000K at 100K interval and plot the diffusivity with respect to temperature. What can you infer from the plot.

5.11. Using [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), calculate monovacancy energy for magnesium.

5.12. Using [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), calculate the magnesium (0001) surface energy.

5.13. Using [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), calculate the substitution formation energy for aluminum in magnesium.

5.14. Using [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), perform a uniaxial compression test along [0001] direction on magnesium.

5.15. Calculate the Young’s Modulus, yield stress and yield strain from Problem 12, and compare/contrast them with experimental observations as well as Problem 5.5.

5.16. Using [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), generate a polycrystalline fcc aluminum, and equilibriate that at 300 K. See how many atoms are still in fcc atom position through Ovito.

5.17. Perform the tensile test for any direction at 300K. What is the difference with Problem 5.5?

5.18. Using [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), generate a polycrystalline magnesium nanowire, and equilibriate it at 300 K.

5.19. Take the sample from Problem 5.18, and perform a tensile test, and mark the difference with Problem 5.14.

5.20. Substitute 10% of magnesium atoms from the generated nanowire with aluminum atoms, and perform the tensile test; what is the difference with Problem 5.19.

**Chapter 6**

**6.1.** (a) Calculate the minimum energy of a photon so that it converts into an electron-positron pair. Find the photon’s frequency and wavelength.

(b) Use the uncertainty principle to estimate the ground state radius and ground state energy of the hydrogen atom.

6.3. An electron is moving freely inside a one dimensional infinite potential box with walls at x=0, and x=a. If the electron is initially in the ground state (n=1) of the box and if we suddenly extend the box size from x=a to x=4a, calculate (i) the probability of finding the electron in the ground state of the new box, and (ii) the first excited state of the box.

6.4. Consider the state | > = 3i |1>-7i|2> and |>=-|1>-2i|2> with |1> and |2> are orthonormal vectors. Calculate the following:

(i) Calculate | + > and < + |.

(ii) Calculate the scalar product < | > and < | >, find if they are equal!

6.5. Determine the cohesive energy of aluminum.

6.6. Calculate the de Broglie wavelength (=h/p) for i) a proton of K.E. 70 MeV, and ii) a 100 g bullet moving at 900 m/S.

6.7. Estimate the uncertainty () in the position of a) a neutron scattering at 5X106 m/S and b) a 50 kg man moving at 2m/S.



6.8. Show that the commutator of two Hermitian operators is anti-Hermitian.

6.9. Consider a matrix A, a ket |> and a bra <|:

A= ; |> = And <| =



Calculate the A|>, <|A|>, and | ><| also, find the complex conjugate, the transpose, and the hermitian conjugate of A, |> and <|.

6.10. Find the eigenvalues and the normalized eigenvectors of the matrix A

A= .



6.11. Consider a particle whose Hamiltonian matrix is H =



i) Is |>= an eigenstate of H? Is H Hermitian?



ii) Find the energy eigenvalues, a1, a2, and a3, and the normalized energy eigenvectors.

iii) Find the matrix corresponding to the operator obtained from ket-bra product of the first eigenvector P = |a1><a2|.

6.12. Consider a one dimensional particle which is confined within the region 0<x<a and whose wavefunction is (x,t) = Sin(πx/a)exp(-iωt). Find the potential V(x). Calculate the probability of finding the particle in the interval a/4 < x < 3a/4.

6.13. A particle of mass m that moves freely inside an infinite potential well of length, is initially in the state  (x,0) = √(3/5a) Sin (3πx/a) + √(1/5a) Sin (5πx/a). Find  (x,t) at any time t. Calculate the probability density ρ(x,t), and the current density, J(x,t). See if the probability is conserved.

6.14. Consider a system whose initial state | (0)> and Hamiltonian are given by

| (0)> = , and H = ,



i) If a measurement of the energy is carried out, what values would we obtain and with what probabilities?

ii) Find the state of the system at a later time t; you may need to expand  (0) in terms of the eigenvectors of H.

iii) Find the total energy of the system at time t=0 and any later time t, are these values different?

6.15. Consider a particle of mass m subject to an attractive delta potential V(x) = -V0δ(x). where V0 is positive.

i) In the case of negative energies, would the particle have bound state? How many? Find the binding energy and wavefunction.

ii) What is the probability that the particle remains bound if V0 is halved and quadrupled suddenly?

iii) Study the scattering case (E>0) and calculate the reflection and transmission coefficients as a function of the wave number k.

6.16. Using the [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), calculate the equilibrium fcc lattice parameter, cohesive energy, and the bulk modulus for aluminum using the computational tools from the cyber infrastructure

(webpage [https://icme.hpc.msstate.edu/mediawiki/index.php/Electronic\_Scale](https://ccg.hpc.msstate.edu/mediawiki/index.php/Electronic_Scale).)

6.17. Using the [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), calculate the equilibrium hcp lattice parameter, cohesive energy, and the bulk modulus for magnesium using the computational tools from the cyber infrastructure.

6.18. Using the PAW-GGA aluminum potential described on the webpage (https://icme.hpc.msstate.edu/mediawiki/index.php/Electronic\_Scale), calculate the equilibrium bcc lattice parameter and the corresponding minimum energy per atom. Compare that with the previously found cohesive energy for aluminum in fcc structure.

6.19. Using the [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu) PAW-GGA Magnesium potential, calculate the equilibrium fcc lattice parameter and the corresponding minimum energy per atom. Compare that with the previously found cohesive energy for magnesium in hcp structure and the minimum energy in a bcc structure. Plot the atomic volume Vs energy curve for three basic structures: fcc, bcc, and hcp.

6.20. Using the [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), calculate the vacancy formation energy for aluminum using the pseudopotential. Note that you need to extend/duplicate the basic unit cell. For orthogonal hcp crystal structure, there are four atoms per unit cell, duplication of 3x3x3 would produce 108 atoms. Check if that many atoms can be handled in your system, otherwise reduce the size.

6.21. Using the [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), calculate the interstitial formation energy for aluminum, using the pseudopotential. Note here, you also need to extend/duplicate the basic unit cell. For fcc system, there are two different interstitial position octahedral and tetrahedral. Calculate the interstitial formation energy for both octahedral and tetrahedral position.

6.22. Using the [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), calculate the interstitial formation energy for magnesium. Check how many interstitial positions could there be.

6.23. Using the [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), calculate the surface energies for aluminum for (100), (110) and (111) surface. Note that along the three directions, your unit cell should be long enough to represent the midway atoms bulk-like.

6.24. Using the [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), calculate the (0001) surface energy for magnesium.

6.25. Using the [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), consider one aluminum atom on top of the magnesium (0001) surface. Find out how many locations could be possible where an aluminum atom can be stable.

6.26. Using the [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), calculate the GSFE curve for aluminum along the direction and on the glide plane of (111).



6.27. Using the [https://icme.hpc.msstate.edu](https://ccg.hpc.msstate.edu), calculate the GSFE curve for magnesium along the direction and on the glide plane of (0001).



**Chapters 7, 8, and 9**

Since these are case studies, an instructor might want the students to have a project for the course that focuses on a new case study of interest. Since it is a graduate course, I often will try to define a problem with the student with the notion of them potentially publishing a journal article. The topic should not necessarily be related to their thesis work and the student’s advisor should definitely be aware of the project ahead of time, so if a paper is published, it is related directly to the course and not related to the funding agent.

**Chapter 10**

10.1 If crashworthiness were the desired performance requirement and a rolled component was going to be designed with this in mind, what electronic structures simulations could be performed to help determine a material that would need to be created for the crashworthiness.

10.2 The next-generation of nuclear reactors are being discussed in terms on making them smaller, safer, and more robust. However, they are projected to last 60 years. In the absence of 60 year old experimental data, explain what the macroscale requirements would be in terms of the thermal, mechanical, and chemical environments. What would be the important structure-property relationships at each scale based upon these requirements.

10.3 If a 30 year old steel bridge experienced a high rate impact of two trucks crashing into each other and then into a main support beam, what performance requirements would need to be evaluated to provide a prognostication about the bridges future.