

Homework 9 Advanced Thermodynamics

Due Monday October 28, 2024

Winter IS, Rudd RE, Oppelstrup T, Frolov T *Nucleation of Grain Boundary Phases* Phys. Rev. Letts. **128** 10.1103/PhysRevLett.128.035701 (2022) discuss a model for nucleation at grain boundaries that is demonstrated using molecular dynamics simulations. They term this “homogeneous” nucleation of grain boundary phases.

- a) Discuss the difference between homogeneous and heterogeneous nucleation. Which does this paper discuss? (Explain/justify this in some detail, this isn't a one-word answer.)
- b) Figure 1a shows the nucleation of an α -phase at a grain boundary from a β -phase. Equation 1 is the base equation to describe nucleation in this confined space. The first two terms are from CNT according to Winter. Explain the first two terms and how they relate to the terms given in class for nucleation. CNT is a 3d theory, what problem is there in applying this to nucleation between two crystalline phases in a 2d environment. Critique the application.
- c) The derivations of equations 2 are given in the supplemental information. Winter doesn't directly describe the terms. v is the Poisson ratio, b is the Burgess vector, R is the radius of the nucleus, ρ is the dislocation core radius, and f has to do with stress differences. Explain each of these terms used in equations 2. Does Winter include a term that accounts for changes in entropy on nucleation? Where or why not?
- d) Winter does a simpler 2D-analysis to obtain a critical size from equation 5. Carry out the minimization of equation 5 to obtain equation 6. Does it make sense that the critical size doesn't depend on the core energy Γ ? Compare this to the critical size obtained from the 3d homogeneous and heterogenous nucleation that we went over in class. To which does it correlate?
- e) Figure 3b shows two plots of the free energy of a nucleus versus the nucleus size. What is the difference between the top and bottom plot? Explain what happens to a nucleus to the left of the peak, to the right of the peak and at the peak. What is the difference in grain growth for positive and negative values of this energy. How is R measured/varied in these simulations? Does that method make sense? What problems to you see with this approach.