MSAE E4215 Homework #1

Yitian Wang

Columbia University
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1. One widely used empirical potential for the energy between two atomswith spacingdis the Morse potential, written as $U(d) = D(e^{-2(d-d_0)} - 2e^{-(d-d_0)})$ Sample values for Cu are$D = 343meV$, $= 1.36A^1$. For a diatomicbond of Cu2,

   (a) Calculate the spring constantf, assuming an interatomic spacing of 0.209 nm.
   apply taylor series expansion on the U near $d = d_0$, we have:

   $$U(d) = D(-1 + 0 + a^2(d - d_0)^2 + -a^3(d - d_0)^3)$$

   $$f = \frac{\partial^2 U}{\partial d^2} = \frac{1}{2}a^2$$

   (b) Calculate the anharmonic coefficientgand parameters

   (c) Calculate the coefficient of thermal expansionfor the bond

   (d) Estimate the ratio of elastic modulus at room temperature to thatat zero temperature, E(300K)/E(0K) considering one bond only.For (FCC) Cu, with lattice parameter 0.36nm,

   (e) calculate the cohesive energy. For simplicity, consider only nearest-neighbor interactions (12 in the crystal).

2. Estimate the yield strength for an absolutely perfect single crystal of Fe (and compare with the experimental value)

3. How is the yield strength defined, conventionally?

4. Brittle or ductile failure: what is better for a structural metal in tension, and why?

5. Why might you want to deform a metal plastically?

6. Examine the stress-strain curve of a perfect Fe whisker (in the presentation, or see notes.) a) is it linearly elastic? b) is it elastic?