

MSAE E4215 Homework #1

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1. One widely used empirical potential for the energy between two atoms with spacing d is the Morse potential, written as $U(d) = D(e^{-2(d-d_0)} - 2e^{-(d-d_0)})$. Sample values for Cu are $D = 343 \text{ meV}$, $d_0 = 1.36 \text{ \AA}$. For a diatomic bond of Cu₂,
 - (a) Calculate the spring constant k , assuming an interatomic spacing of 0.209 nm.
 - (b) Calculate the anharmonic coefficient α and parameters β and γ .
 - (c) Calculate the coefficient of thermal expansion for the bond.
 - (d) Estimate the ratio of elastic modulus at room temperature to that at zero temperature, $E(300\text{K})/E(0\text{K})$ considering one bond only. For (FCC) Cu, with lattice parameter 0.36 nm.
 - (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?