

**Problem 1.** Three different materials, A, B and C, have different potential curves described by the general expression below:

$$V_i(r) = 4\varepsilon_i \left[ \left( \frac{\sigma_i}{r} \right)^{12} - \left( \frac{\sigma_i}{r} \right)^6 \right], \quad i = A, B, C.$$

The material parameters are listed below. (Here,  $\sigma_i$  is not a stress.)

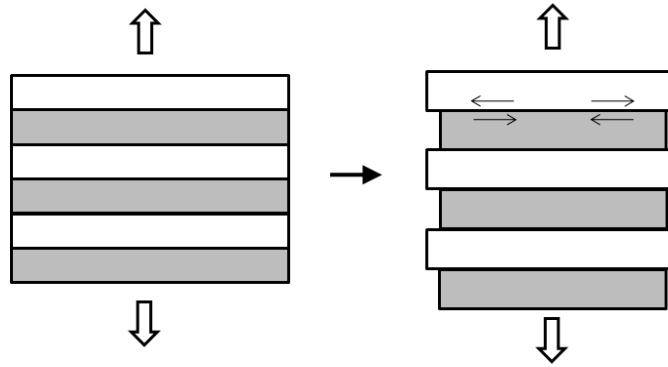
- Material A :  $\varepsilon_A = 0.3 \text{ eV}$ ,  $\sigma_A = 3 \text{ \AA}$
- Material B :  $\varepsilon_B = 0.9 \text{ eV}$ ,  $\sigma_B = 3.4 \text{ \AA}$
- Material C :  $\varepsilon_C = 0.6 \text{ eV}$ ,  $\sigma_C = 3.8 \text{ \AA}$

For each of these materials:

- Plot the potentials and see whether the given expression shows the typical shape (asymmetric and anharmonic) of potential curve (*hint* : plot the curves within the range of  $r = 3 \sim 7 \text{ \AA}$ ,  $V = -1 \sim 0.5 \text{ eV}$ ).
- Calculate the lattice parameters and the binding energies at 0 K.
- Estimate the Young's moduli at 0 K. Which one material is the stiffest?
- Estimate the thermal expansion coefficients when heated from 0 K to the room temperature (300 K). Which one has the largest thermal expansion coefficient ( $l$ ) ?

The increase in thermal energy is given roughly by  $\Delta V_{thermal} \approx k \cdot \Delta T$ , where  $k$  is the Boltzmann constant ( $8.617 \times 10^{-5} \text{ eV / K}$ ). The thermal expansion coefficient ( $l$ ) can be obtained by using the relation,  $l \cdot \Delta T = \varepsilon^{th}$ , where  $\varepsilon^{th}$  is the thermal strain given by  $\varepsilon_{T=300K}^{th} = \frac{a_{T=300K} - a_{T=0K}}{a_{T=0K}}$

**Problem 2.**  $\frac{\nu_A}{E_A} = \frac{\nu_B}{E_B}$  is the necessary condition for stable deformation of composites. If this condition is not satisfied, the Poisson contraction of the layer A is different from that of the layer B, which would lead either to interfacial failure or to developing a complex stress state.



< Schematic diagram of elastically deformed composite when  $\frac{V_A}{E_A} \neq \frac{V_B}{E_B} >$

To avoid these situations, both constituent materials must be contracted by the same amount.

Prove that the condition,  $\frac{V_A}{E_A} = \frac{V_B}{E_B}$ , guarantees the same lateral strains in both materials.

**Problem 3.** Consider two different materials: “Coffeemugium” is a brittle ceramic (get it?) and “Paperclipite” is a polycrystalline metal. Uniaxial tensile tests of both materials give you their load displacement curves until fracture. The data are included in the Excel file on the website. The initial geometries (the initial cross-sectional area,  $A_o$ , and the initial length,  $L_o$ ) of two materials are

- Coffeemugium :  $A_o = 0.025 \text{ m}^2$ ,  $L_o = 0.05 \text{ m}$
- Paperclipite:  $A_o = 0.05 \text{ m}^2$ ,  $L_o = 0.15 \text{ m}$ .

For both materials,

(a) Plot the true stress-strain curves, calculate yield stresses and work hardening rate.

(hint: to obtain the true stress, you need to know the instantaneous cross-sectional area at any given time (or strain). To get it, use the volume conservation,  $L_o A_o = LA$ . Here,  $L = L_o + d$ , where  $d$  is the measured displacement.)

(b) Make two thin plates from each material. For the 2D multi-axial loading conditions shown below (directions 1 and 2 are the lateral directions of the plate), determine whether yield occurs. (hint to use the yield criteria, you have to use a 3D stress state even though there is no component being applied along direction 3). In the case of the Paperclipite, check both Tresca and von Mises’s criteria.

- Coffeemugium:  $\sigma_{11} = 70 \text{ MPa}$ ,  $\sigma_{22} = 120 \text{ MPa}$ ,  $\sigma_{12} = 60 \text{ MPa}$ .
- Paperclipite:  $\sigma_{11} = 85 \text{ MPa}$ ,  $\sigma_{22} = -111 \text{ MPa}$ ,  $\sigma_{12} = 56 \text{ MPa}$ .