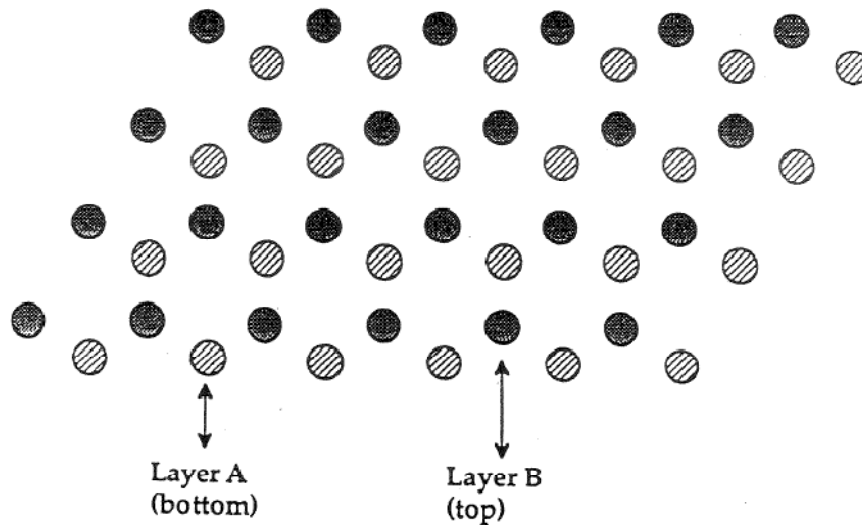
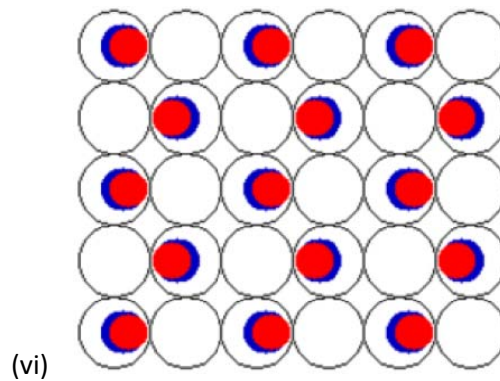
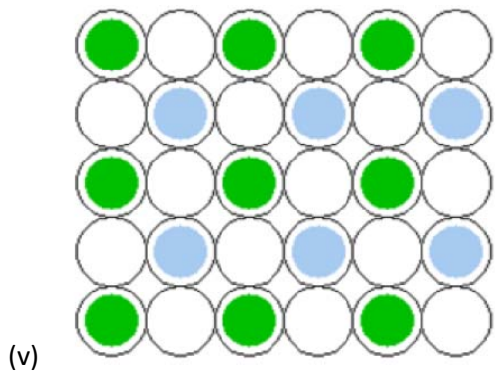
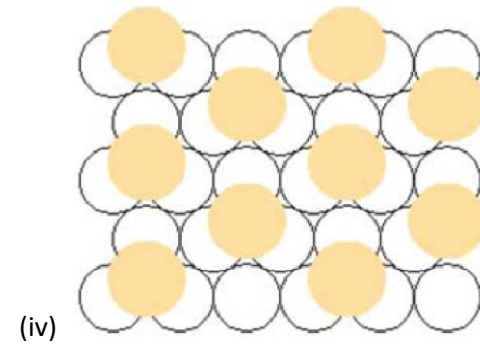
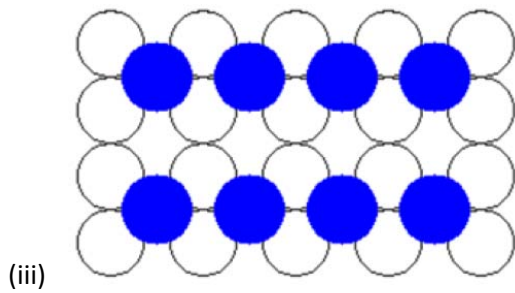
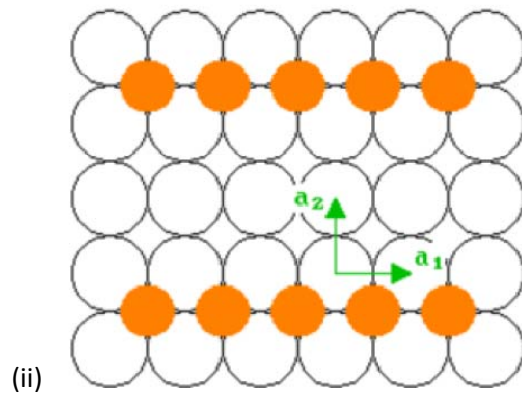
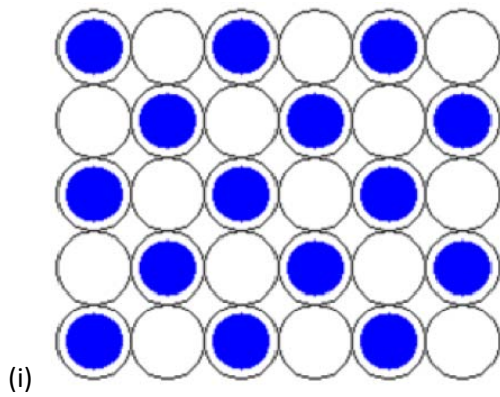


1. Consider a hypothetical two dimensional crystal with a simple square unit cell. Suppose that the γ -plot of the surface tension has deep cusps in the $\{10\}$ directions, however, these cusps are different in the orthogonal directions. That is, $\gamma_{10} = \gamma_{\bar{1}0}$ and $\gamma_{01} = \gamma_{0\bar{1}}$ but $\gamma_{10} \neq \gamma_{01}$.
 - (a) Assume that $\gamma_{10} = 200$ erg/cm and $\gamma_{01} = 400$ erg/cm. Sketch the equilibrium crystal shape (be sure to have the proper ratio of lengths of the edges). Calculate the total edge energy, assuming a crystal of unit area.
 - (b) Now, assume that a change in the interatomic interactions (perhaps the result of a high temperature anneal) results in a new set of deep cusp in the surface tension along the $\{11\}$ set of directions. All of these cusps have the same magnitude, that is $\gamma_{11} = \gamma_{1\bar{1}} = \gamma_{\bar{1}1} = \gamma_{\bar{1}\bar{1}}$. What is the maximum value of γ_{11} such that one of the edges that is stable in part (a) disappears in favor of $\{11\}$ faces? Which edge disappears? Calculate the total edge energy of this new equilibrium shape and show that it is less than that of part (a). Again, assume a crystal of unit area.
 - (c) Suppose that γ_{11} continues to decrease with further annealing steps. At what value of γ_{11} will the only $\{11\}$ edges remain? For this value of γ_{11} calculate the total edge energy and, again, show that the total energy (for a crystal of unit area) is less than that calculated in part (b).

2. Consider a hexagonal close-packed plane. If several such planes are stacked in an ABCABC... sequence, the crystal structure is face centered cubic (fcc). If the stacking sequence is ABABAB... then the crystal structure is hexagonal close packed (hcp). Two such planes are shown below, stacked in an AB sequence.
 - (a) Indicate on the diagram where the next layer of atoms would be if the crystal were fcc. Repeat this exercise (with a different symbol) for the hcp structure.
 - (b) Suppose that this surface were a Cu(111) surface and you were depositing additional Cu atoms from an evaporation source. Into what site would you expect the Cu atoms to go. Explain your answer.



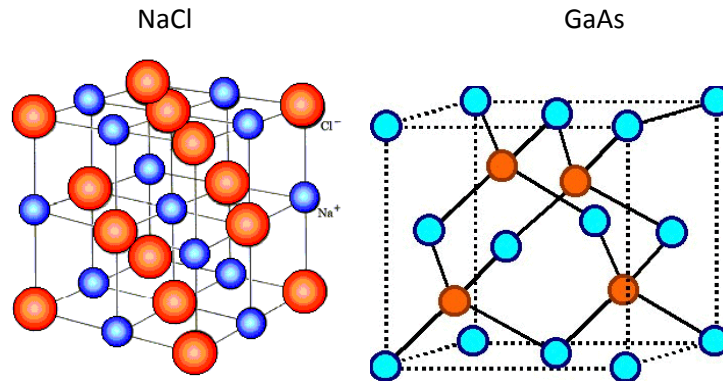
3. Consider the overlayer surface structures below:



For each structure:

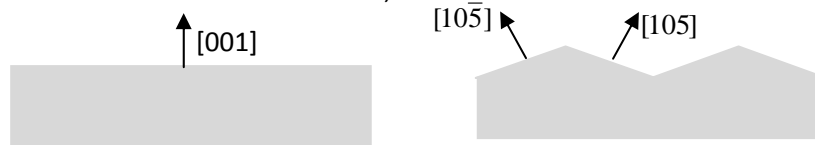
- Draw the primitive unit cell and unit cell vectors for both the substrate and the overlayer.
- Calculate the ideal coverage (in monolayers) of the surface layer.
- If the primitive cell can be named with Wood's notation, do so. If not, try to identify a non-primitive cell which can be so named.
- Give the matrix notation for the primitive surface unit cell of the overlayer.
- Classify the overlayer structure as simple or coincident.
- Does the surface have rotationally equivalent domains? If so describe.

4. For structures (i), (ii), and (iv) above, sketch the magnitude and direction of the reciprocal lattice vectors for both the substrate and the overlayer. Sketch the expected LEED pattern. Use different symbols to distinguish between the substrate and overlayer spots.
5. The figure below show the bulk cubic cell for NaCl and GaAs.



For each of these structures:

- (a) Sketch the geometry of the (111) surface. Also indicate the location of atoms in the second layer. In each case, identify the different atoms.
- (b) As you can imagine, each of these surfaces have high energy owing to the bonds that must be broken to create the surface. Comment on which surface might have higher energy (and why), and suggest a surface atomic rearrangement that might reduce the surface energy.
6. Consider an fcc crystal which is cut and polished to expose the (001) surface. Surprisingly, it is found that when the surface is exposed annealed in oxygen, the surface spontaneously restructures into an array of (105) and $(10\bar{5})$ facets. Suppose the surface tension of each surface is denoted by γ_{001} , γ_{105} , and $\gamma_{10\bar{5}}$, where the latter two surface tensions are equal. Owing to the fact that the surface facets, determine the maximum value of the ratio $105/\gamma_{001}$.



7. (a) Assume small particles of Au and of H₂O, each at their respective melting points. Using the Kelvin equation, calculate the particle sizes for which the vapor pressure is twice the value for a flat surface.
- (b) Calculate the percentage of atoms that are surface atoms in particles containing 125 atoms. Repeat for 1000 atoms. Assume a simple cubic geometry.
8. Tungsten (W) is bcc and palladium (Pd) is fcc, however their atomic radii are essentially identical (1.36 Å). Calculate the surface density of atoms in the topmost layers of Pd(111), Pd(110), W(111) and W(110). Express each in units of atoms/cm².