

# Atomistic Modeling of Materials

## **3.320 Lab Exercise 1:** Using empirical potentials to perform simple defect calculations



# Objectives

## OBJECTIVE

Understand commonly used approaches for calculating properties of materials

- use of supercells
- definition of defect energies
- convergence issues

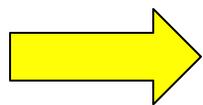
## METHOD

Lennard Jones Potentials and Embedded Atom Potentials with GULP program (General Utility Lattice Program)\*

\* Julian Gale

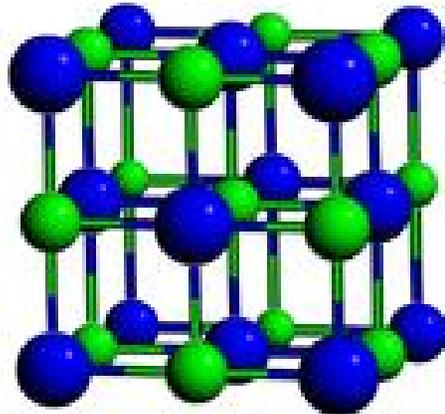
# Problem 1: Lattice Constant and Energy

In general one starts with some estimate for atomic positions and lattice parameters. This can be obtained from experimental information, related compounds, or simply guessing based on heuristic rules (Vegard's Law, atomic sizes, etc.)

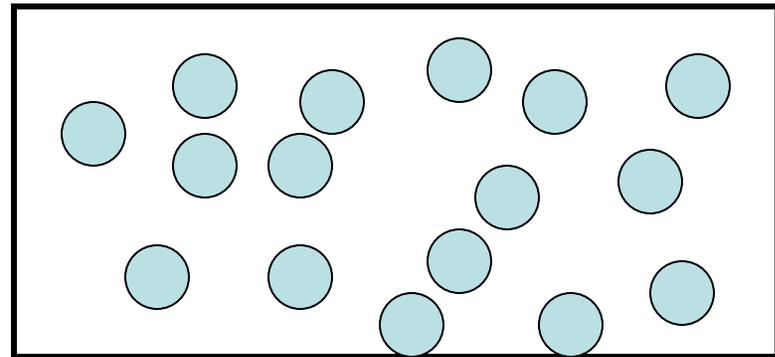


usually need to "relax" the structure to find lowest energy lattice parameter and atomic positions

## Simple High Symmetry Structure



## Low symmetry: Cell + Internal Coordinates



**Note that only a local minimum will be found**

# Defects: The Vacancy Formation Energy

## How to calculate it ?

Vacancy formation is the process of removing an atom from a lattice site and adding it to the bulk. NOTE: The number of atoms in this process remains constant

$$\Delta E_{\text{vac}} = \left[ \begin{array}{c} \text{N atoms on} \\ \text{N+1 sites} \end{array} \right] - \left[ \begin{array}{c} \text{N atoms on} \\ \text{N sites} \end{array} \right]$$

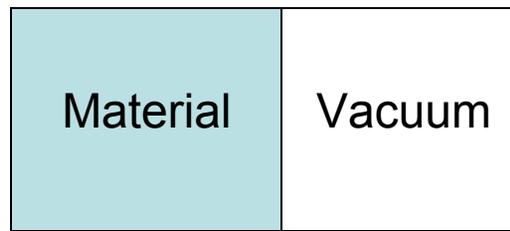
$$E_{f, \text{vacancy}} = E_{\text{cell with } (n-1) \text{ atoms on } n \text{ sites}} - \frac{n-1}{n} * E_{\text{perfect}}$$

# Vacancy formation energy

- Study the convergence of the vacancy formation energy with respect to the size of the supercell ?
- Does it matter which atom you replace from the supercell ?
- Compare the vacancy formation energy to the cohesive energy per atom. Do you notice a difference between the results obtained from the Lennard-Jones potential and the Embedded Atom Method ?
- Connect what you see in the simulation to the lectures on empirical energy methods

# Surface energy

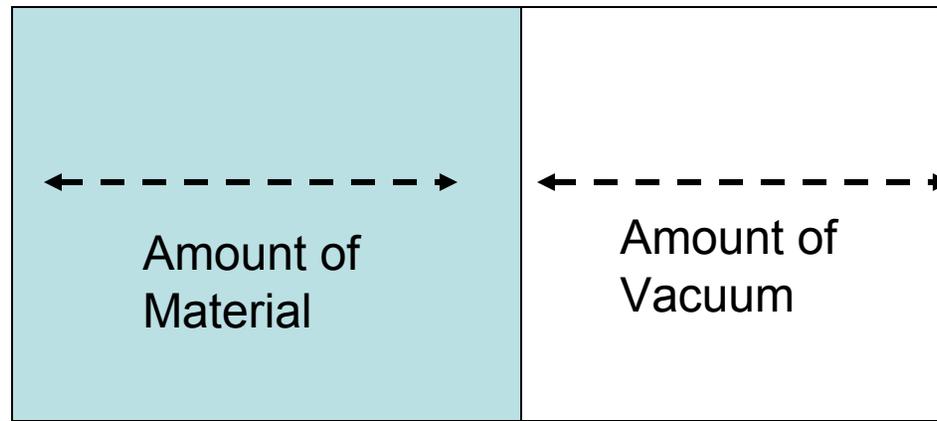
Concept of using supercell is similar to previous problem



Note that there are two surfaces ! Can see this from translating the boundaries of the cell



# Convergence Issues



Which variables to relax ?

freeze some atoms in the center of the slab of atoms  
so as to better approximate bulk

no need to relax the cell shape/parameters

# Surface energies

Compare the surface energies in the Embedded Atom Method and the Lennard Jones Potential. Also look at what happens to the distance between the first and second layer. Can you understand why the two potential models are different ?