Evaluate Phases and Orientations of Given Atomic Structures
S. Shankar, Intel Corporation

Summary: *Ability to identify both crystal structures and orientations for given positions of atoms.*

The project intent is to develop a software prototype that will take as inputs atomic positions for inorganic materials (and element information) and output crystal phase information (BCC, FCC, HCP etc..) orientations (100, 110, 111, 120 etc… including close-packed directions with higher order surfaces) and average lattice parameters (dimensions, compositions). In addition to the software, the expectation is that outputs are also in a file viewable or editable.

As a stretch goal, Identification of point groups on surfaces as well as the 3D groups in these structures.

The crystal structure database for this project is primarily intended to assist the areas of material science and solid-state physics in identifying structural information of inorganic materials. The crystal structures are classified into 14 Bravais lattices as given below.

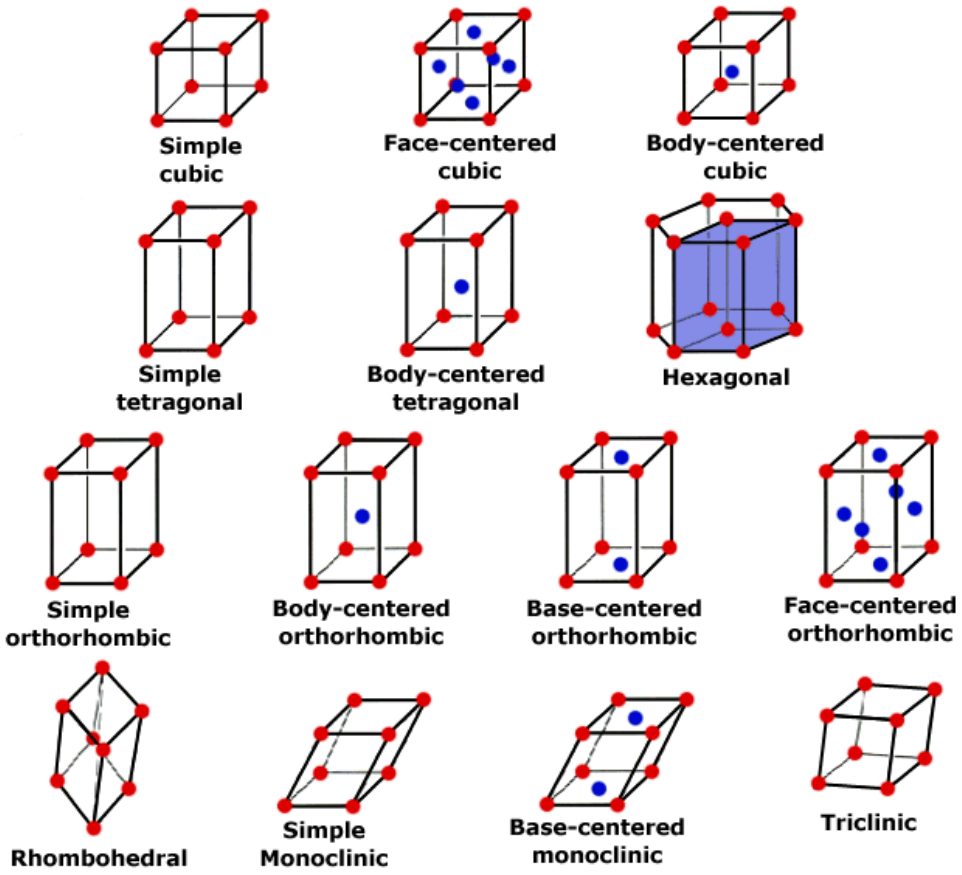


Figure 1: 14 Bravais Lattices

There are 230 unique space symmetry groups in 3D crystal structures. The ability to match a given set of atomic model to these structures implies having a look-up table with distinct groups. The structural arrangements of the atoms in solids and liquids are fundamentally important to the study of their properties. In addition, materials design depends intensely on the structural arrangements of the component phases (e.g. single crystalline, amorphous etc..). Shifting the positions of atoms in a solid material by one means or another, or substituting one chemical species for another, alters the multiple properties of that material. The complete understanding of properties of solids cannot be accomplished without an accurate characterization of the atomic arrangements. While the possibilities for atom arrangements and repetition are infinite in theory for pure bulk crystals, the requirement of different symmetries and arrangements impose rules on these possibilities in real systems. Hence characterization of the structural arrangements in solids is important.

The intent of the project is the ability to identify different Miller Indices (Figure 2) for surfaces or interfaces.

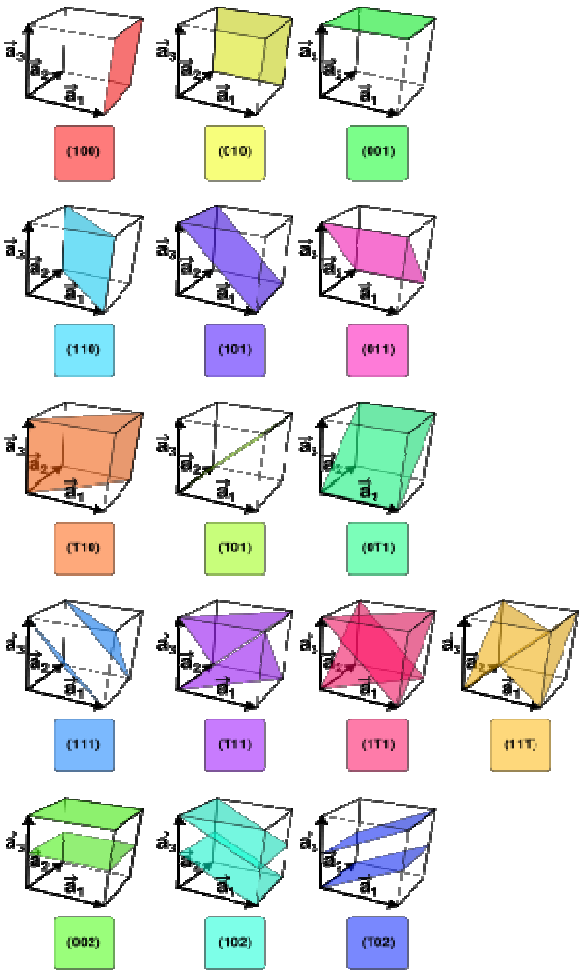
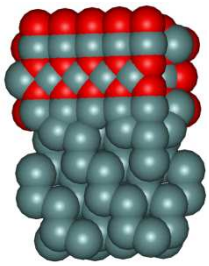


Figure 2: Miller Indices (http://en.wikipedia.org/wiki/File:Miller_Indices_Felix_Kling.svg)

The two primary sources of atomic models are either generated by different tools or manually as shown in the following figures.



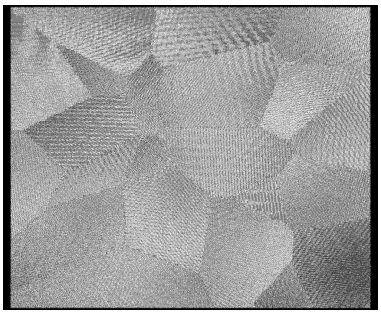


Figure 3: (A). Structure with 3 different surfaces combined together; (B) Poly-crystalline materials.

The work itself can be based on extending the tool Debyer(http://code.google.com/p/debyer/). This particular tool calculates diffraction patterns, pair distribution function (PDF) and related function of atomistic model from simply a set of atomic symbols and positions, either in periodic boundary conditions (PBC) or not. Further, this tool is able to handle tens of millions of atoms. Subsequent methods have been developed for reducing noise in the calculation of structure function (PHYSICAL REVIEW B **73**, 184113 , 2006)

The following operations expected out of the software or tool;

1. Access given atomic structures (given as input files in some standard format)
2. Identify bulk crystal structure phases (number of bulk structures or semi-infinite surfaces)
3. Identify their orientations (Miller indices)
4. If possible, identify point groups and other symmetries
5. Calculations to estimate statistics of lattice dimension
    a. Single crystalline,
    b. Multi-crystalline or poly-crystalline
    c. Amorphous
    d. Quasi-crystalline
6. Calculations to estimate other variables ("pseudo" unit cell dimensions, multi-directional dimensions, element statistics)
7. Run simulations to minimize noise, if needed
8. Output variables that can be plotted, read, and imported for further processing.