February 1, 2007
Lecture #06
Centering of a Crystal Lattice
Fig. 2-5 Types of centering of lattices. (a) Four-unit cells (not necessarily cubic). (b) Body centering, showing all four unit cells. (c) All-face centering, showing only one unit cell for clarity. (d) One-face centering, showing one unit cell. (e) An impossible way to center a lattice. (f) A projection of four trigonal unit cells. (g) Rhombohedral centering of these cells. (h) A rhombohedral unit cell in a rhombohedral lattice. The corresponding hexagonal cell, which is three times larger, is also shown.
Fig. 2-6 (a) through (c) Several aspects of centering a monoclinic lattice. (d) and (e) Several aspects of centering a tetragonal lattice.
FIG. 3-7 Rhombohedral lattice. The triply primitive hexagonal cell has axes $a, b, c$ and lattice points at $0,0,0; \frac{1}{3}, \frac{1}{3}; \frac{1}{3}, \frac{1}{3}, \frac{1}{3}$. Vectors from $0,0,0$ to $\frac{1}{3}, \frac{1}{3}, \frac{1}{3}; -\frac{1}{3}, \frac{1}{3}, \frac{1}{3};$ and $-\frac{1}{3}, -\frac{1}{3}, \frac{1}{3}$ define the primitive rhombohedral cell. Note that this destroys the $S_6$ symmetry of the hexagonal cell. However, if it is considered to be trigonal, the symmetry (which is $C_3$) is retained in these cases. It is possible to choose a primitive cell satisfying $a = b = c$, (i.e., $A_1, B_1, C_1$) $\alpha = \beta = \gamma$. This lattice is called rhombohedral (symbol $R$). There are three equal axes inclined at equal angles with each other (Fig. 3-7). The trigonal threefold (or $\bar{3}$) axis in this case is along the body diagonal of the lattice. 

Note that $\bar{3} = C_6$. 

FIG. 3-8 Rhombohedral lattice projected parallel to the threefold axis. Numbers next to points indicate $z$ coordinates referred to hexagonal axes.