Energy-bands in 1-Dimension

- useful for visualizing band structure with the many k-dependent bands and also the band splitting at Bragg planes

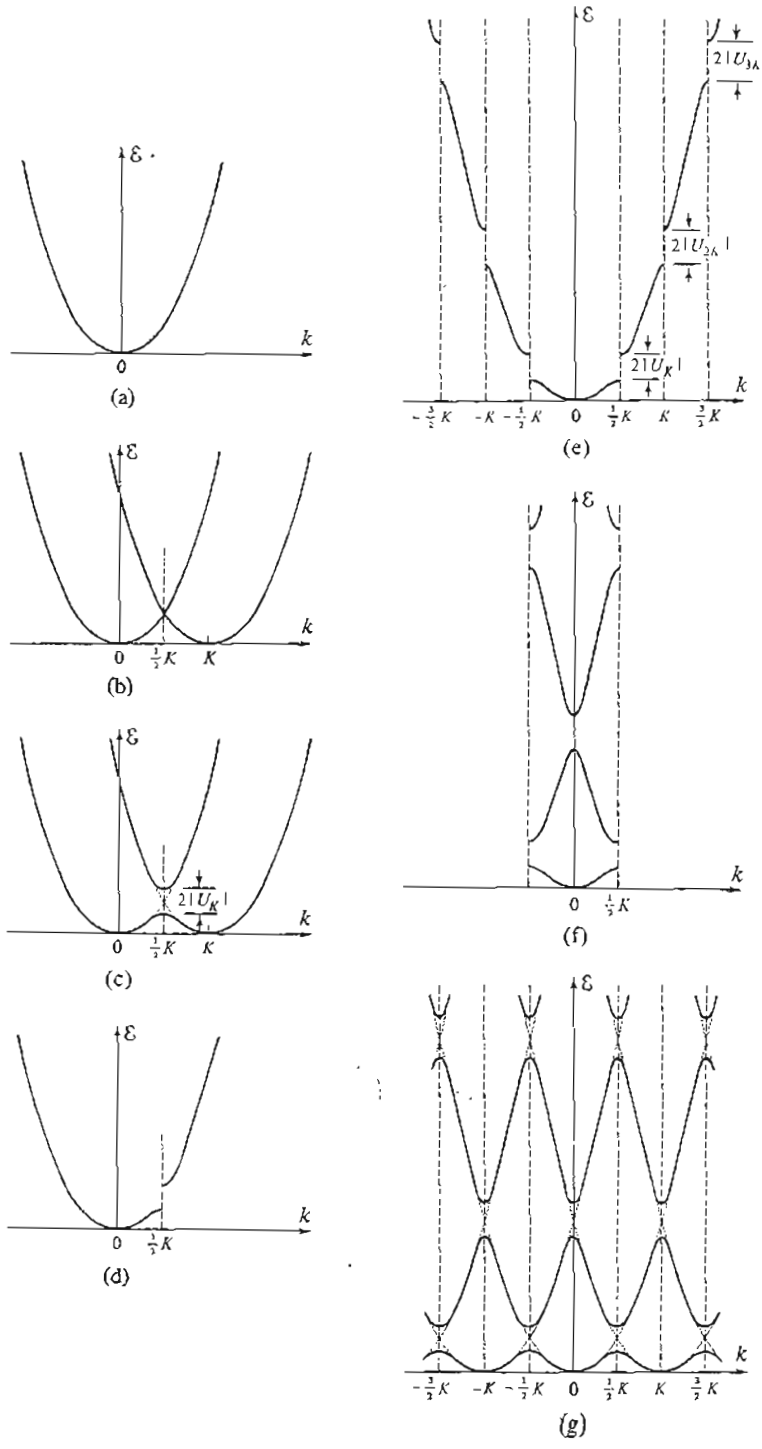

Figure 9.4
(a) The free electron ε vs. k parabola in one dimension. (b) Step 1 in the construction to determine the distortion in the free electron parabola in the neighborhood of a Bragg "plane," due to a weak periodic potential. If the Bragg "plane" is that determined by K, a second free electron parabola is drawn, centered on K. (c) Step 2 in the construction to determine the distortion in the free electron parabola in the neighborhood of a Bragg "plane." The degeneracy of the two parabolas at $K/2$ is split. (d) Those portions of part (c) corresponding to the original free electron parabola given in (a). (e) Effect of all additional Bragg "planes" on the free electron parabola. This particular way of displaying the electronic levels in a periodic potential is known as the *extended-zone scheme*. (f) The levels of (e), displayed in a *reduced-zone scheme*. (g) Free electron levels of (e) or (f) in a *repeated-zone scheme*.

Ashcroft & Mermin, p. 160

Energy-Wave Vector Curves in 3-D

generally use the reduced zone scheme

"gamma point" → Γ point is the zero-point in k-vector space

only at the Γ-point is the energy $E = 0$

then the zones are determined by defining points of high symmetry on the surface of the Brillouin zone

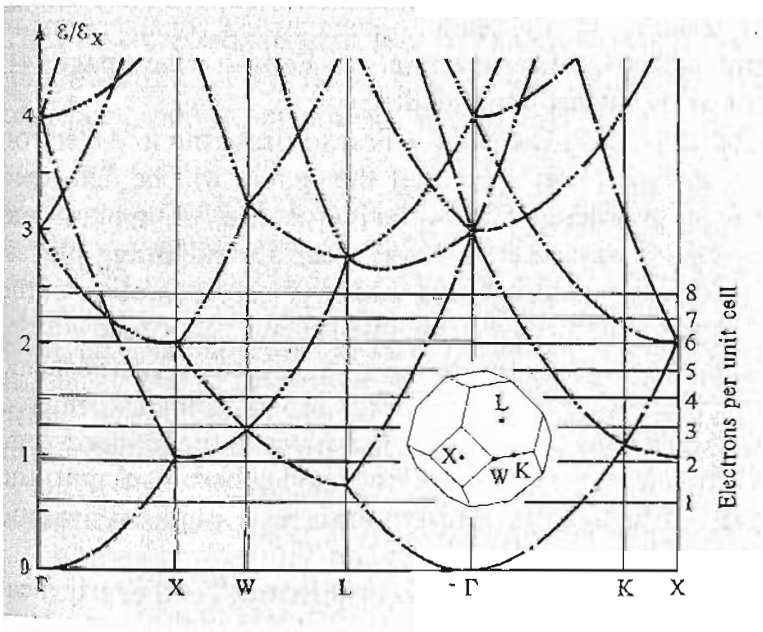

Figure 9.5
Free electron energy levels for an fcc Bravais lattice. The energies are plotted along lines in the first Brillouin zone joining the points $\Gamma(\mathbf{k} = \mathbf{0})$, K, L, W, and X. $\mathcal{E}_x$ is the energy at point X ($[\hbar^2/2m][2\pi/a]^2$). The horizontal lines give Fermi energies for the indicated numbers of electrons per primitive cell. The number of dots on a curve specifies the number of degenerate free electron levels represented by the curve. (From F. Herman, in *An Atomistic Approach to the Nature and Properties of Materials*, J. A. Pask, ed., Wiley, New York, 1967.)

- Ashcroft & Mermin, p. 161

- Energy E is plotted along straight lines connecting the points of high symmetry.
- Zones along different directions are often shown in the same graph