

Section 10

Bandstructure in Real Materials (Si, Ge, GaAs)

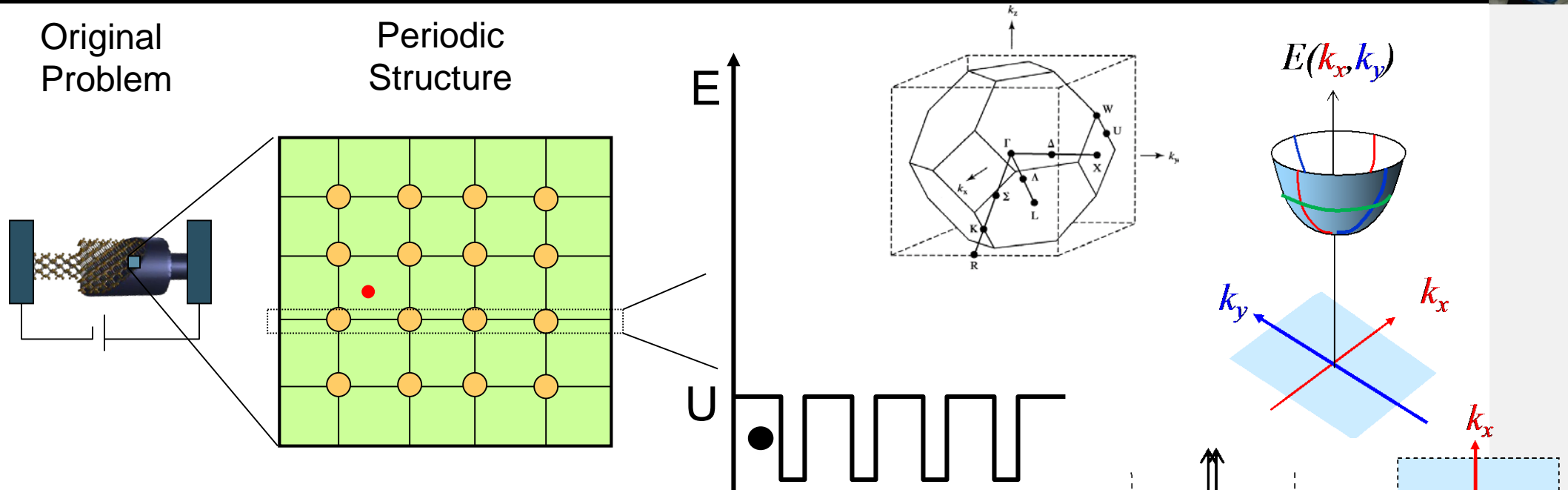
Gerhard Klimeck

gekco@purdue.edu



School of Electrical and
Computer Engineering

Section 10 Bandstructure in Real Materials (Si, Ge, GaAs)



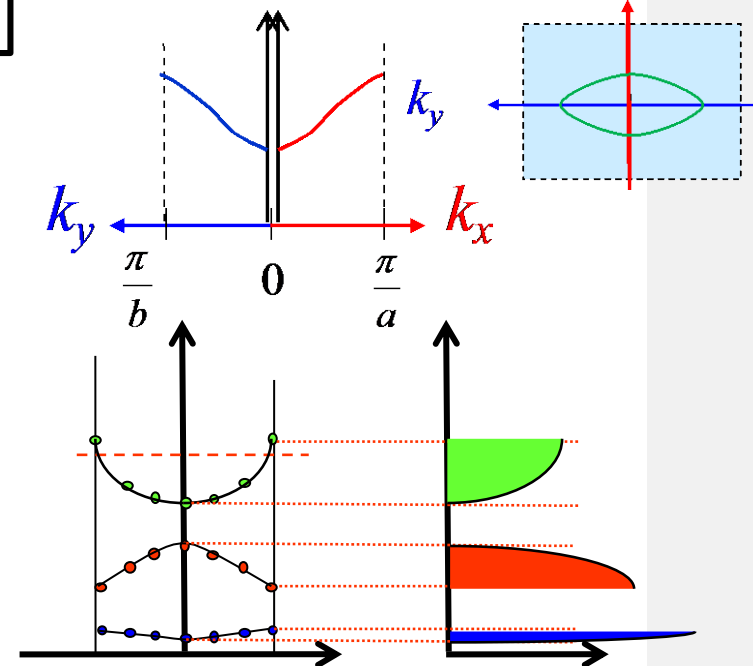
Section 7 – Bandstructure in 1D Periodic Potentials

Section 8 – Brillouin Zone - Reciprocal Lattice

Section 9 – Constant Energy Surfaces & DOS

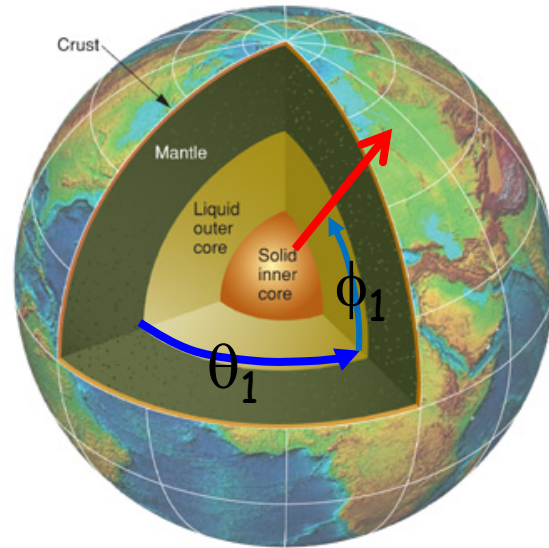
- 10.1 $E(k)$ diagrams in specific crystal directions
- 10.2 Constant Energy Surfaces – Effective Mass Tensor
- 10.3 Density of States Effective Mass

Reference: Vol. 6, Ch. 3

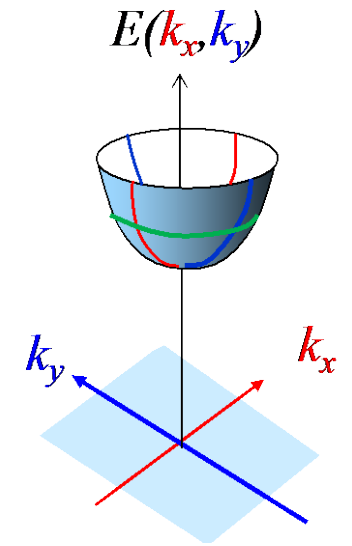
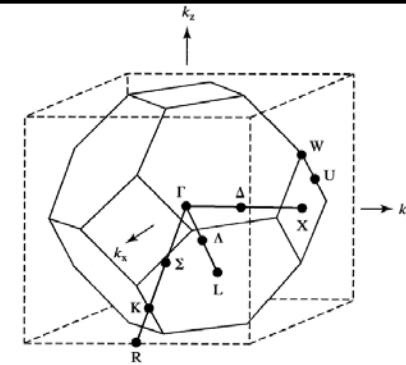


Analogy for E-k Diagram: 4D info through 2D Plots

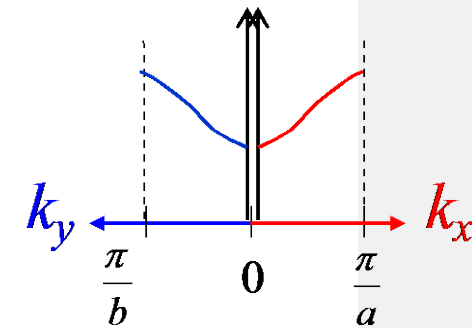
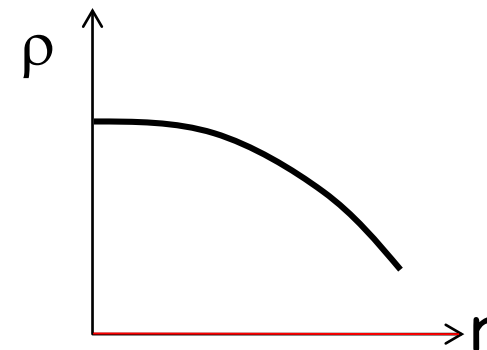
Density (x,y,z)
4D information



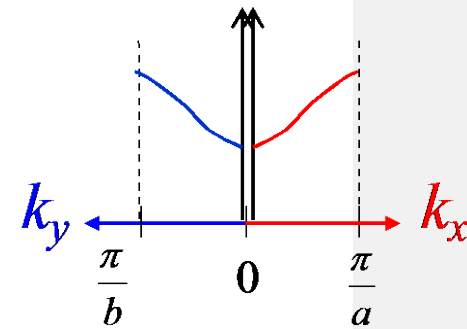
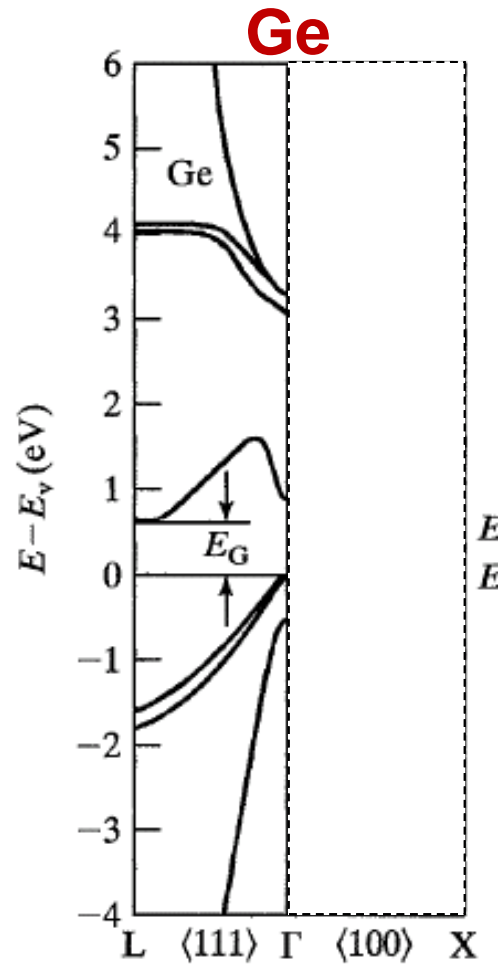
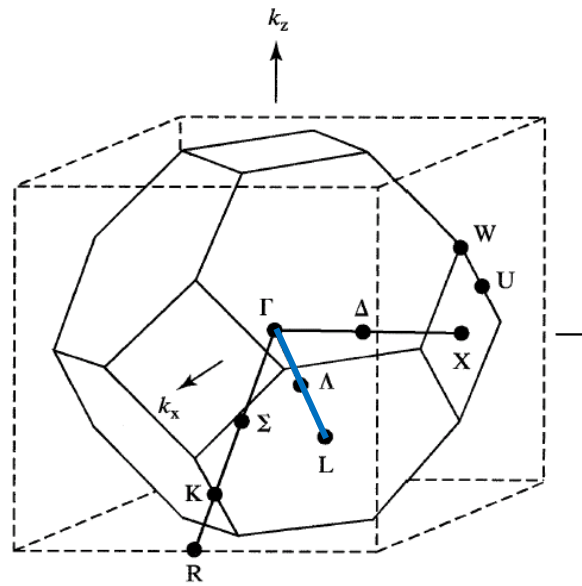
A series of line-sections can
Represent the 4D info in 2D plots



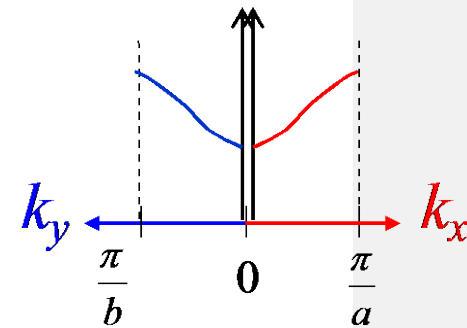
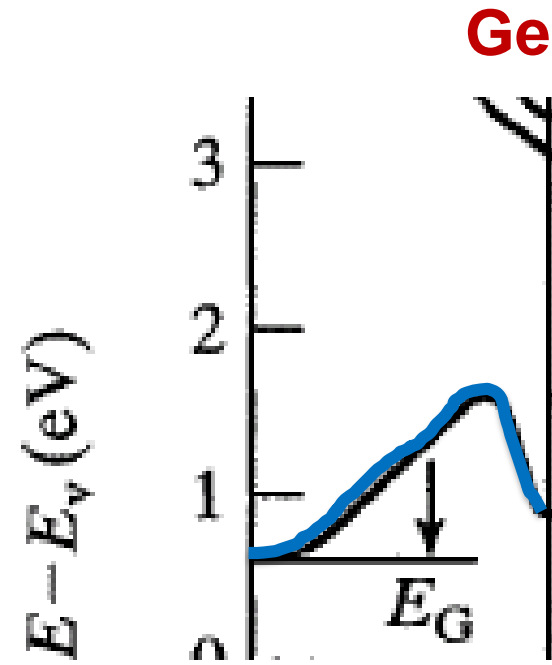
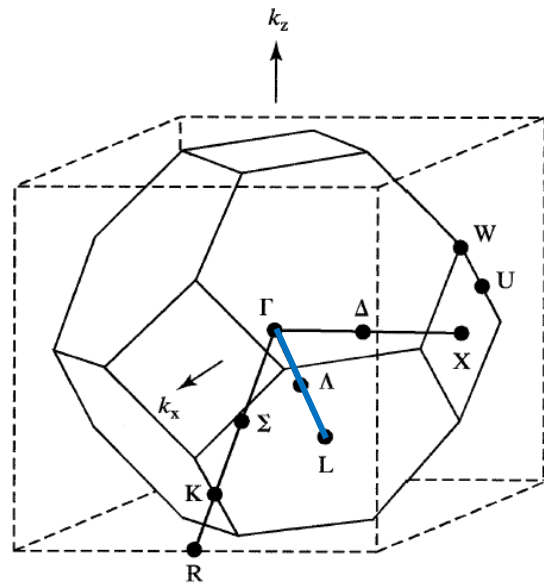
Cut along $(\theta_1, \phi_1) \dots$



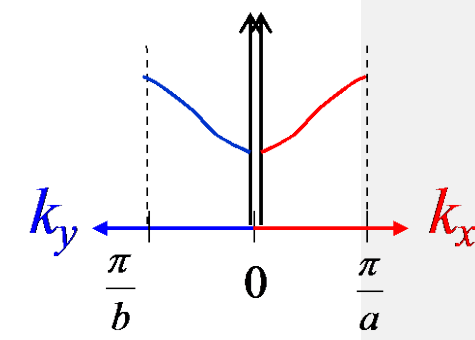
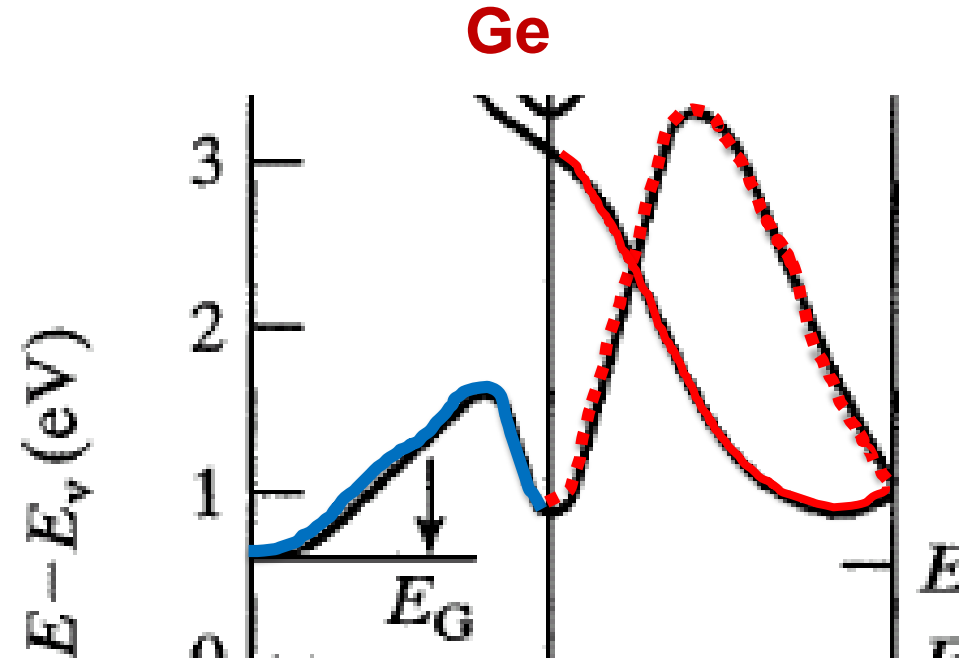
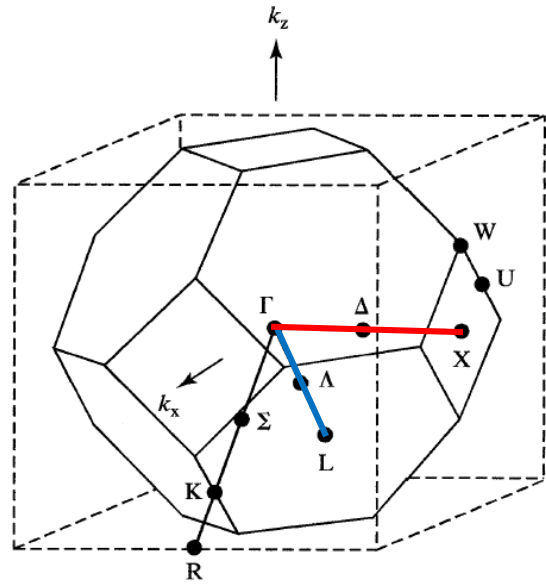
E-k along Γ -X Direction



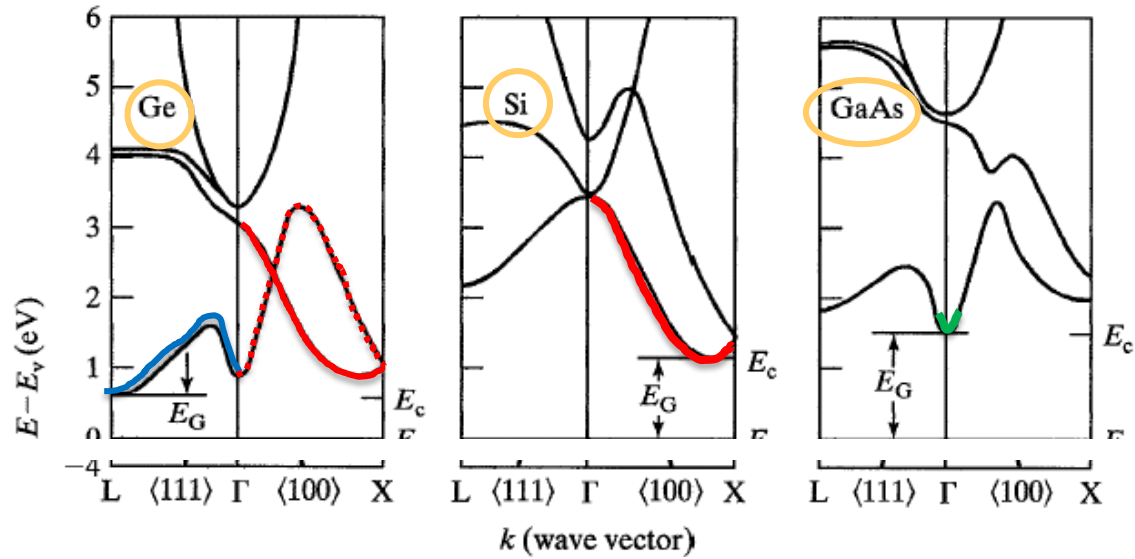
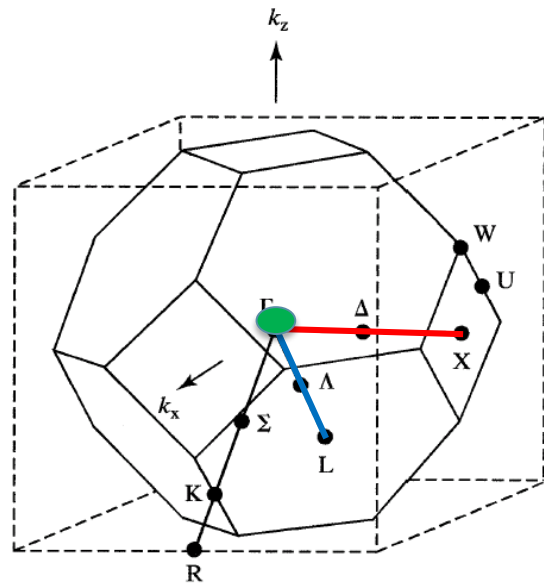
E-k along Γ -X Direction



E-k along Γ -X Direction

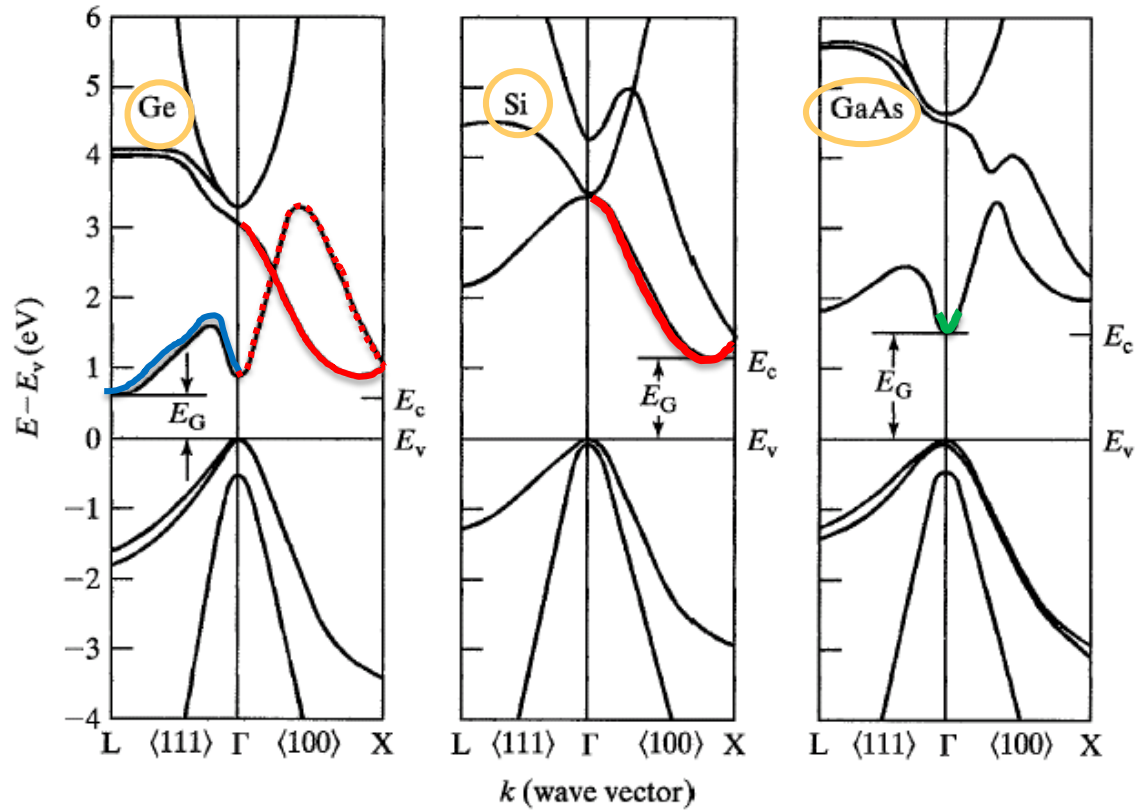
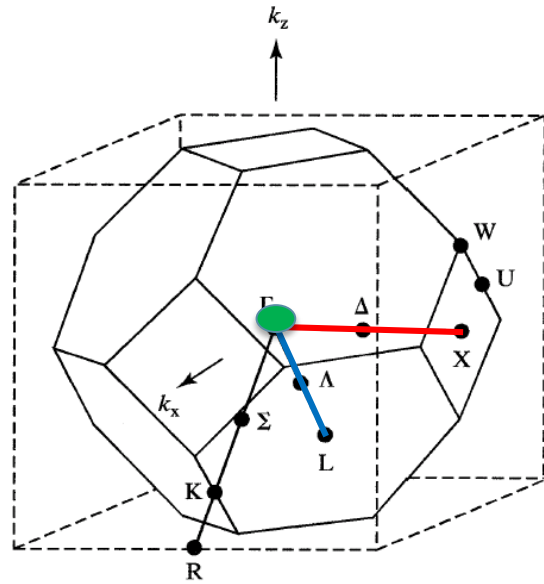


E-k Diagram - Dispersion for Ge, Si, GaAs



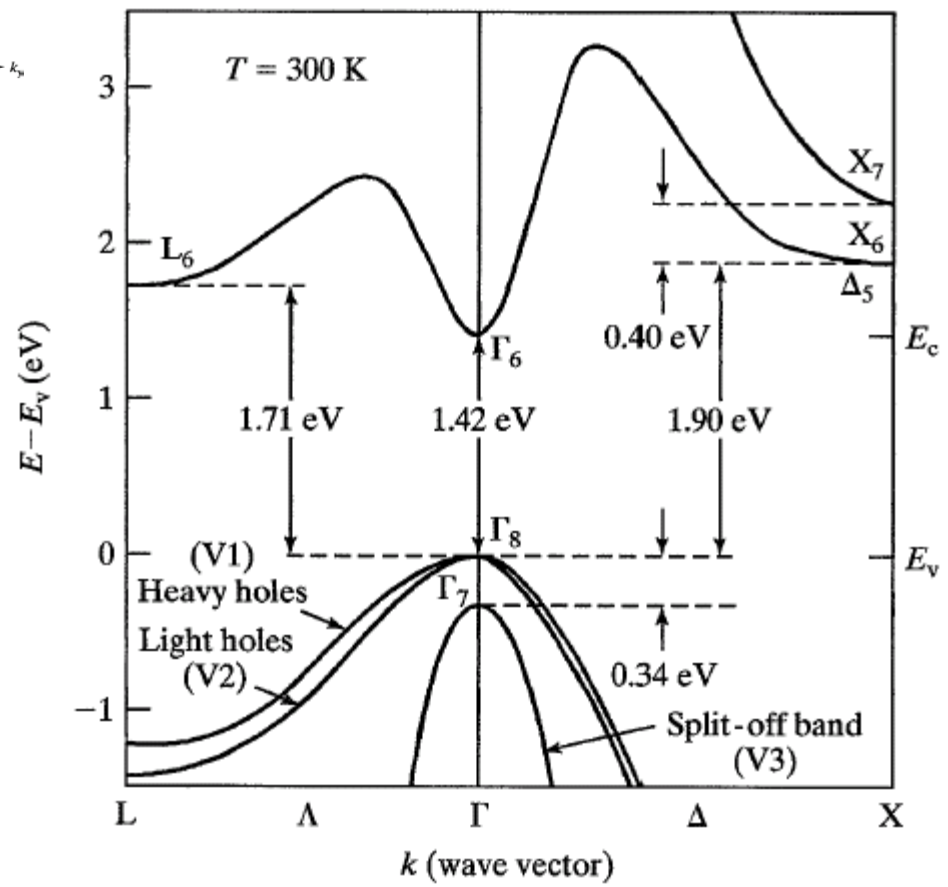
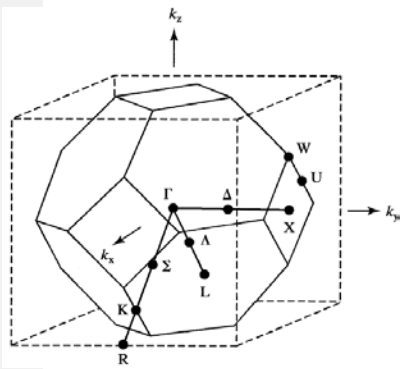
- Minima may not be at zone center
- (Ge: 8 L valleys, Si: 6 X valleys, and GaAs: Γ valleys)

E-k Diagram - Dispersion for Ge, Si, GaAs



- Minima may not be at zone center
- (Ge: 8 L valleys, Si: 6 X valleys, and GaAs: Γ valleys)
- 3 valence bands (light hole, heavy hole, split-off)
valence bands near $k=0$ is essentially $E \sim k^2$

E-k diagram for GaAs

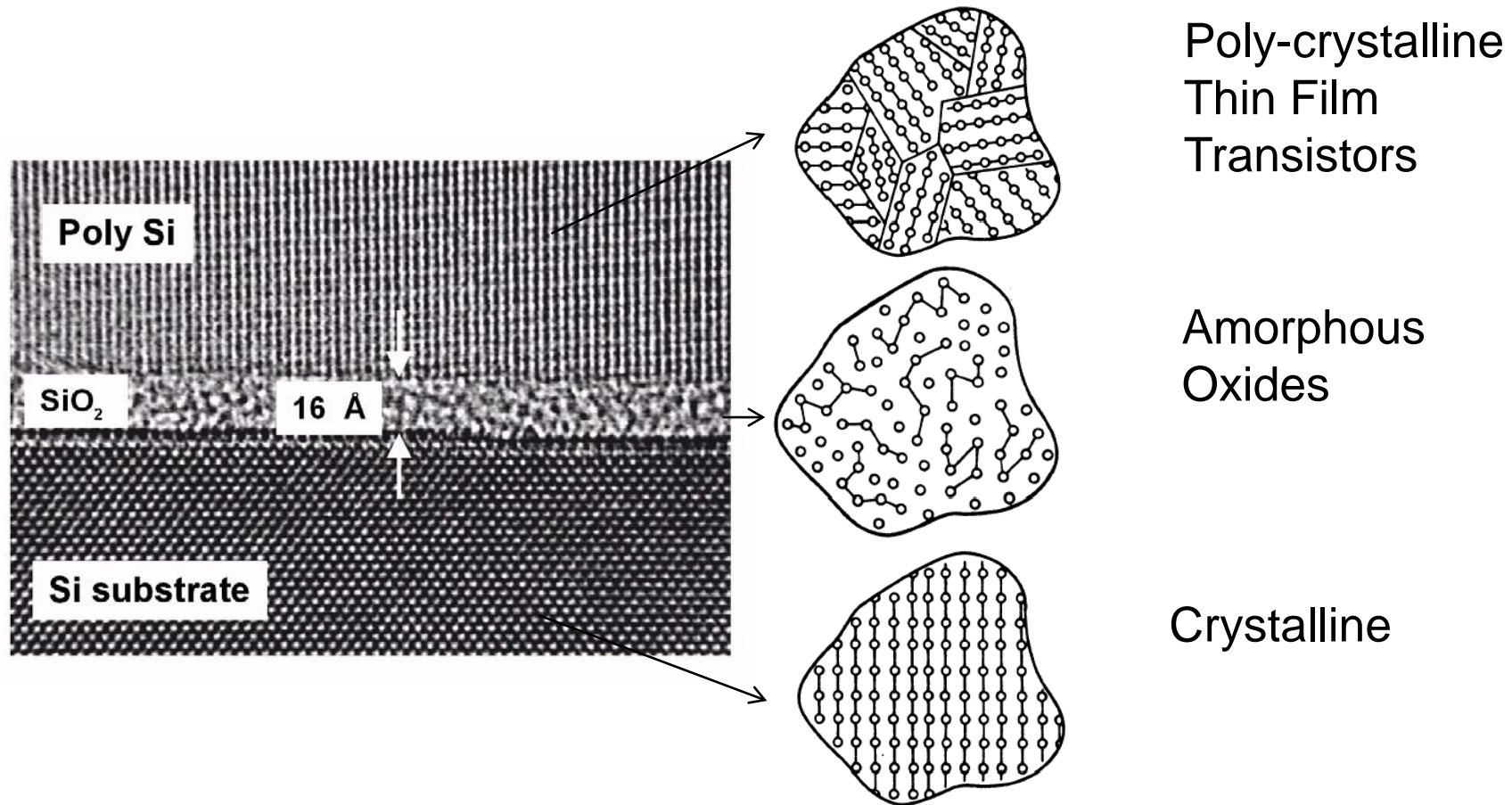


Direct bandgap material

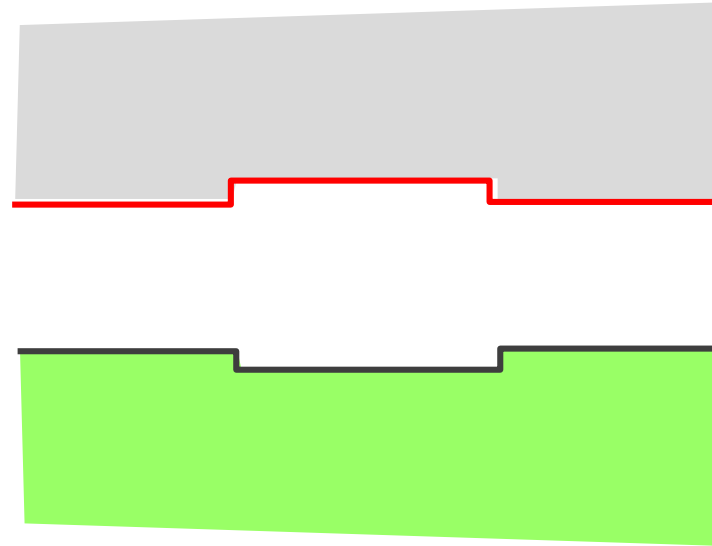
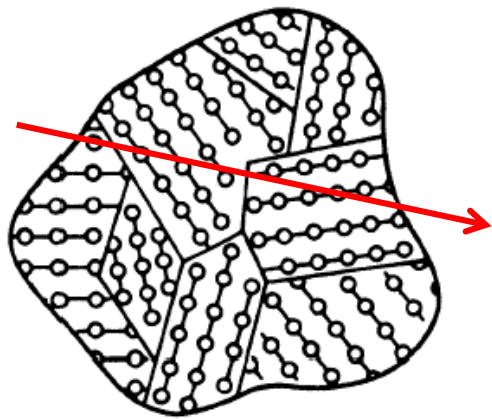
Zone-edge gaps ($L_6 - \Gamma_8$, $X_6 - \Gamma_8$) close to direct gap

Has important implications
For transport

Arrangement of Atoms

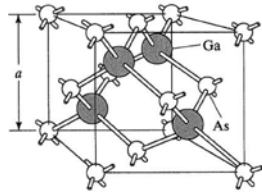


Poly-crystalline material

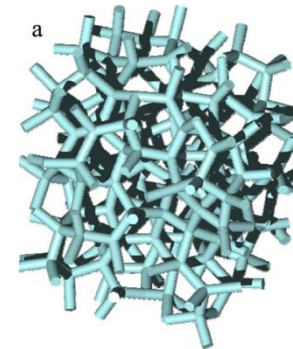
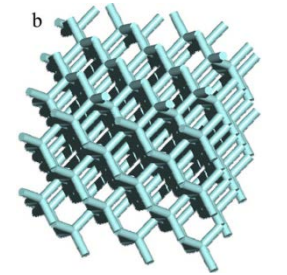
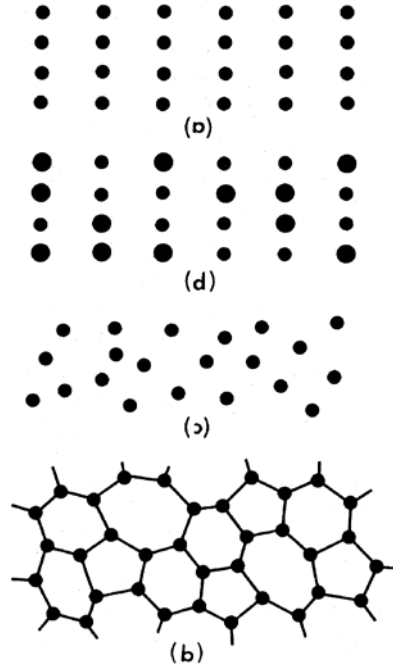


Isotropic bandgap and increase in scattering

Band-structure and Periodicity



PRB, 4, 2508, 1971



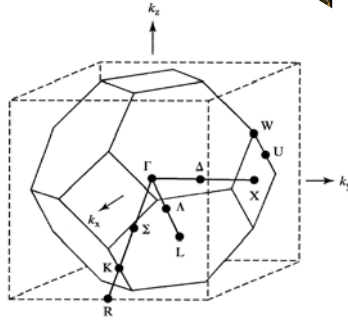
Edagawa, PRL, 100,013901, 2008

Periodicity is sufficient, but not necessary for bandgap.
Many amorphous material show full isotropic bandgap

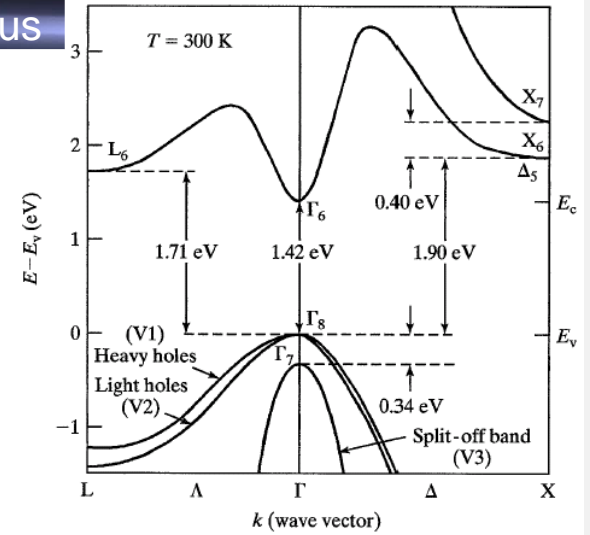
Section 10

Bandstructure in Real Materials (Si, Ge, GaAs)

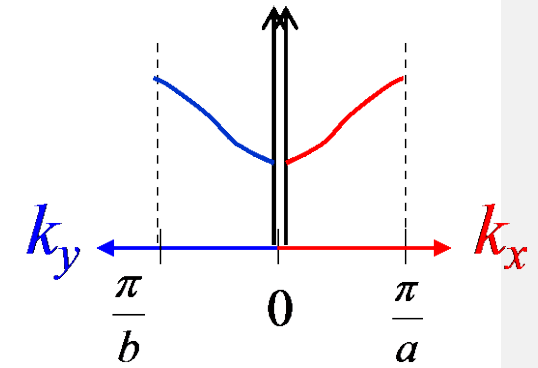
- 10.1 E(k) diagrams in specific crystal directions



status



- 10.2 Constant Energy Surfaces – Effective Mass Tensor



- 10.3 Density of States Effective Mass

One Video Segment

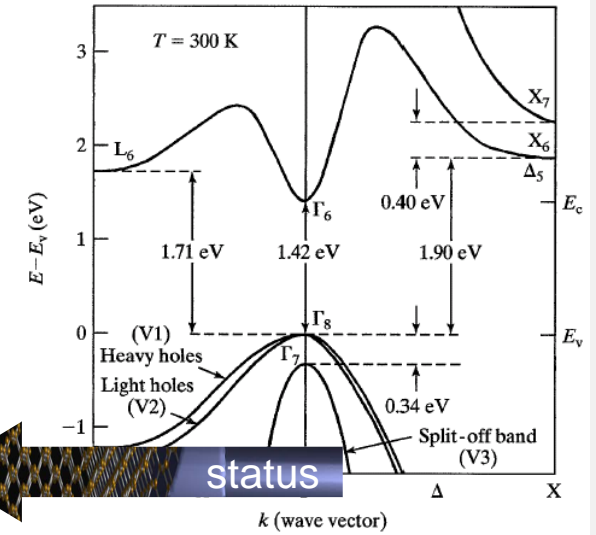
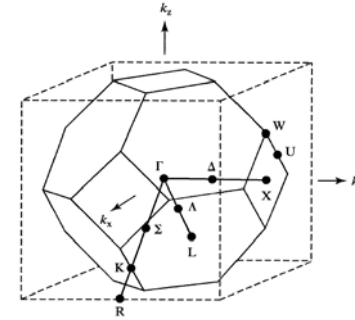
One Video Segment

One Video Segment

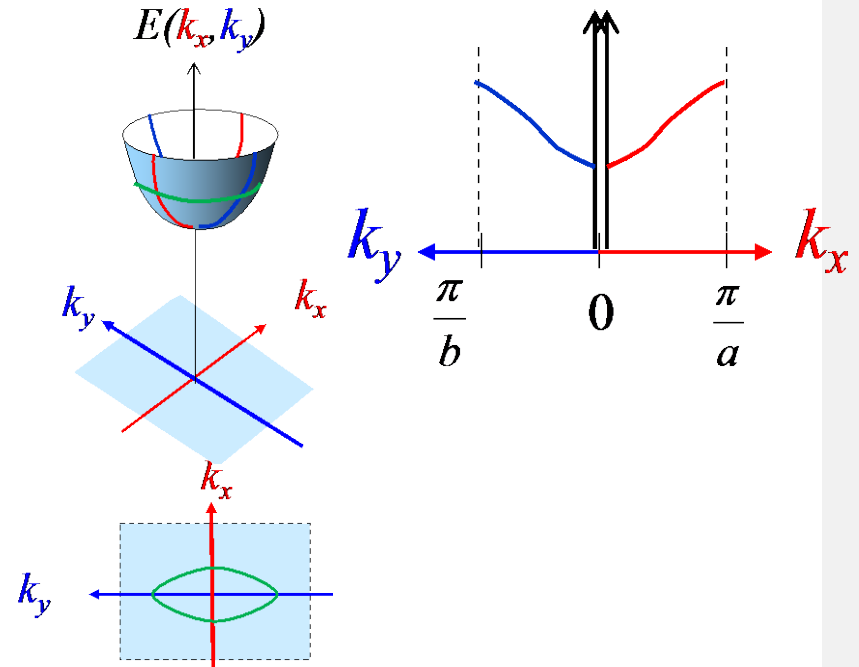
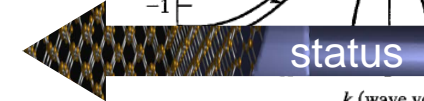
Section 10

Bandstructure in Real Materials (Si, Ge, GaAs)

• 10.1 E(k) diagrams in specific crystal directions



• 10.2 Constant Energy Surfaces – Effective Mass Tensor



• 10.3 Density of States Effective Mass

One Video Segment

One Video Segment

One Video Segment