Introduction to hydrogenated amorphous silicon

Yifan Yuan

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Street, R. A. (2005). Hydrogenated Amorphous Silicon.
United Kingdom: Cambridge University Press.

1. Basic concepts of amorphous semiconductors

- *Atomic structure*
  - The amorphous material has the same short range order as the crystal but lacks the long range order.

  - The disorder is represented by the atom pair distribution function, which is the probability of finding an atom at distance R from another atom.

Fig. 1.2. Schematic diagram of the atom pair distribution functions for a crystalline and amorphous solid and a gas, scaled to the average separation of nearest neighbor atoms, R_{av}, showing the different degree of structural order.
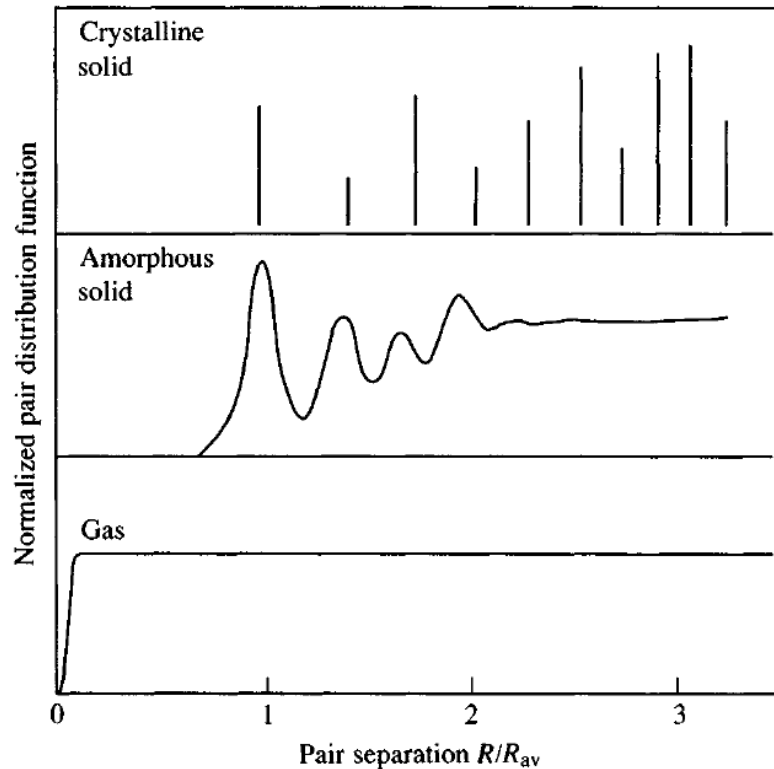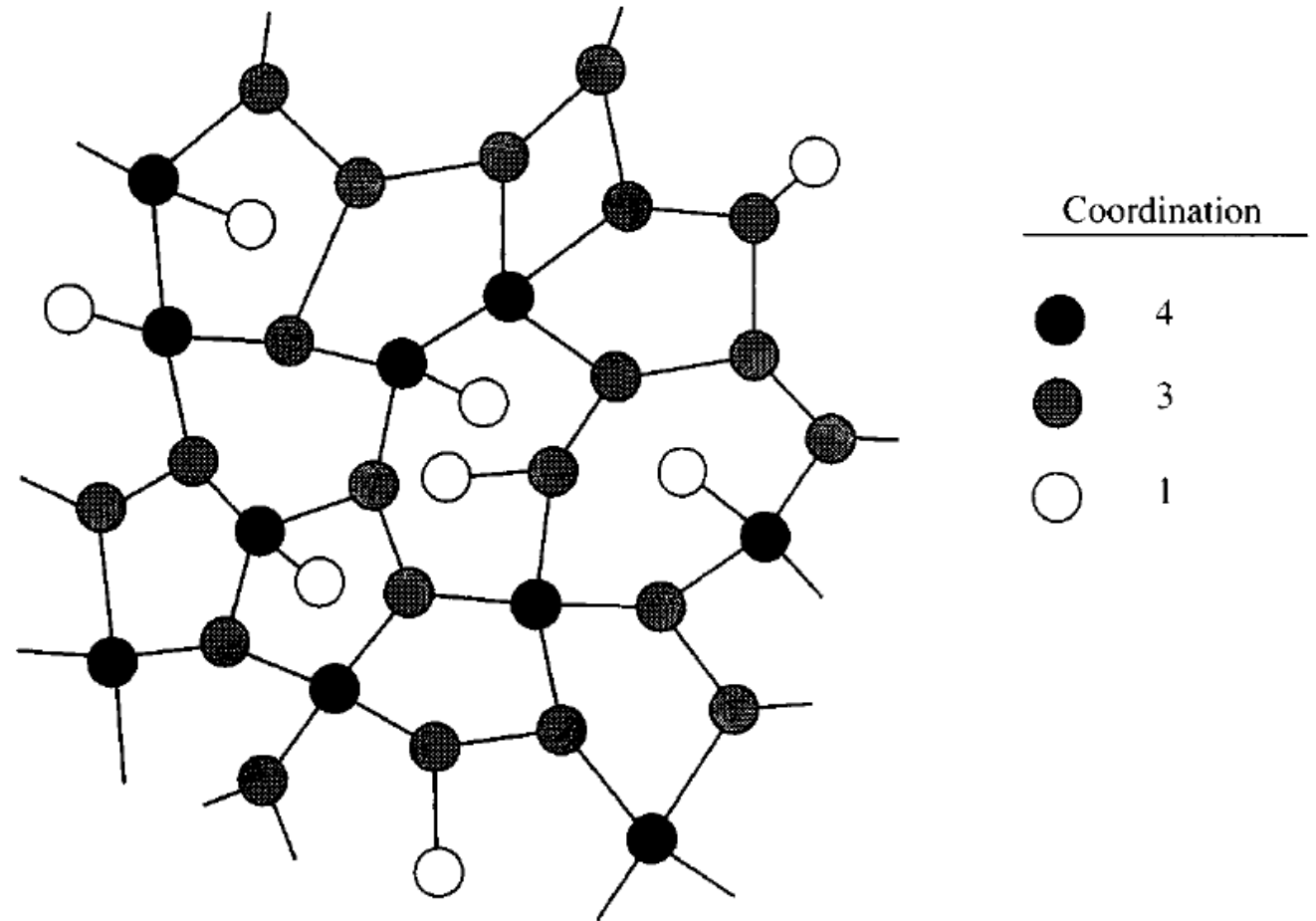
1. Basic concepts of amorphous semiconductors

- *Random network model*

Easily incorporating atoms of different coordination

Crystalline lattice in which impurities are generally constrained to have the coordination of the host

Fig. 1.3. An example of a continuous random network containing atoms of different bonding coordination, as indicated.

| Coordination	
●	4
●	3
○	1

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- *Definition of defects*

  Any atom which is out of place in a crystal is a defect - the simplest such defects are vacancies and interstitials.

  The elementary defect of an amorphous semiconductor is the **coordination defect**, when an atom has too many or too few bonds

Fig. 1.4. An illustration contrasting the different types of simple defects in (a) crystalline and (b) amorphous networks.
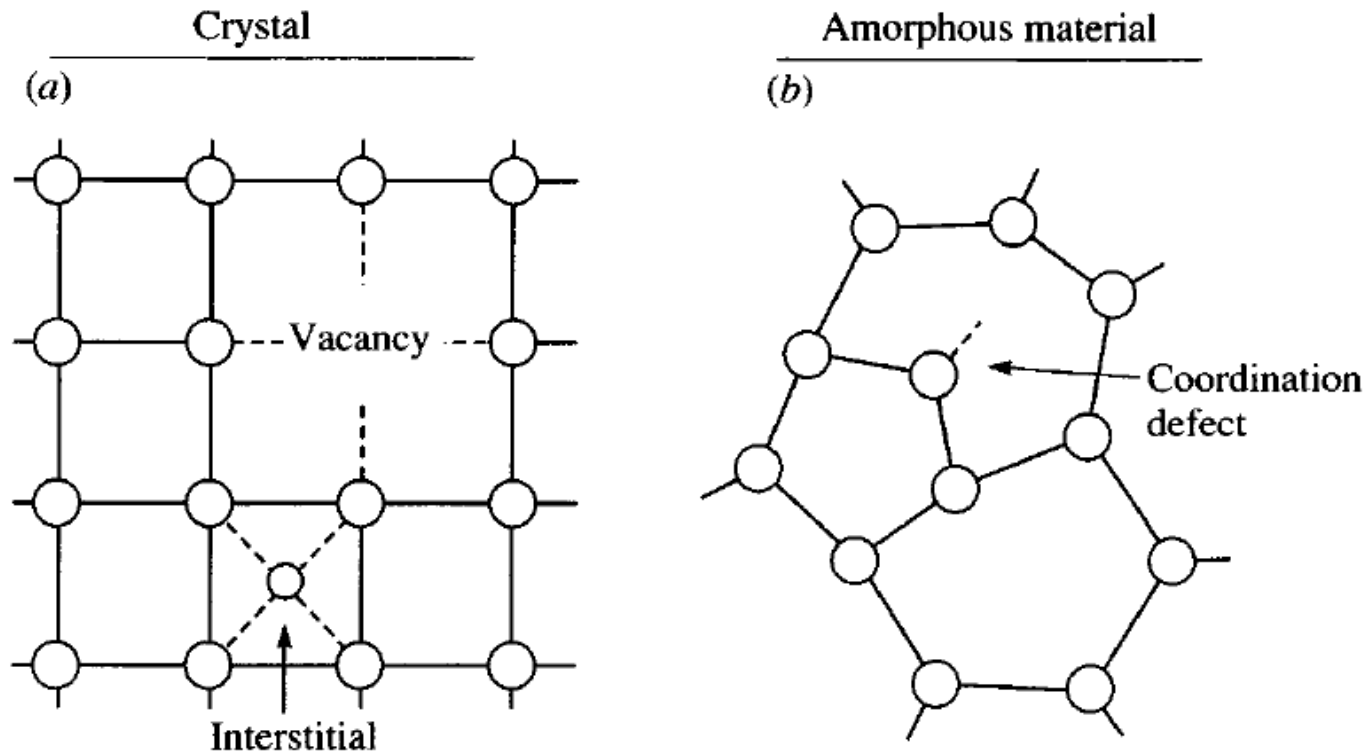
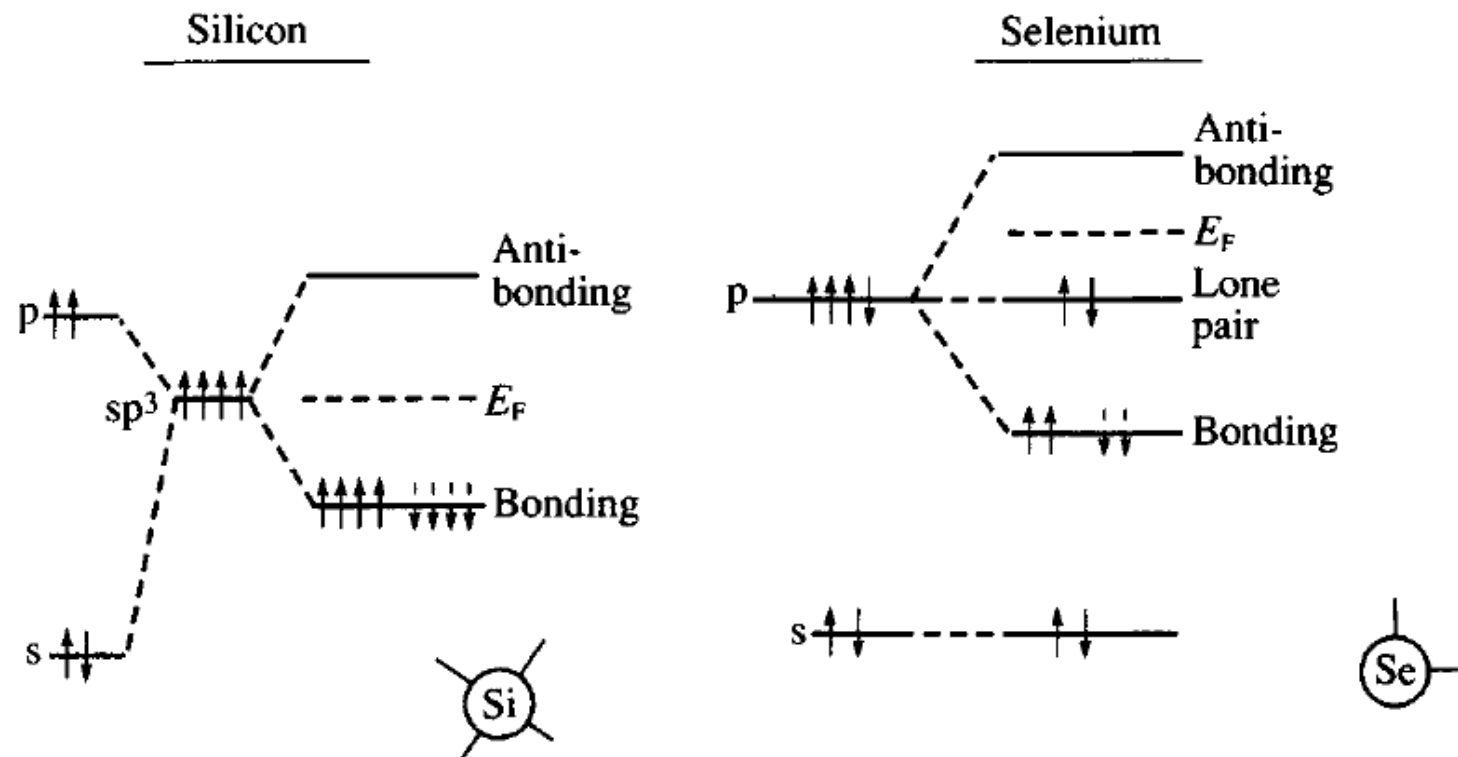# 1. Basic concepts of amorphous semiconductors

- *Electronic structure*

- The electrons of an isolated silicon atom occupy two 3s and two 3p states

- The electron interaction splits the valence states into bonding and anti-bonding levels

- The four silicon valence electrons combine to give four sp3 orbitals.

In selenium,

Six valence electrons

- There is no sp3 hybridization and the s state and one of the p states are filled with electron pairs, forming nonbonding states known as lone pairs.

- The remaining two singly occupied p states form covalent bonds, splitting into bonding and anti-bonding orbitals

Fig. 1.5. Illustration of the bonding configuration of (*a*) silicon and (*b*) selenium atoms constructed from hybridized molecular orbitals. The position of the Fermi energy, E_F, is indicated.

Silicon

Selenium

Anti-bonding

E_F

Lone pair

Bonding

Anti-bonding

E_F

Bonding

Si

Se

1. Basic concepts of amorphous semiconductors

- *Electronic structure*

- the band gap is a consequence of the periodicity of the crystalline lattice

Why amorphous silicon has band gap?

- Also, the band gap is equivalently described by the splitting of the bonding (or lone pair) and anti-bonding states of the covalent bond

- The bands are most strongly influenced by the short range order, which is the same in amorphous and crystalline silicon and the absence of periodicity is a small perturbation.

(a)
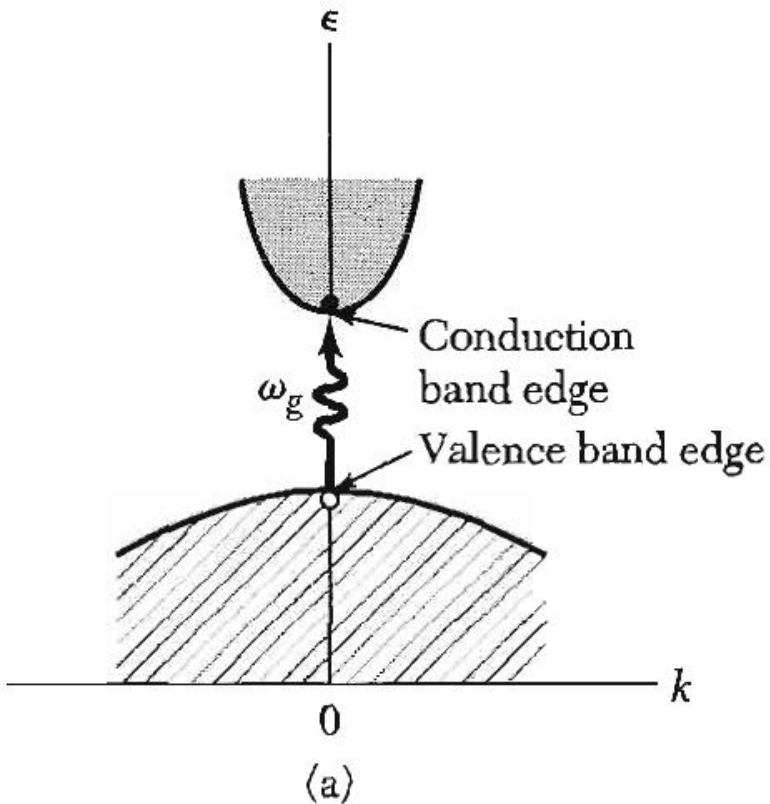
The bonding is described by a tight binding Hamiltonian of the form

$$H = V_1 \sum_{j \neq j'} |\Phi_{ij}\rangle\langle\Phi_{ij'}| + V_2 \sum_{i \neq i'} |\Phi_{ij}\rangle\langle\Phi_{i'j}|. \qquad (1.3)$$

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The wavefunctions, Φ, are the sp3 hybrid orbitals of the tetrahedral silicon bonding

a sum over interactions for which the two wavefunctions Φ_{ij} belong to the same atom

sums pairs of orbitals that belong to the same bond

Hamiltonian describes the short range bonding information, but contains no information about the long range order, and so applies equally to amorphous and crystalline silicon.

The interaction strength V_1 / V_2
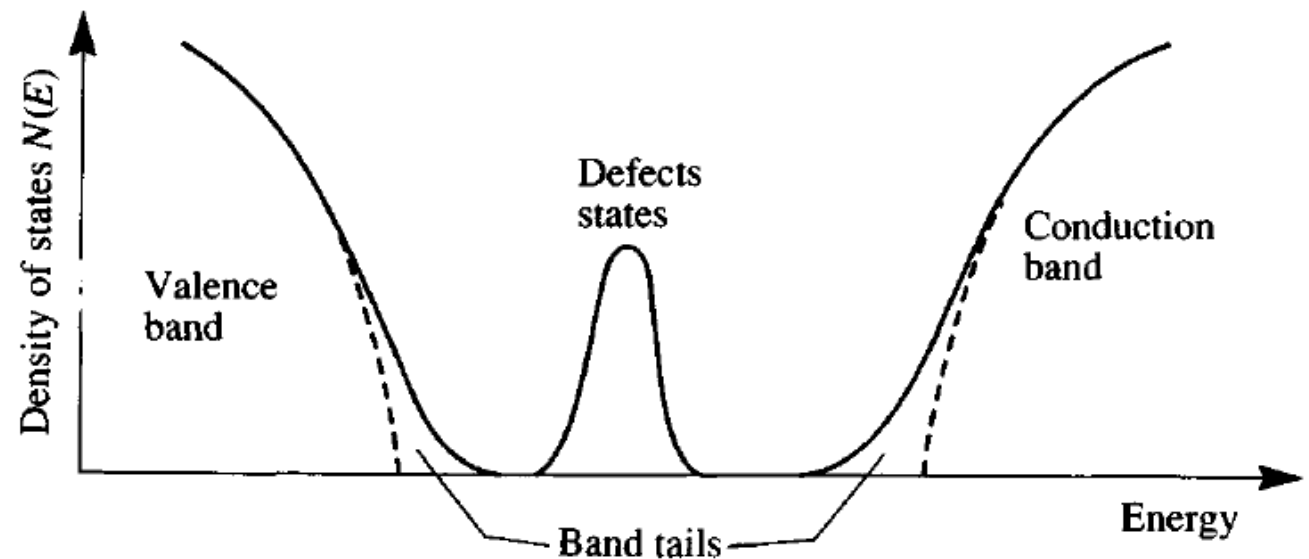
1. Basic concepts of amorphous semiconductors

- ## *Electronic structure*

- Three principal features of the structure of amorphous semiconductors are the **short range order** of the ideal network, the **long range disorder** and the **coordination defects**.

- The preservation of the short range order results in a similar overall electronic structure of an amorphous material compared to the equivalent crystal.

- Broadened band tail of states extending into the forbidden gap, which originates from the deviations of the bond length and angle arising from the long range structural disorder.

Fig. 1.6. Schematic density of states distribution for an amorphous semiconductor showing the bands, the band tails, and the defect states in the band gap. The dashed curves are the equivalent density of states in a crystal.
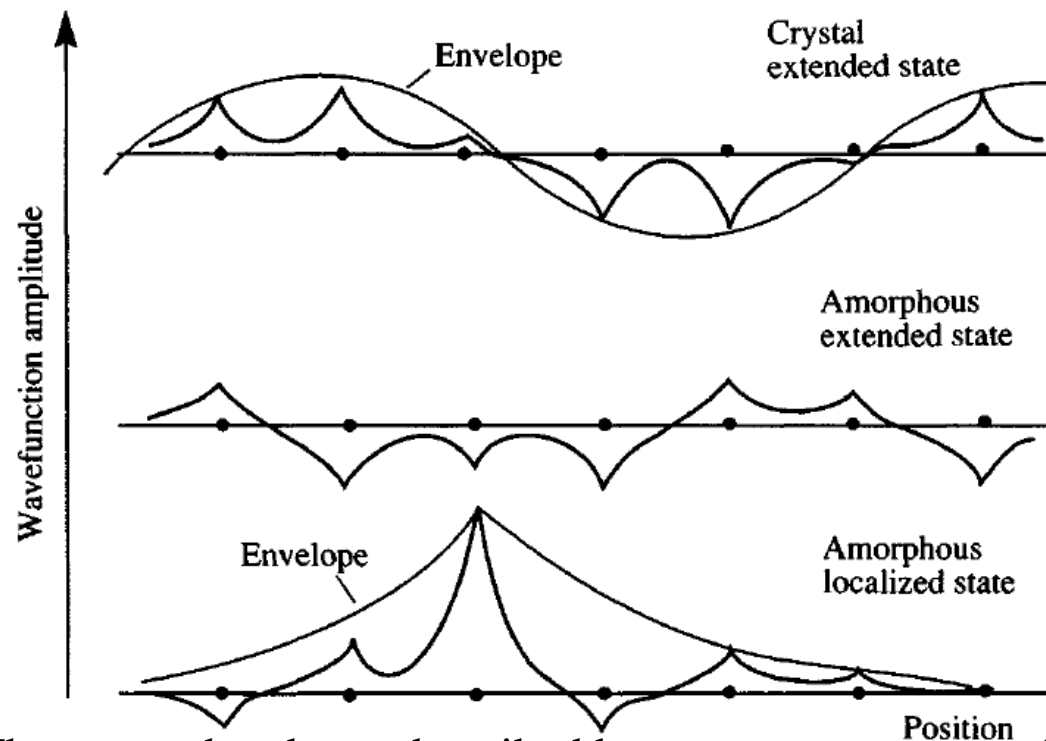
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- *Electronic properties*

$$-\frac{h^2}{2m}\nabla^2\Phi + V(\mathbf{r})\Phi = E\Phi \qquad (1.4)$$

$$\Phi(\mathbf{r}) = \exp(i\mathbf{k}\cdot\mathbf{r})\, U_k(\mathbf{r}) \qquad (1.5)$$

The periodic potential of the ordered crystal leads to the familiar Bloch solutions for the wavefunction

Fig. 1.7. Illustration of the wavefunctions of extended and localized states of an amorphous material, compared to the extended states of a crystal.

The disordering effect of an amorphous semiconductor is strong enough to cause such frequent scattering that the wavefunction loses phase coherence over a distance of one or two atomic spacings.

loss of k-conservation

The energy bands are described by energy-momentum *(E-k)* dispersion relations,

1. Basic concepts of amorphous semiconductors

- Some consequences of the loss of k-conservation are:

(1) The energy bands are no longer described by the E-k dispersion relations, but instead by a density-of-states distribution $N(E)$ illustrated in Fig. 1.6.

(2) The disorder reduces the carrier mobility because of frequent scattering and causes the much more profound effect of localizing the wavefunction.

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- *Localization, the mobility edge and conduction*
- An increasing disorder potential causes first strong electron scattering and eventually electron localization
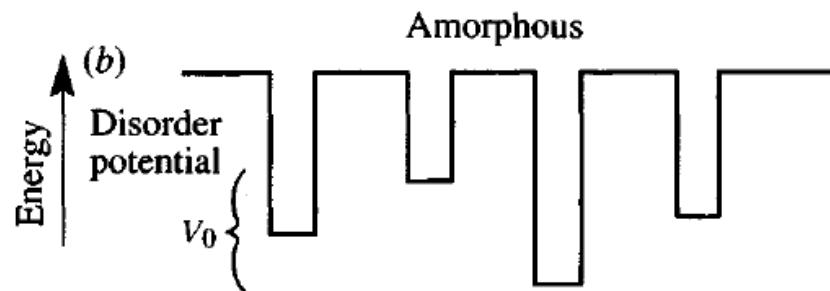
Fig. 1.8. The Anderson model of the potential wells for (a) a crystalline lattice and (b) an amorphous network. V_0 is the disorder potential.
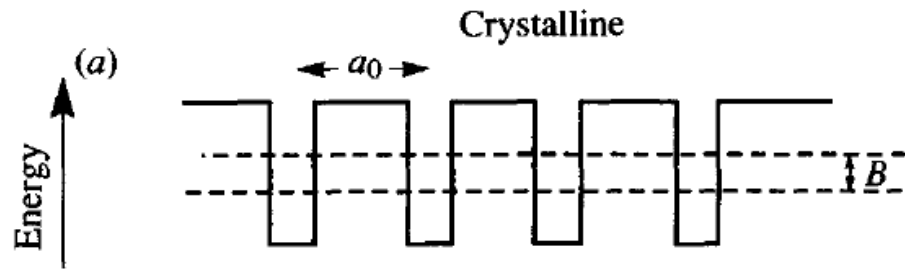
atomic potential wells

band width B

random potential with average amplitude V_0

when V_0/B exceeds a critical value, there is zero probability for an electron at any particular site to diffuse away

Anderson's theory of localization

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- *Localization, the mobility edge and conduction*

- However, even when the disorder of an amorphous semiconductor is insufficient to meet the Anderson criterion, some of the states are localized and these lie at the band edges

- The center of the band comprises extended states at which there is strong scattering and states at the extreme edges of the bands are localized.

- The extended and localized states are separated by a mobility edge at energy E_c, which derives its name because at zero temperature, only electrons above E_c are mobile and contribute to the conduction.

Fig. 1.9. The density of states distribution near the band edge of an amorphous semiconductor, showing the localized and extended states separated by the mobility edge.
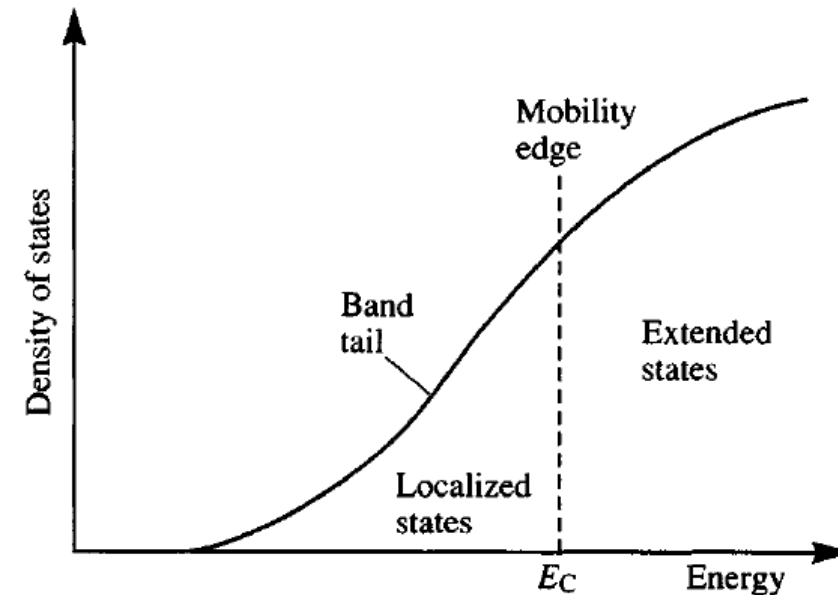
1. Basic concepts of amorphous semiconductors

- *Localization, the mobility edge and conduction*

- the disorder also influences the mobility of the electrons and holes above the mobility edges

- There is no metallic conduction, but instead there are several other possible conduction mechanisms, which are illustrated in Fig. 1.11.

Fig. 1.11. Illustration of the three main conduction mechanisms expected in an amorphous semiconductor.
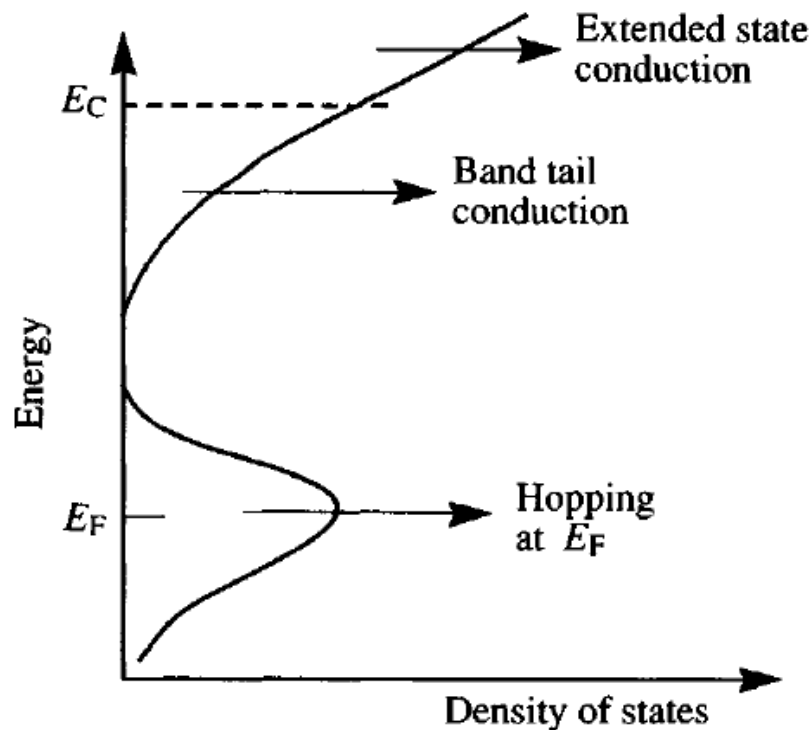
(1)   *Extended state conduction*
Conduction is by thermal activation of carriers from E_F to above the mobility edge and follows the relation,

$$\sigma_{ext} = \sigma_{oe} \exp\left[-(E_C - E_F)/kT\right] \tag{1.11}$$

(2)   *Band tail conduction*
Although carriers cannot conduct in localized states at zero temperature, conduction by hopping from site to site is possible at elevated temperatures. Hopping conduction in the band tail is given by,

$$\sigma_{tail} = \sigma_{ot} \exp\left[-(E_{CT} - E_F)/kT\right] \tag{1.12}$$

THANK YOU!
Any questions?