

Introduction to Condensed Matter

PHY 251/PHY 420

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— ASSIGNMENT 4 — SOLUTIONS

(Undergraduate students do not have to answer the questions marked with the symbol ■.)

Intrinsic Carrier Concentration (15 points)

Indium arsenide (InAs) is a semiconductor crystalline compound made from the elements indium (In) and arsenide (As). It is used in a number of modern advanced technologies including construction of infrared photovoltaic photodiodes and diode lasers. Calculate the intrinsic carrier concentration in InAs at 300 K and 600 K. (Note that the sum of heavy and light hole has to be included.)

SOLUTION:

At 300 K the band gap of InAs is 0.35 eV and the electron effective mass is $0.027m_0$. The hole density of states mass is $0.40m_0$. The intrinsic concentration is

$$n_i = p_i = 2 \left(\frac{k_B T}{2\pi \hbar^2} \right)^{3/2} (m_e^* m_h^*)^{3/4} \exp \left(\frac{-E_g}{2k_B T} \right) = 1.025 \times 10^{15} \text{cm}^{-3}$$

The concentration at 600 K becomes

$$n_i = 2.89 \times 10^{15} \text{cm}^{-3}.$$

Shallow Donors in InSb (15 points)

Indium antimonide (InSb) is a semiconductor crystalline compound made from the elements indium (In) and antimony (Sb). It is a narrow-gap semiconductor material used in infrared detectors, including thermal imaging cameras, infrared homing missile guidance systems, and in infrared astronomy. InSb has energy gap $E_g = 0.23 \text{eV}$; dielectric constant $\epsilon = 18$; and electron effective mass $m_e = 0.015m$. Calculate

(a) the shallow donor ionization energy;

$$\text{(CGS)} \quad E_d = (13.6 \text{ eV}) \frac{m^*}{m} \frac{1}{\varepsilon^2} \simeq 6.3 \text{ eV}$$

(b) the radius of the ground state orbit;

$$\text{(CGS)} \quad E_d = (0.53 \times 10^{-8}) \frac{m^*}{m} \varepsilon \simeq 6 \times 10^{-6} \text{ cm}$$

(c) at what minimum donor concentration will an impurity band occur?

Band overlap will be significant at a concentration

$$\text{(CGS)} \quad N = \frac{1}{\frac{4\pi}{3} r^3} \simeq 10^{15} \text{ cm}^{-3}$$

Static Magnetoconductivity Tensor (30 points)

Using the Drude model, show that in presence of a static electric (E) and magnetic field (H) the static current density flowing in a wire can be written in matrix form as

$$\begin{pmatrix} j_x \\ j_y \\ j_z \end{pmatrix} = \frac{\sigma_0}{1 + (\omega_c \tau)^2} \begin{pmatrix} 1 & -\omega_c \tau & 0 \\ \omega_c \tau & 1 & 0 \\ 0 & 0 & 1 + (\omega_c \tau)^2 \end{pmatrix} \begin{pmatrix} E_x \\ E_y \\ E_z \end{pmatrix}.$$

In the high magnetic field limit $\omega_c \tau \gg 1$, show that $\sigma_{yx} = nec/H = -\sigma_{xy}$. In this limit $\sigma_{xx} \simeq 0$, to order $1/\omega_c \tau$. The quantity σ_{yx} is called the *Hall conductivity*.

SOLUTION:

From the magnetoconductivity matrix we have

$$j_y = \sigma_{yx} E_x = \frac{\omega_c \tau}{1 + (\omega_c \tau)^2} \sigma_0 E_x$$

$$\text{For } \omega_c \tau \gg 1, \text{ we have } \sigma_{yx} \simeq \frac{\sigma_0}{\omega_c \tau} = \frac{nec}{H}.$$

Semiconductor Heterostructures (40 points)

Semiconductor heterostructures offer the unique opportunity to manipulate the behavior of electrons and holes through *band engineering*. A first approach to construct energy band diagrams

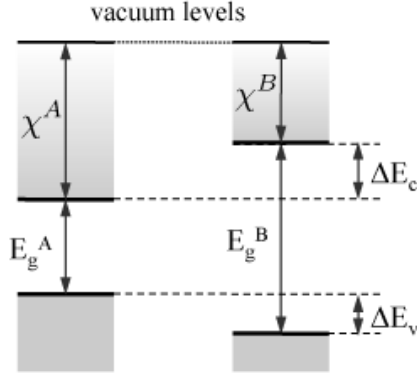


Figure 1: A/B heterojunction; energy band diagram.

(i.e. band-edge potential profile) of the heterojunction between two semiconductor materials (A and B) is the Anderson's rule, Fig 1. This is based on the electron affinity (χ) of the materials, the energy required to take an electron from the bottom of the conduction band E_c to the vacuum, that is, to escape from the crystal.

Electron affinity is nearly independent of the position of the Fermi level. Anderson's rule states that once the vacuum levels are aligned it is possible to use the electron affinity ($\chi^{A,B}$) and band gap ($E_g^{A,B}$) values for each semiconductor to calculate the conduction band (ΔE_c) and valence band (ΔE_v) offsets.

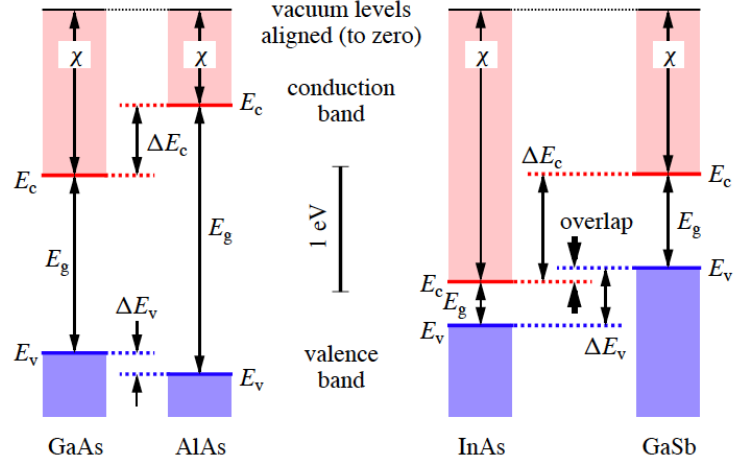
1.1) Estimate $\Delta E_{c,v}$ (at the Γ -point and $T = 300$ K) for the nearly lattice-matched systems, GaAs/AlAs, $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{InP}$, and InAs/GaSb . (A possible source of data for semiconductor is <http://www.ioffe.ru/SVA/NSM/>.) How well do the results agree with the accepted values in literature?

In many important devices, semiconductor are doped to enable a significant additional potential (e.g. p-n junction in inhomogeneous semiconductors) due to the large number of charge carriers. At equilibrium the additional electrostatic potential $V_\rho(z)$ arising from the the spatial charge distribution (ρ) has to satisfies the Poisson's equation $\nabla^2 V_\rho = -\rho/\epsilon_r \epsilon_0$.

1.2) Sketch the band diagram for the heterojunction $\text{n-Al}_{0.33}\text{Ga}_{0.67}\text{As}/\text{GaAs}$ (i.e. n-doped $\text{Al}_{0.33}\text{Ga}_{0.67}\text{As}$ and undoped GaAs) and show that this can trap a two-dimensional electron gas (2DEG) at the interface. Repeat for $\text{p-Al}_{0.33}\text{Ga}_{0.67}\text{As}/\text{n-GaAs}$ and elaborate on the possible formation of a two-dimensional carrier gas.

1.3) Sketch the band diagram for both p-n and n-p generic heterojunctions of type II (or staggered alignment). Determine whether electrons or holes can be trapped at the interface.

Figure 2: Anderson's rule for the alignment of the bands at GaAs/AlAs and InAs/GaSb heterojunctions.



1.4 ■) Consider an undoped InAs/GaSb heterojunction (type III or broken gap alignment). Sketch the band diagram at equilibrium. Next, suppose that a sequence of narrow InAs/GaSb layers is grown. Each layer of InAs now behaves as a quantum well for electrons, and the lowest state is raised above the bottom of the conduction band. The energy of the lowest state for holes in GaSb is raised too. For very thin layers the states will be raised so far in energy that they no longer overlap. Estimate the threshold thickness for alternating layers of equal thickness. (Treat the wells as infinitely deep.)

SOLUTION:

1.1) Taking the vacuum level as zero, the energy of the conduction band is given by $E_c = -\chi$ and the valence band is at $E_v = -(\chi + E_g)$. Conduction and valence band offsets ($\Delta E_{c,v}$) according to Anderson's rule are reported in following table. (The vacuum level is taken as zero and all energies are in eV.)

	GaAs	AlAs	ΔE	InAs	GaSb	ΔE	InGaAs	InP	ΔE
χ	4.07	3.50		4.90	4.06		4.50	4.38	
$E_g(\Gamma)$	1.42	2.17		0.35	0.73		0.74	1.34	
E_c	-4.07	-3.50	0.57	-4.90	-4.06	0.84	-4.50	-4.38	0.12
E_v	-5.49	-5.67	-0.18	-5.25	-4.79	0.46	-5.24	-5.72	-0.48

GaAs/AlAs and $\text{In}_{0.53}\text{Ga}_{0.47}\text{As}/\text{InP}$ have type I alignment. InAs/GaSb has type III band alignment

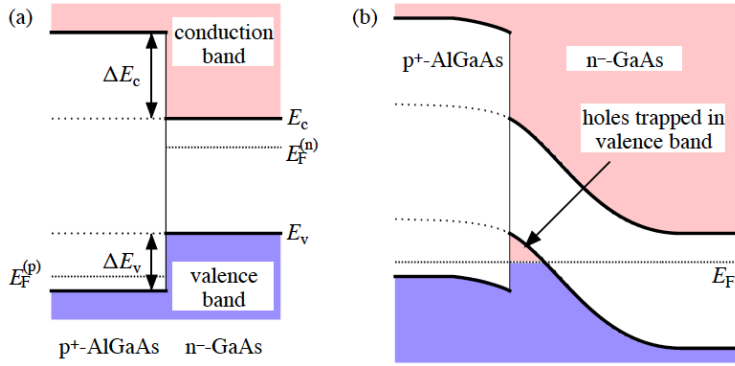


Figure 3: Heterojunction band diagram for heavily-doped p-Al_{0.33}Ga_{0.67}As and lightly-doped n-GaAs. (a) Flat bands at non-equilibrium showing the different Fermi levels (E_F) on the two sides. (b) Band bending at equilibrium after electrons have moved from the n-GaAs to the p-AlGaAs. Holes are trapped in the n-GaAs at the junction.

(broken-gap) as the gap of GaSb lies wholly above that of InAs.

Band offsets values estimated with Anderson's rule are not very accurate mainly because of the difficulty to measure the electron affinity. In fact, it depends strongly on the cleanliness of the surface, roughness, and orientation of the surface may also be important.

1.2) For the n-Al_{0.33}Ga_{0.67}As/GaAs heterojunction bands are bent near the interface as they would be in a p-n diode, but the band discontinuity add a new feature and electrons may be trapped in a nearly triangular potential well next to the junction.

For the p-Al_{0.33}Ga_{0.67}As/n-GaAs heterojunction bands are flat before any charge can flow from one material to another (Fig. 3a). The system is in non-equilibrium as the Fermi levels are misaligned. When equilibrium is reached bands are bent (Fig 3b). If the AlGaAs is heavily p-doped (but still non-degenerate) and GaAs only lightly n-doped, holes are accumulated at the interface (Fermi energy cuts the well). The precise outcome depends on the positioning of the Fermi level in each material, which is in turn a function of the doping. If the energy levels in the triangular well are well separated, a two-dimensional hole gas (2DHG) is formed.

1.3) From Fig. 4 we can see that p-n heterojunctions show no potential well, but the n-p heterojunctions has wells in both conduction and valence bands. The occupation of these wells will depend on the Fermi level and doping of both sides. Very few carriers would be trapped for the materials sketched (just what caused by temperature). With more doping the n-p heterojunction would be more likely to trap electrons.

1.4) The equilibrium is reached by spontaneous transfer of electrons from GaSb to InAs. This creates holes in the valence band of GaSb and electrons in the conduction band of InAs near the junction until the Fermi level becomes flat (Fig. 5). Such a system is particularly interesting

Figure 4: Top sketches how flat bands, with different Fermi levels on the two sides. The corresponding bands at equilibrium are shown below. Neither electrons nor holes are localized near the p-n junction, but either may be trapped with n-p doping.

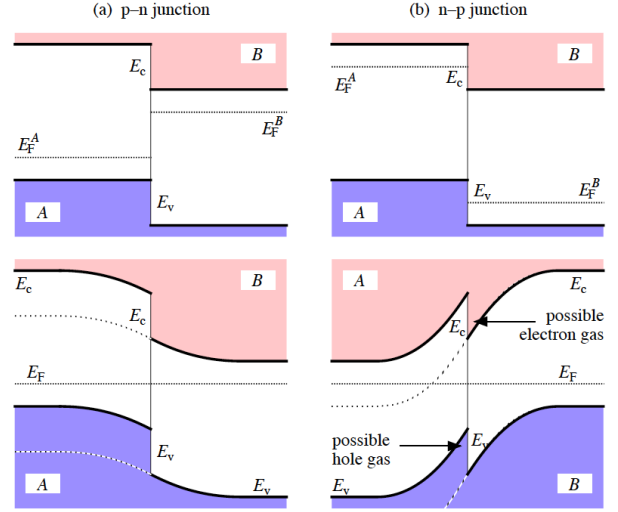
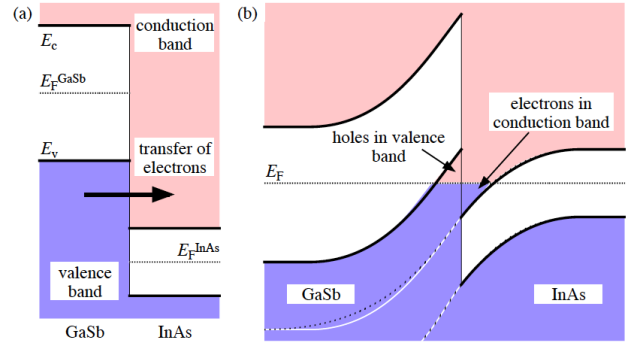


Figure 5: Band diagram for the type III GaSb/InAs heterojunction.



because it contains mobile carriers without the need for doping. A sequence of narrow A/B layers will form a so-called *superlattice*, Fig. 6.

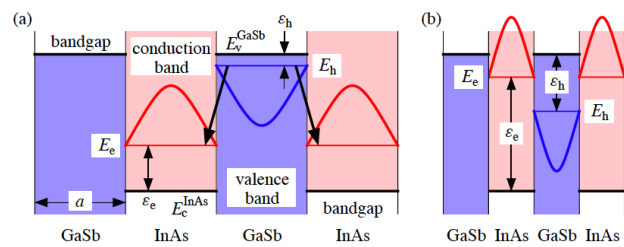


Figure 6: