Problem Set 3 **ECE 236A** Due 19 February 2008
IN CLASS

**Problem solutions are to be turned in at the beginning of class on the due date. Solutions to all problems will be provided after problem sets are collected in class. SHOW ALL WORK.**

1. Consider an $In_xGa_{1-x}As$ film coherently strained to the lattice constant of GaAs at 300K, $a$ = 5.65Å. Assume that epitaxial growth is on the (001) plane, and assume the following parameters for $In_xGa_{1-x}As$ can be obtained by linear interpolation from the values for GaAs and InAs: $a$, $c_{11}$, $c_{12}$, $a_c$, $a_v$, $b$, and $\Delta_{so}$. The values for GaAs and InAs are as given below.

| | $a$ (Å) | $c_{11}$ (Mbar) | $c_{12}$ (Mbar) | $a_c$ (eV) | $a_v$ (eV) | $b$ (eV) | $\Delta_{so}$ (eV) |
|---|---|---|---|---|---|---|---|
| GaAs | 5.65 | 1.223 | 0.571 | -7.17 | 1.16 | -1.7 | 0.34 |
| InAs | 6.08 | 0.833 | 0.453 | -5.08 | 1.00 | -1.8 | 0.38 |

   (a) Calculate, i.e., obtain numerical values, and plot the critical thickness for strain relaxation in the $In_xGa_{1-x}As$ layer as a function of the In concentration $x$. You may use the results you obtained (or that are in the written solutions) for Problem Set 2. For dislocations, assume that the Burgers vectors are of the form $(a_{GaAs}/2)\langle 110\rangle$, $\beta$=60°and that $b_{\text{edg},\|}=b/2$.

   (b) Calculate, i.e., obtain numerical values, and plot the energies $E_{v,av}$, $E_{hh}$, $E_{lh}$, and $E_{so}$ in the $In_xGa_{1-x}As$ layer as functions of the In concentration $x$, taking $E_{hh}$(GaAs)=$E_{lh}$(GaAs)=0 and assuming, for simplicity, that $\Delta E_{v,av}$ between unstrained InAs and unstrained GaAs is zero.

   (c) Now assume that the average valence band offset, i.e., $\Delta E_{v,av}$, between unstrained InAs and unstrained GaAs is 0.25eV, with $E_{v,av}$ for InAs being higher in energy than $E_{v,av}$ for GaAs. Repeat part (b). You may assume that the valence-band offset for the unstrained InGaAs/GaAs heterojunction can be obtained by linear interpolation between zero and the unstrained InAs/GaAs heterojunction. The process outlined in parts (b) and (c) allows valence-band offsets in strained heterojunctions to be determined.

2. Consider the conduction-band structure of Si, which has six conduction-band minima, one in each of the {100} directions in reciprocal space. Suppose Si is subjected to strain by adjusting the value of the in-plane lattice constant $a_\|$. Calculate and plot the energies of the (100), (010), and (001) minima, assuming $a_\|$ is the lattice constant in the (001) plane, i.e., along the [100] and [010] directions, as a function of $\varepsilon_\|$ for $-0.02<\varepsilon_\|<0.02$. Assume that $\Xi_u$=8.7eV, $a_c$= 4.18eV, $c_{11}$=1.675Mbar, and $c_{12}$=0.650Mbar, and let $E_c$(Si)=0 for unstrained material.

3. The boundary conditions for envelope functions at a heterojunction interface are typically determined by the requirements that the envelope function $f(\mathbf{r})$ be continuous, and that the particle current density be continuous. For a heterostructure in which only a single energy band, e.g., the conduction band, is relevant, the expression for the particle current density $\mathbf{j}$ can be derived from Schrödinger's equation and the requirement that the following continuity equation be satisfied:

$$\frac{\partial}{\partial t}\left(f^* f\right)+\nabla\cdot\mathbf{j}=0$$

   Recall that the form of Schrödinger's equation when the effective mass is a function of position is

$$\hat{H}f=i\hbar\frac{\partial f}{\partial t}\text{ with }\hat{H}=-\frac{\hbar^2}{4}\left\{\nabla^2,\frac{1}{m^*(\mathbf{r})}\right\}+V(\mathbf{r})\text{ where }\left\{\hat{A},\hat{B}\right\}\equiv\hat{A}\hat{B}+\hat{B}\hat{A}$$

   Using these expressions, derive an expression for the particle current density $\mathbf{j}$, and then show that the boundary condition that must be satisfied by the envelope function, in addition to the requirement of continuity of the envelope function, is

$$\frac{1}{m^*(\mathbf{r})}\nabla f(\mathbf{r})\text{ continuous}$$