Chapter 2 Theoretical background for photoluminescence in semiconductors

To study optical properties of semiconductors, laser beams with photon energy higher than the band gap energy of the semiconductor are usually used to excite electrons from the valence band to the conduction band and leave holes in the valence band. The excited electrons and holes may scatter and relax to the bottom of the conduction band and the top of the valence band through the carrier-phonon interaction. Some electrons could be attracted by holes through Coulomb interaction to form excitons. Excitons could be further trapped by acceptors or donors. Excitons or trapped excitons could recombine radiatively and emit photons. Electrons/holes could also radiatively recombine with acceptors/donors. This re-emission of light after absorbing a photon of higher energy is called photoluminescence (PL). In some semiconductors, non-radiative transitions, which involves electrons and holes recombine with defects, could dominate, so weak PL intensity was detected. Radiative recombination processes include (1) band to band transition, (2) excitonic recombination, and (3) defect (donor and/or acceptor) related transitions. A schematic diagram for the above mentioned PL processes is shown in Fig. 2-1.

(1) Band to band transition

Band to band transition involving free electrons in the conduction band minimum and holes in the valence band maximum usually occurs in direct-gap materials with the momentum conservation. The electron-hole pairs (e-h) will recombine radiatively. The recombination rate is almost proportion to the product of electron and hole concentrations.

(2) Free exciton transition

E-h pairs attract each other by the Coulomb interaction to form free excitons. The transition energy of free excitons is $h\nu=E_g-E_n$, where h is the Plank's constant, ν is the photon frequency, E_g is the semiconductor band gap, E_n is the free exciton's binding energy. $E_n = \frac{2\pi^2 m^* e^4}{h^2 \varepsilon^2 n^2}$, where m* is the reduced mass, n is the quantum number, ε is the dielectric constant.

(3) Defect related transition

For the semiconductor with few intrinsic defects, instead of free exciton recombination, emission from the recombination of excitons bound to acceptor and/or donors could be a dominant feature in the PL spectrum. Electrons localized at neutral donor sites could also recombine with free holes, or holes confined at neutral acceptor sites can also recombine with free electrons.

Electrons and holes can also be created at the D^+ and A^- sites to produce neutral D^0 and A^0 centers. Electrons localized at neutral donor sites could recombine with holes attracted by neutral acceptors. Transition from donor levels to acceptor levels can be expressed as $D^0 + A^0 \rightarrow D^+ + A^- + h\upsilon$. The transition energy is $h\upsilon = E_g - (E_D + E_A) + \frac{e^2}{\varepsilon R}$, where E_D and E_A are the binding energy of donors and acceptors, ε is the dielectric constant, R is the distance between donors and acceptors.

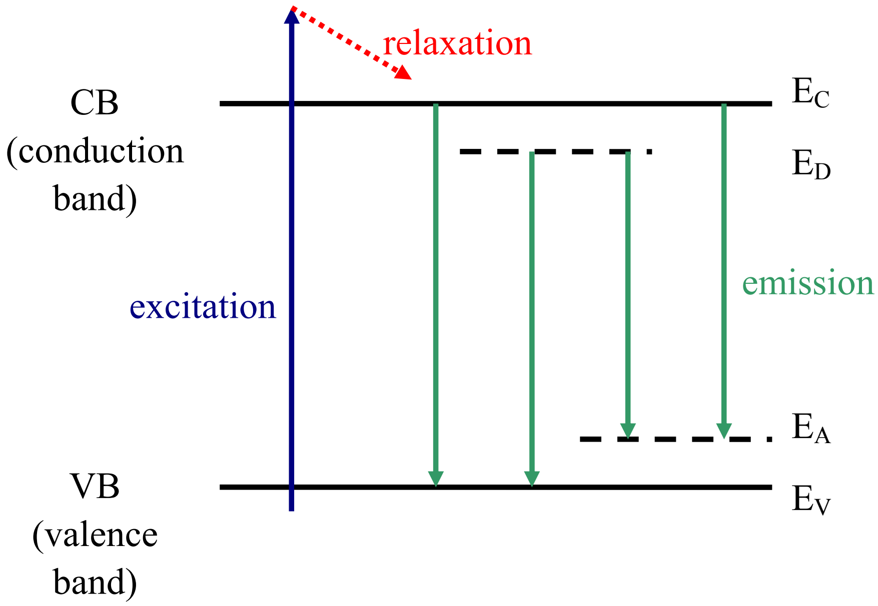

Fig. 2-1. Schematic diagram for PL transitions in semiconductors.