

Intermediate bands versus levels in non-radiative recombination

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Abstract

There is a practical interest in developing semiconductors with levels situated within their band gap while preventing the non-radiative recombination that these levels promote. In this paper, the physical causes of this non-radiative recombination are analyzed and the increase in the density of the impurities responsible for the mid-gap levels to the point of forming bands is suggested as the means of suppressing the recombination. Simple models supporting this recommendation and helping in its quantification are presented.

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1. Introduction

The use of intermediate bands (IB) or levels lying within the band gap of a semiconductor has been proposed [1–3] as a means of manufacturing solar cells with efficiencies of up to 63.3% in ideal conditions. These cells have been implemented with quantum dots that provide the mid-gap level [4], but actual efficiencies have been limited to 10% as a result of weak sub-band absorption and excessive non-radiative recombination among other reasons. We believe that the use of alloys containing a large density of centers able to absorb sub-band gap photons has a higher potential than solutions based on nanotechnology.

Mid-gap levels in semiconductors have been well known for long time. They constitute the so-called deep energy traps and are known to act as very effective recombination centers, thus jeopardizing the potential of IB solar cells.

In this paper we give arguments that suggest that, surprisingly, sufficiently high densities of traps introducing deep energy levels will suppress the non-radiative recombination and thus produce promising IB materials for solar cells.

We looked at this conjecture [5] before publishing the arguments here and have subsequently promoted research, using band calculation methods, for alloys producing a suitable IB [6–11].

Recombination can be radiative and non-radiative. The first mechanism is unavoidable because it is a detailed balance counterpart of the generation through light absorption. A solar cell in which recombination processes are exclusively radiative may reach its efficiency limit [12].

For non-radiative recombination, several mechanisms are known to exist [13–16]. In Auger recombination, the energy of a recombining electron–hole pair is transmitted to another electron. It can be enhanced by impurities but, in general, it is not important except in highly doped semiconductors or at very high levels of carrier injection. In the rest of the non-radiative recombination processes, the energy is transferred to phonons. The statistics of this mechanism were studied in the pioneering works by Shockley, Read and Hall (SRH) [17,18]. However, the physical nature of the mechanism underlying this recombination has remained obscure for years as the energy to be removed from a recombination event is much larger than the energy of a single phonon; in fact, it amounts to a few hundreds of millielectronvolts. For this type of recombination, several mechanisms have been proposed. Among them, the currently most widely accepted one is the lattice

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relaxation multiphonon emission (MPE) mechanism, which was first proposed by Lang and Henry [19]. They based their work on the early model suggested by Seitz [20], in connection with the quenching of luminescence and which was further developed by Huan and Rhys [21] to explain the absorption line broadening of F-centers in alkaline halides.

The most important points of our argumentation are related to the so-called Anderson [22] and Mott [23] transitions, which determine whether the eigenfunctions of the Hamiltonian of an array of atoms will be a set of wave functions associated to the different atoms or they will be extended wave functions expanding over all the atoms in the array.

This paper is organized as follows: after this introduction we devote a section to refreshing the fundamentals upon which the mechanisms governing the recombination are based, including the use of the so-called configuration diagrams. Then, the lattice relaxation multi-phonon emission mechanism, which is responsible for the SRH recombination, is described. Finally, the argumentation on how to suppress this mechanism is developed, first according to the Anderson mechanisms based on the lack of homogeneity followed by the Mott mechanisms associated to the basic electron–electron interaction. A rough quantification of these effects is introduced, in the first case, with the help of a simplified model.

2. Background

2.1. Fundamentals

For the analysis of solids, advantage is taken of the big difference in mass between electrons and nuclei. First, a Schrödinger equation associated to the fast electrons is solved in which the positions of the nuclei are taken as parameters that provide the external potential. Once this is done, the electronic energy obtained is introduced into the total Hamiltonian leading to a purely nuclear equation in which the electronic energy appears thus completing the potential energy of the nuclei.

The difference between the aforementioned treatment and the non-approximated Hamiltonian leads to a non-adiabatic term which may be treated as a perturbation that induces transitions from state to state, where the states are those defined in the adiabatic framework.

For the solution of the fast electronic Schrödinger equation, the multi-electronic eigenvectors are split into a set of one-electron eigenvectors (Slater determinants) and a self-consistent calculation [24] is undertaken using one-electron Hamiltonians in which the influence of the other electrons appears as Coulomb repulsion and exchange terms. Every one-electron wave function is expressed as a linear combination of previously selected base functions. The obtained solutions for the one-electron eigenvectors correspond to a given set of nuclei positions. Now we must move the nuclei positions until a lattice-relaxed minimum

energy is achieved for the total nuclei-plus-electrons system.

In the preceding calculation, not all the one-electron eigenstates (as many as base functions) are filled with electrons, but only some of them, up to the number of total electrons in the crystal. Only the filled states participate in the Coulomb repulsion and the exchange terms. Selecting them in order to get the lowest energy is the choice that leads to the calculation of the fundamental state.

In materials with an “impurity”, the impurity produces a potential that is different from those of the host atoms and provides special base functions which are also different from those of the host atoms (if the base function is made up of localized functions, rather than a set of plane waves). For certain impurities, one or several energy eigenvalues will appear in the middle of the semiconductor gap and their eigenfunctions will have a strong projection on the base functions provided by the impurity.

Deep-level impurities, with eigenvalues in the mid-gap, will produce eigenfunctions which are strongly localized and that may be empty and then filled (or vice versa) during the recombination process. In the case of a metallic IB material (e.g. Ti in GaAs and GaP and Cr in ZnS and ZnTe) some filled one-electron wave functions in the fundamental state are in the IB [6–11].

2.2. Configuration diagrams

The electronic energy (of all the electrons) for unrelaxed lattice situations becomes a part of the potential energy of the nuclei necessary to study the lattice dynamics. The nuclear energy is usually combined with the electronic energy to draw the so-called “combined potential energy” configuration diagrams. The deviation of the nuclei with respect to their equilibrium position can be expanded to the second order leading to a quadratic form of the combined potential energy of the type $U = \sum_{i,j} b_{ij} \delta R_i \delta R_j$. This expression can be represented as a two-dimensional plot if, for example, we set a value for all the δR_i save one. However, the most illustrative of these two-dimensional plots are those representing the potential energy along a line of maximum slope parameterized by q (the length of the line in the multidimensional δR_i space).

In the configuration diagrams the electronic energy usually refers to a single electron while the nuclear energy is associated to the whole crystal. We can divide the latter by the number of electrons to account for homogeneous concepts.

An example of a configuration diagram is represented in Fig. 1. Let us consider, for the moment, the branches in the figure associated to the valence band (VB) and the conduction band (CB). For them, in the position of equilibrium ($q = 0$), the energy corresponds to the top of the VB and the bottom of the CB. For other values of q , the branches represent the total potential energy (of electrons and nuclei referred to one electron) as described above and, by definition, the curve in the CB is just a

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