Wigner-Weyl description of radiative processes in correlated disordered semiconductor alloys

Jean-Philippe Banon[1,*], **Pierre Pelletier**[1], **Claude Weisbuch**[1], **Svitlana Mayboroda**[2], **Marcel Filoche**[1]

[1]Laboratoire de Physique de la Matière Condensée, CNRS, Ecole Polytechnique, Institut Polytechnique de Paris, 91120 Palaiseau, France

[2]School of Mathematics, University of Minnesota, Minneapolis, Minnesota 55455, USA

[*]Email: jean-philippe.banon@polytechnique.edu

Abstract

We present a model for light absorption and luminescence in correlated semiconductor alloys based on an approach in phase space combined with the localization landscape. The model was recently shown to give reliable results at low computational cost for uncorrelated disordered InGaN alloys when compared with a model based on the direct solution of the Schrödinger equation. We study the influence of compositional correlation on the absorption and spontaneous emission spectra.

Keywords: Disordered semiconductor alloys; phase space representation;

Introduction

Light absorption and emission measurements are commonly used to study the electronic and optoelectronic properties of semiconductor alloys, and to characterize devices made of heterostructures of such alloys such as LEDs. The absorption and luminescence spectra are in general affected by several processes: thermal processes, electric fields, Coulomb interaction, and alloy disorder. Alloy disorder corresponds to the random configuration of atoms of different species on the crystal lattice, and consequently, breaks the periodic symmetry of the ion lattice potential. In order to understand and predict the effect of alloy disorder on the optoelectronic properties of alloys and devices, we have developed a model of light absorption [1] and spontaneous emission based on a formulation in phase space (also called the Wigner-Weyl approach) for the electronic states and on results from the localization landscape theory [2,3]. The derived model is simple, computationally efficient and was shown to yield good approximations when compared with eigenstate-based computations. In this contribution, we apply the Wigner-Weyl-localization-landscape model to the case of light absorption and emission by correlated InGaN alloys.

1 Correlated alloys

The electronic properties of the disordered InGaN alloy are modeled in the framework of the effective mass approximation. The energy eigenstates of the electrons near the edges of the valence and conduction bands are sought as products of a Bloch-lattice-periodic cell function and of an envelope function satisfying an effective Schrödinger equation. The effective masses and potentials appearing in the conduction and valence effective Schrödinger equations are obtained via a continuous local indium concentration which is a regularization of the discrete atomic indium configuration on the InGaN wurtzite lattice. The indium ions are drawn randomly on the cation sites following a Bernoulli law either independently (uncorrelated alloy) or with some correlation by drawing them preferentially close to already present indium ions following the model proposed by Di Vito and co-workers [4] (a fraction p_u of the In ions being drawn first without correlation).

2 Radiative processes in phase space

In Ref. [1] we have derived a model for the absorption coefficient which is based on a phase space approach and which draws inspiration from the modified Weyl law based on the localization landscape for the integrated density of states [3]. In the dipole approximation, the absorption coefficient was shown to be proportional to

$$\alpha(\omega) \propto \int\int\int \mathcal{D}^{(c)}(\mathbf{r},\mathbf{k},\varepsilon+\hbar\omega) \times \mathcal{D}^{(v)}(\mathbf{r},\mathbf{k},\varepsilon)\,\mathrm{d}\varepsilon\,\frac{\mathrm{d}^3r\,\mathrm{d}^3k}{(2\pi)^3}\,, \quad (1)$$

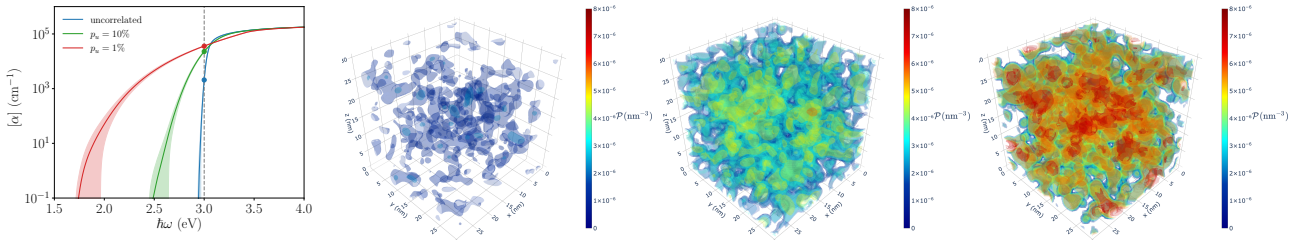

Figure 1: Absorption coefficient spectra for In-concentration $x = 10\%$ and different distributions: uncorrelated, $p_u = 10\%$ and $p_u = 1\%$. Absorbed power density for $\hbar\omega = 3$ eV and for a realization of the alloy for three values of p_u: uncorrelated, $p_u = 10\%$, $p_u = 1\%$. Average In-concentration $x = 10\%$.

where $\mathcal{D}^{(c,v)}(\mathbf{r}, \mathbf{k}, E)$ are *densities of states in phase space,* whose definitions are given in Ref. [1]. A similar expression can be obtained for the spontaneous emission spectrum. Approximations for the densities of states in phase space can then be derived using the localization landscape, resulting in the following closed form expression for the absorption coefficient [1]

$$\alpha(\omega) = K(\omega) \int_\Omega \left[\frac{2m_r(\mathbf{r})}{\hbar^2}\right]^{3/2} \times \Big(\hbar\omega - E_g^{(\mathrm{eff})}(\mathbf{r})\Big)_+^{1/2} \mathrm{d}^3 r\,. \quad (2)$$

Here $K(\omega)$ is a know material dependent function of the light angular frequency ω, m_r is the local reduced effective mass and $E_g^{(\mathrm{eff})}$ is an effective band gap profile derived from the localization landscape theory. The effective band gap profile can be viewed as a smoothed version of the original disordered band gap profile. This smoothed version accounts for the typical length scale of the lowest energy eigenstates and their energy without having to resort to a diagonalization of the Hamiltonians. We can also derive an approximation of the absorbed power density which we show to be directly proportional to the integrand in Eq. (2). This allows for an intuitive physical interpretation. For a given value of $\hbar\omega$ the electromagnetic power is deposited in the volume defined by $\hbar\omega - E_g^{(\mathrm{eff})} > 0$, and thus contributes to the absorption coefficient at frequency ω. As $\hbar\omega$ increases the contributing volume increases to finally fill the whole space when $\hbar\omega > \max E_g^{(\mathrm{eff})}$.

3 Results

Figure 1 displays absorption coefficient spectra obtained with the Wigner-Weyl-localization-landscape model [Eq. (2)] for uncorrelated alloy, and correlated alloys. As the degree of correlation increases (p_u decreases) the low energy absorption tail exhibits a broadening. The broadening of the absorption tail is attributed to the lowering of the conduction and valence potentials, and hence, of the energies of the eigenstates close to the band edges. This is captured by the effective band gap profile in our model. Figure 1 shows 3D maps of the absorbed power density for a fixed photon energy $\hbar\omega = 3$ eV and for the three values of p_u studied in Fig. 1. We observe that as the correlation length increases, the volume contributing to the absorption increases and so does the absorbed power. The typical volumes in which the power density is localized correspond to In-rich regions in which the local band gap is lowered.

4 Acknowledgments

J.-P. B. P. P. and M. F. are supported by the Simons foundation grant 601944. S. M. is supported by the NSF RAISE-TAQS grant DMS-1839077 and the Simons foundation grant 563916. C. W. is supported by the Simons foundation grant 601954 and NSF Raise-TAQS grant DMS-1839077.

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