Advanced Modeling of Hot Carrier Effects in 3rd Generation Solar

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Objectives

The concept of hot carrier solar cells is based on the use of the carriers excess energy induced by above band gap photons absorption, and on the collection of carriers before thermalization with the lattice. Previous experiments [1] showed that hot carriers thermalization rates can be reduced under strong excitation in nanostructures to the point that conversion efficiencies over 50% under concentration are possible. The thermalization rate is tightly related to the phonon-carrier interaction, and ultimately is limited by the zone centre longitudinal optic-phonon (LO) anharmonic decay. Increase the LO-phonon lifetime though enhances the chance to collect charge carriers at still a high energy. We aim at understanding LO decay process in promising III-V semiconductors and the influence of its lifetime on the extracted current in hot carrier solar cells, to draw a phonon engineering strategy in order to increase its relaxation time, and therefore enhance cell efficiencies.

Methodology

- Phonon density of state computed on very tight mesh (density functional perturbation theory, QUANTUM ESPRESSO package [2]) ;
- Deriving the three-phonons decay process within energy and momentum conservation, and the eventual LO phonon lifetime.

Main Results

- 34% of incoming photon flux is absorbed.
- Photon re-emission and Impact Ionization processes are negligible.
- Maximum extracted current achieved for Energy Selective Contacts close to band edges.
- Auger recombinations are the main current loss processes.
- Heating of electron populations through hot phonon effect possible for artificially long (but achievable) LO phonon lifetime.
- The extracted current is not significantly impacted by the hot phonon effect in the lifetime range investigated.

Methodology

The Ridley and Gupta approach [3] :

\[ \tau_{\text{LO}} = \frac{1}{\alpha_\text{ex} + \beta_\text{ex} + \alpha_\text{em} + \beta_\text{em}} \]

The model succeed in reproducing temperature dependence of LO phonon lifetime in III-V semiconductors.

Conclusions

The LO phonon lifetime can be calculated with a simple model in bulk semiconductors. In addition to a large mass difference, a ideal hot carrier solar cell absorber must show a low LO-TO splitting. Indeed, it leads to low contributor channels in the rate integral, so higher lifetimes.

First realistic modulation of a Hot Carrier Solar Cell has been carried with the test material InGaAs. There is no compensation between Auger and Impact Ionization processes, and Auger recombinations constitute the main current loss process. Raw LO phonon lifetime in common III-V semiconductors cannot trigger the hot phonon effect efficiently. However, longer lifetimes can cause the heating of carrier populations in the absorber.

Perspectives

Works are in progress to investigate the optical phonon decay in nanostructures materials. In such a system, phonon engineering may allow us to prevent the Klemens channels from occuring. Further studies on the hot carrier solar cell modelling will permit to investing the J(V) characteristics of the simulated cell.

References:

Figure 1 : GaAs dispersion relation (red) and LO two-phonon decay final state.

Figure 3 : (L)-Optical phonon lifetime temperature dependence calculated for various III-V semiconductors. The points refer to experimental data [4-10], except for AlSb for which they refer to calculated values [9].

Figure 4 : Two-phonons final states resulting from a optical-phonon decay by various III-V and IV-VI semiconductors ( three-phonons process ) Colour scale indicates the weight of each channel in the Ridley (3) integral (see the right section).

Figure 5 : The model succeed in reproducing temperature dependence of LO phonon lifetime in III-V semiconductors.