EXTENSIBLE MODELLING FRAMEWORK FOR NANOSTRUCTURED III-V SOLAR CELLS

Markus F Führer[1], Jessica GJ Adams[1], Keith WJ Barnham[1], Ben C Browne[1], Ngai LA Chan[1], Daniel J Farrell[1], Louise Hirst[1], Kan-Hua Lee[1], Ned J Ekins-Daukes[1], Akio Ogura[2], Katsuhisa Yoshida[2], Yoshitaka Okada[2]

[1]Imperial College London, London, United Kingdom
[2] Research Center for Advanced Science and Technology, The University of Tokyo, Tokyo, Japan

ABSTRACT

The use of nanostructures has been shown to provide practical performance enhancements to high-efficiency III-V based solar cells by permitting sub-bandgap tuneable absorption. Nanostructures present a fertile ground for new solar cell technologies, and an improved understanding of fundamental processes may even lead to functional intermediate band and hot-carrier devices. As the fundamental processes occurring in nanostructured solar cells are complex and not easily observable, the study of such devices often requires the analysis of data derived from experimental characterisation techniques using computer models. Models exist for many individual aspects of these nanostructured solar cells, but as yet no comprehensive modelling solution exists. We report on our progress to produce an extendable abstract modelling framework written in the high-level programming language Python. The framework is intended for deployment both as back-end to a variety of interfaces for specialised modelling purposes, and as a library of methods and classes for use at source-code level, allowing adaptation to a wide variety of research problems. Significant code abstraction, such as sequestering complex materials parameterisation behind a simple material object allows simple scripts to do complex work. Modules underway cover several device simulation tiers, including fundamental processes such as quantum well and dot absorption and recombination, as well as device level simulations such as spatial bias mapping using equivalent circuits and multijunction IV characteristics. These simulations correlate with and derive experimental data from characterisation techniques including spatially and temporally resolved electro- and photoluminescence spectroscopy, fourier-transform infrared spectroscopy, and others.

NANOSTRUCTURED III-V SOLAR CELLS

The incorporation of nanostructures such as quantum wells or quantum dots into the intrinsic region of p-i-n solar cells has been studied extensively. Recent results show that directional emission from strained quantum wells provides a small but fundamental efficiency enhancement to such devices [1]. An improved understanding of the fundamental processes in these structures may even lead to functional high efficiency cell concepts, such as hot-carrier devices, wherein above-bandgap carriers are collected prior to thermalisation, and intermediate-band devices, where an additional band in the band-gap permits sub-bandgap absorption as a two step process. Preliminary evidence of non-equilibrium carrier populations suggesting delayed cooling is actively being investigated [2,3].

A more immediate benefit to nanostructures comes in the form of subcell bandgap tuning in multijunction solar cells: the inclusion of lower bandgap regions in current-limiting junctions trades extra current for a slight reduction in junction voltage, allowing the other junctions to operate closer to their maximum power point [4], as well as permitting multijunction cells to be tuned to particular insolation spectra. The recent world-record efficiency achieved by a single-junction quantum well solar cell shows that even single-junction nanostructured devices show promise. [5]

Nanostructure Example: Quantum Well Solar Cells

The production of quantum well solar cells involves growing several interleaved layers of different band-gap lattice-matched materials. There are no binary or ternary alloys with a suitable band-gap that are lattice-matched to GaAs. One candidate, InGaAs, satisfies the band-gap constraints, but its larger lattice constant limits the number of quantum wells; only a few can be grown under compressive strain before relaxation occurs and dislocations form. To counter this problem, it is possible to space the quantum wells not with GaAs, but rather with another material with a smaller lattice constant, such as

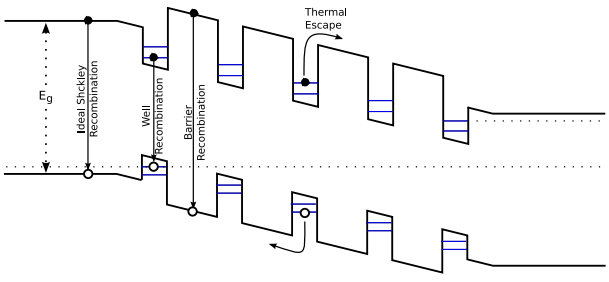

Figure 1: Quantum Well Solar Cell band structure

GaAsP. The compressive strain in the InGaAs wells can be balanced by the tensile strain in the GaAsP barriers. In this fashion, many wells may be grown without any observable dislocations [6]. The band-structure of such a device is illustrated in Figure 1.

SOL-CORE: CHARACTERISATION AND SIMULATION

Attempting to understand the processes that occur in this structure system poses a unique set of challenges. Materials in a nanostructured system do not retain the same physical parameters (eg. absorptivity) as the same material would have in bulk form, and so the extraction of such parameters from devices requires special characterisation methods in conjunction with appropriate simulations.

Models exist for many individual aspects of these solar cells, but as yet no comprehensive, extensible modelling solution exists. We have been developing SOL-CORE, an extensible programming framework designed to simulate aspects of nanostructured PV from cell level to systems level. It is written in high-level programming language Python, and aimed at deployment both as a code-level library and as back-end to more specialised applications.

Design goals

The SOL-CORE project has several guiding doctrines, summarised below.

Simple objects doing complex work: the problems being addressed are complicated, but significant abstraction is possible and desirable. The user of the Sol-Core framework should have to manipulate as few numbers as possible – greater understanding can be gained by manipulating concepts. For example, solar cell structures are represented as an ordered collection of layer objects, each consisting of a material object and a thickness. The material object is a collection of material parameters calculated from a variety of sources such as Vurgaftman [7] (see figure 2) or Hamaker parameterisation [8], or interpolated from databases such as the Sopra nk database[9]. These calculations are transparently performed in the background, and the parameters available when needed, retrievable via single lines of code, e.g.:

```
mat = InGaAs(indium_fraction=0.18, T=300)
E = mat("band_gap")
A = mat("lattice_constant")
```

While intuitive unit conversion functions are available, by default all modules pass variables in SI-units, simplifying calculations and readability.

Flexibility: Specialised software for addressing specific problems exist. By producing a framework intended primarily for use as part of other programs, greater flexibility is achieved. For example, a specialised program might calculate the quantum efficiency of a particular structure. If this process is instead available as an importable library, it is possible to write a simple program that iterates over a particular parameter in order to study the quantum efficiency dependence on that parameter, and it is possible to write a program that optimises cell structure to a particular incident spectrum.

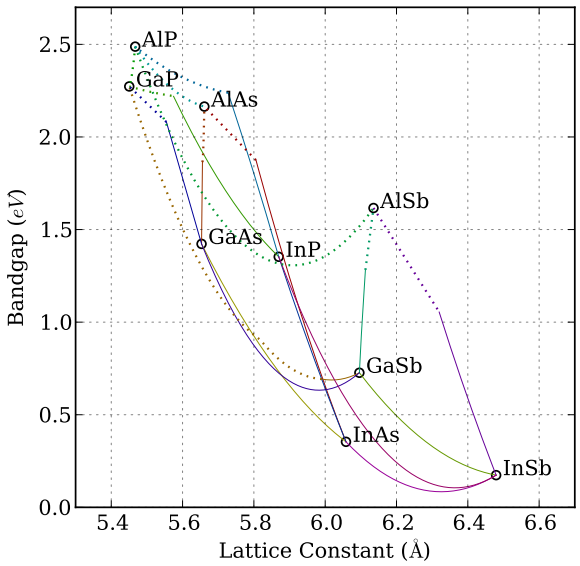

Figure 2: Vurgaftman ternaries parameterisation – dashed lines indicate indirect band gaps

Expandability and Customisation: it is not possible to address all possible needs, and therefore important that specific simulations can be added as necessary. Sol-core consists of a core body of methods, data structures, and protocols, but most physical methods are implemented as extensions that can be as simple as a single file containing several functions or data structures. It is therefore possible to implement new material systems or simulations with relative ease, compared to developing a new stand-alone product.

Deployability: If a particular script is repeated often with very similar input, it may be beneficial to deploy this script as a stand-alone product with a non-code user interface. This should require as few changes to existing code as possible.

To meet these design goals, the high-level object-oriented programming language Python was chosen as a base for the framework. Python is an interpreted language that can make use of compiled code for speed, with the stated aim of combining "remarkable power with very clear syntax" [10]. Python is free, open source, available for a wide range of operating systems, and actively being developed.

Sol-core Module examples

Within Sol-Core, **Quantum Efficiency** [11] and **IV characteristics** can be modelled by considering material absorptivities, the spectral intensity as a function of depth, as well as the drift and diffusion of carriers within the solar cell. Shockley Read Hall recombination in the depletion region accounts for the ideality 2 current. Ideality 1 currents include bulk recombination, as well as radiative recombination in the nanostructures. Absorption coefficients of nanostructures are calculated by solving the Schrödinger equation for the confined electron and hole states, calculating overlap integrals and applying Fermi's golden rule to compute the transition strengths. In this fashion, high quality fits to experimental quantum efficiencies and IV curves can be obtained. [12]

The **dark-IV fitting** module produces fast, high-quality fits of the current equation (equation 1) to experimental DIV data (figure 3) by finding the boundary point between the n=1 and n=2 regime numerically in data and equating the result to the analytic expression for the boundary point (equation 2). This relates several key parameters at one experimental data point, significantly reducing fitting complexity and time. Shunt resistance is extracted from data by treating the cell as an ohmic resistor at low bias. In this manner, the ideality parameters n_1 and n_2, reverse saturation currents J_{01} and J_{02}, temperature T, series resistance, and shunt resistance can be extracted.

$$J_{\text{div}} = J_{01}\left(\exp\left(\frac{qV}{n_1 kT}\right) - 1\right) + J_{02}\left(\exp\left(\frac{qV}{n_2 kT}\right) - 1\right) \quad (1)$$

$$\text{where } \frac{\mathrm{d}^3}{\mathrm{d}V^3}\ln\left(J_{\text{div}}(V = V_{\text{inflection}})\right) = 0$$

$$V_{\text{inflection}} = \frac{kT}{q}\ln\left(-\frac{J_{01}n_2^3}{J_{02}n_1^3}\right)\frac{n_1 n_2}{n_1 - n_2} \quad (2)$$

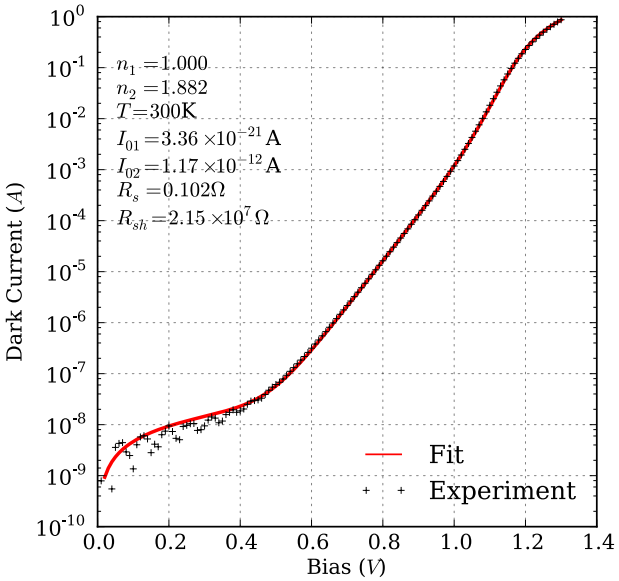

Figure 3: Experimental IV data and fit

Spectral Luminescence is modelled using a combined Kirchhoff and generalised Planck formalism, using the experimental quantum efficiency as a stand-in for absorption parameters. Fitting experimental data by varying parameters such as temperature and chemical potential allows information about the carrier populations to be extracted from spectra.

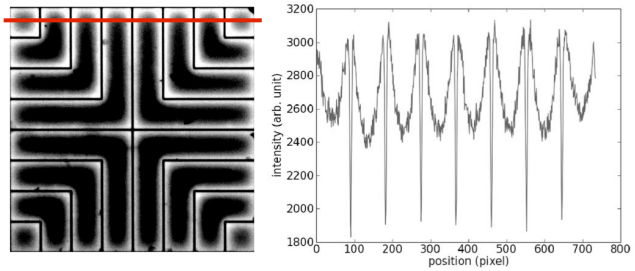

Figure 4: Spatial electroluminescence inhomogeneity due to low front metallisation

Spatial Luminescence is modelled using a SPICE- based circuit analysis module, which assembles a spatially discretised analogous circuit out of a unit cell circuit (figure 5), and determines the connections between unit cells based on the metallisation pattern to be simulated. This approach has been shown to produce reliable results [13] and allows calculation of spatial bias (Figure 6), luminescence, and radiative efficiency distributions. Comparison with experimental data allows key front-metallisation grid parameters to be optimised faster than by a purely experimental approach (Figure 4), which requires iterated production of samples. This methodology also allows for the non-experimental characterisation of more complicated masks than a purely analytic approach.

Other modules being developed include atmospheric conditions and spectral irradiance models.[14]

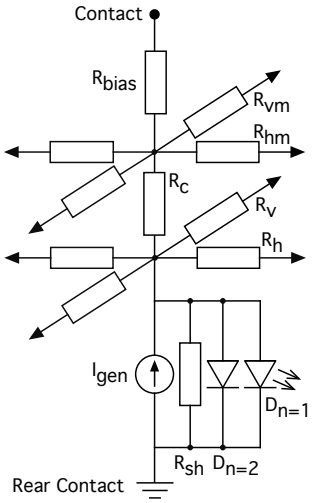

Figure 5: Spatial Grid Equivalent circuit

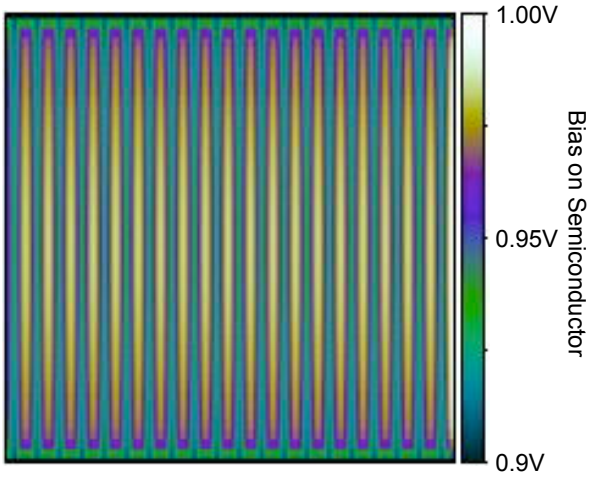

Figure 6: Spatial bias distribution across a 10cm × 10cm simulated GaAs solar cell

CONCLUSION

We are developing a comprehensive modular and extendable nano-PV modelling tool-suite taking the form of a programming framework in the accessible programming language Python. Modules underway include solar cell IV, QE, and spatial/spectral EL/PL characterisation, simulation and fitting, as well as atmospheric conditions and spectral irradiance models, and a nanostructured materials module. These modules add to a core functionality that includes an easy to use materials system that sequesters complex parameterisations and data behind simple objects. This allows specialised applications to make use of an simple but extensive common code-base, simplifying the development of future device simulations.

ACKNOWLEDGEMENTS

This project is conducted in collaboration with the Research Center for Advanced Science and Technology at the University of Tokyo, funded by the New Energy and Technology Development Organization (NEDO), and Ministry of Economy, Trade and Industry (METI), Japan.

REFERENCES

[1] J.G.J. Adams, W. Elder, et al. “Efficiency Enhancement in Strain-Balanced Quantum Well Solar Cells Via Anisotropic Emission”. Proc. 24th European Photovoltaic Solar Energy Conference, Hamburg, Sep 2009.

[2] L. Hirst et al. “Hot Carrier Dynamics In InGaAs/GaAsP Quantum Well Solar Cells”. Abstract submitted to 37th IEEE PVSC, 2011.

[3] G.J. Conibeer, et al. “Slowing of carrier cooling in hot carrier solar cells, Thin Solid Films”, 516 (20), Proceedings on Advanced Materials and Concepts for Photovoltaics EMRS 2007 Conference, Strasbourg, France, 2008, pp. 6948-6953.

[4] K.W.J. Barnham et al, “Photonic Coupling in Multi-Junction Quantum Well Concentrator Cells”, Proc. 25th European Photovoltaic Solar Energy Conference / 5th World Conference on Photovoltaic Energy Conversion (2010) pp 234 - 240.

[5] J. Adams, et al., "Higher Limiting Efficiencies for Nanostructured Solar Cells", *Proceedings of the SPIE Photonics West 2010 Conference* **7597**, 2010.

[6] D.B. Bushnell, N.J.Ekins-Daukes, K.W.J.Barnham et al., Sol. Energy Mater. Sol. Cells 75 (2003) 299

[7] I. Vurgaftman et al. “Band parameters for III–V compound semiconductors and their alloys”. Journal of Applied Physics **89** (11), 2001, pp 5815-5875.

[8] H.C. Hamaker. “Computer Modeling Study Of The Effects Of Inhomogeneous Doping And Or Composition In GaAs Solar-Cell Devices”. Journal of Applied Physics **58** (6),1985, pp. 2344-2351

[9] Sopra NK database. http://www.sopra-sa.com/index2.php?goto=dl&rub=4, last access date 20/02/2011

[10] Python FAQ. http://docs.python.org/faq/general#what-is-python, last access date 20/02/2011

[11] M. Paxman, J. Nelson, B. Braun, J. Connolly, K.W.J. Barnham, C.T. Foxon, J.S. Roberts, J.Appl.Phys. 74, 1 (1993) 614

[12] J. Connolly et al., Proc. 19th European Photovoltaic Solar Energy Conference, Paris, 2004.

[13] M. Steiner et al. “Validated front contact grid simulation for GaAs solar cells under concentrated sunlight”. Progress in Photovoltaics: Research and Applications, **19**. pp 73–83.

[14] N. J. Ekins-Daukes, Y. Kemmoku, K. Araki, T.R. Betts, R. Gottschalg, D.G. Infield, M. Yagamuchi. “The design specification for Syracuse: A multi-junction concentrator system computer model”, Proc. 19th European Photovoltaic Solar Energy Conference, Paris, 2466-2469. (2004)