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# Equivalent-circuit and transport-based mobility models of microcrystalline silicon solar cells

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**Abstract**

Microcrystalline silicon thin film solar cells exhibit optimal PV efficiency when the absorber layer contains similar proportions of crystalline and amorphous phases. When the crystalline fraction is reduced below 30%, efficiency falls very steeply, from around 8% to as low as 2%, and does not recover until fully amorphous growth conditions are established. We demonstrate that an electrical model, comprising two parallel-connected diodes scaled to reflect material composition, qualitatively predicts the features observed in the PV parameters. However the scale of the reduction in fill-factor is not reproduced. As an alternative approach, a homogeneous transport model is proposed in which carrier mobilities are scaled in accordance with values determined by the time-of-flight experiment. This model predicts a large reduction in fill-factor for low-crystallinity absorbers more in keeping with measurement. A novel carrier transport landscape is proposed to account for mobility variations.



*Keywords*: Microcrystalline silicon; solar cells; computer modelling; carrier transport; mobility

## 1. Introduction

The structural and optoelectronic properties of thin-film silicon may be controlled by the use of a process gas consisting of silane diluted in hydrogen. At silane concentrations $SC = [SiH_4]/([H_2] + [SiH_4])$ typically below 10% under VHF PECVD conditions, mixed-phase microcrystalline silicon of good optoelectronic quality, consisting of

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similar volumes of crystalline and amorphous material, may be deposited. By careful adjustment of process parameters, solar cells with optimized PV conversion efficiencies in excess of 8% can be achieved, with open-circuit voltages $V_{OC}$ in the region of 500-550 mV [1].

As *SC* is varied either side of this optimum concentration there is a reduction in solar cell efficiency. In the more crystalline material deposited at low *SC*, this may be linked to an increase in spin density [2] arising from silicon dangling bonds at the crystalline column boundaries. Such bulk defects may be responsible for reduced cell performance [3]. It is believed that the column boundaries are passivated to some extent by the amorphous phase in mixed-phase material, leading to improved electronic properties. As *SC* is increased, the crystalline fraction continues to fall and the optical band-gap of the absorber and $V_{OC}$ increase. Ultimately a point is reached where both the fill-factor *FF* and short-circuit current density $J_{SC}$ decrease rapidly, and PV efficiency drops to as low as 2%. Further increase in *SC* yields nominally amorphous films containing no detectable crystalline volume fraction when analyzed by Raman spectroscopy, and the efficiency begins gradually to improve. By re-optimization of the deposition conditions in this regime good-quality solar cells may again be obtained, with $V_{OC}$ now in the region 850-1000 mV [4]. Thus there are two regimes which, when approached from the microcrystalline and amorphous 'ends' of the silane : hydrogen dilution spectrum, may yield efficient solar cells, albeit with quite different spectral response, short-circuit current and open-circuit voltage.

Why solar cells with 'low-crystallinity' or 'Raman amorphous' absorber layers, lying between these two regimes, exhibit such poor PV performance forms the central question of this work. ESR studies [2] have shown that paramagnetic defects remain at a low level, and thus there is no reason to suspect an increase in defect-mediated recombination. It has been suggested that changes in growth conditions may instead give rise to local degradation of the *p-i* interface [5] and the formation of a space-charge which acts as a barrier to transport. This view is supported by the improved performance of cells containing buffer layers (see reference [6] for example), but these appear only to defer the decline in performance. More recently, time-of-flight (TOF) transport measurements [7, 10] have been carried out which indicate that in the low-crystallinity regime, both electron and hole bulk mobilities are significantly reduced relative to their values in optimized microcrystalline silicon films [11]. Indeed, the electron mobility appears even lower than in good-quality *amorphous* films. These variations in transport properties with composition were recently investigated by the present authors and their co-workers, by means of two-beam photogating measurements [12].

Here we consider two alternative modelling approaches to explain solar cell behaviour in the low-crystallinity region, each based on bulk, rather than interface, properties. The first may be termed an equivalent-circuit method. This is a more quantitative PSPICE [13] implementation of a proposal by the UniSolar group [14, 15] in which microcrystalline and amorphous phases in an inhomogeneous absorber layer are represented by two parallel-connected photodiodes, the photocurrent generation and diode transport parameters being scaled in proportion to the volume fraction of the constituents. This model was shown to predict *qualitatively* the observed increase in $V_{OC}$ with increasing amorphous content, and with light-soaking, and is consistent with conductive AFM measurement of local current flows in mixed-phase material down to quite low volume fractions. We note that a similar approach comprising a mesh of discrete diode-resistor elements was proposed by the IPE Stuttgart group [16] to investigate the related issue of statistical fluctuations in homogeneity in a generalised solar cell. The second approach used here is based on solution of the transport equations, assuming multiple-trapping kinetics in a model density of states (DOS) consisting of exponential conduction and valence band tails and a Gaussian distribution of amphoteric dangling bond mid-gap defect states. Specifically, we investigate the influence of varying the electron and hole extended-state mobility, in keeping with the TOF results, on the solar cell parameters.

## 2. Experimental

### *2.1. Solar cell preparation*

Cells were prepared in p-i-n sequence using a cluster-tool system, as described previously [17, 18]. The i-layer was deposited by PECVD at 20 W VHF power, at a rate of typically 0.3 - 1 nm/s onto a 10 cm × 10 cm glass substrate held at 200 °C. A series of depositions at *SC* between 5% and 15% were carried out, with nominal i-layer