Numerical Modeling of CuInSe₂ and CdTe Solar Cells

Annual Subcontract Report
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1. INTRODUCTION

1.1 Objectives

There are two primary objectives of this project:

1. The development of a numerical model, ADEPT (A Device Emulation Program and Tool), specifically for application to thin film CIS and CdTe based solar cells.
2. The application of ADEPT to the analysis and design of CIS and CdTe based solar cells.

An additional objective is to interact with researchers in industry, universities, and the national laboratories through distribution of ADEPT and consultations on the analysis of CIS and CdTe solar cells.

1.2 Period Covered

This report covers the period March 1, 1994 to February 28, 1995.

2. ADEPT DEVELOPMENT

As stated above, a primary objective of this project is the development of a detailed numerical model for CdTe and CIS based solar cells. This section will briefly review the current status of this development. ADEPT (A Device Emulation Program and Tool) is a detailed numerical model for a wide variety of semiconductor devices. An objective of this project has been its development for application to thin film CdTe and CIS based solar cells. First, however, a brief overview of basic characteristics of ADEPT will be given.

2.1 ADEPT

ADEPT generates a numerical solution to a set of three coupled nonlinear partial differential equations commonly referred to as the semiconductor equations. These are Poisson's equation and the hole and electron continuity equations and are shown below for steady state isothermal conditions.

$$\nabla \cdot D = q(p - n + N) \quad (1)$$

$$\nabla \cdot J_p = q(G - R) \quad (2)$$

$$\nabla \cdot J_n = q(R - G) \quad (3)$$

Coupled with the following auxiliary equations, these are solved for the electrostatic potential, V , and the hole and electron concentrations, p and n , on a domain defined by the

device structure subject to appropriate boundary conditions (at the contacts, for one-dimensional simulations) and the device operating conditions (the applied bias, operating temperature, and incident light flux).

$$D = \nabla V \quad (4)$$

$$J_p = -q\mu_p \left[p \nabla (V - V_p) - \frac{kT}{q} \nabla p \right] \quad (5)$$

$$J_n = -q\mu_n \left[n \nabla (V + V_n) - \frac{kT}{q} \nabla n \right] \quad (6)$$

As can be seen by examining equations (1) through (6), there are only a modest number of parameters to be set in order model any device constructed from any semiconductor material, so long as the assumptions regarding transport are not violated. These parameters are: N , the trapped charge density; G , the optical generation rate; R , the net recombination rate; ϵ , the electric permittivity; μ_p and μ_n , the carrier mobilities; and V_p and V_n , the band parameters. While this is a convenient way to express the model equations, it is a somewhat misleadingly simple representation. All the information regarding device structure and material characterization is contained in these terms.

The numerical solution of the preceding equations is achieved through a finite box discretization on a discrete mesh, resulting in a set of coupled nonlinear difference equations. This set is then solved using a generalized Newton iteration.

2.2 Modeling CdTe and CIS Based Solar Cells

The main issues in developing the numerical model for CdTe and CIS based solar cells revolves around three basic issues:

1. Determination of appropriate material parameters.
2. Adequate knowledge of the device structure.
3. Availability of device characteristics, especially light and dark I-V characteristics and the spectral response.

As yet, a complete self consistent model for CdTe and CIS solar cells able to predict, *a priori*, cell performance is not possible. Continued analysis, using ADEPT, of existing cells, as well as parameter sensitivity studies is necessary to further refine the numerical model. Work is continuing in further improvement of the particular material models needed. In particular, this includes development of material models appropriate to graded band gap structures.

In addition, work is continuing on the development of a user friendly release of ADEPT along with detailed code documentation.

3. ADEPT APPLICATIONS

During the period covered by this report, ADEPT has been used to analyze several issues related to the performance of CdTe and CIS based solar cells. Papers presenting this analyses are reproduced in the Appendices. These papers give results of the analysis of possible mechanisms for the "second junction" sometimes observed in CIS cells (especially at low temperatures) and a preliminary analysis of the issues relevant to the modeling and design of graded band gap solar cells.

4. SUMMARY

This report is a brief update of status of the development of ADEPT and its use in analyzing CdTe and CIS based solar cells. Future work will include further development and application of ADEPT, as well as continued interaction with NREL's Thin Film Partnership participants.

3 conf papers cycled separately. ds

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