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A modelling and multiobjective optimisation study of the light induced degradation parameters influencing the variation of distribution of annealing activation energies in a-Si:H

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Abstract

We have utilized multiple linear regression analysis using up to date distributions of annealing activation energies given in the literature in order to investigate the variation of these distributions with light induced degradation parameters as light intensity, degradation duration and degradation temperature in a-Si:H. We have also optimised these parameters using multiobjective optimisation method. Results we have obtained are in a way, complementary and in accord with suggestions in our previous works [J. Non-Cryst. Solids 255 (1999) 132; Mater. Sci. Eng. B 95(1) (2002) 67], where we have showed both at room temperature and at low temperatures defects with higher annealing activation energies are created at higher light intensities.

Keywords: a-Si:H; Staebler–Wronski effect; Regression analysis; Model fitting; Optimisation; Distribution of annealing activation energies

1. Introduction

Light induced degradation of the optoelectronic properties of hydrogenated amorphous silicon (a-Si:H) is one of the most challenging problems in the field of amorphous semiconductors. Illumination with strong light creates metastable dangling bonds (DB), which are indistinguishable from native DBs originally present in the mid-gap of the material. These metastable defects can be completely annealed at temperatures above 170 °C [1,2]. Accordingly, creation as well as

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annealing of these metastable defects was studied as a function of illumination intensity, illumination duration and their effect on a range of properties of the material at various illumination temperatures [2–8].

Distribution of annealing activation energies (DAAE) is a valuable tool that distinguishes the metastable defects from one another in terms of the height of the barriers between stable and metastable states [4–8]. A wider full width at half maximum (FWHM) of distribution of annealing activation energies are needed to account for the annealing behaviour of the defects created at low temperatures [3–5,7]. This distribution is described by a narrow peak at about 1.1 eV for room temperature degradations [1,3,5,8]. In one of our previous works, [7] we have confirmed that at low temperatures, light induced defects with lower annealing activation energies are created at the earlier stages of the illumination. In another previous work [8] for the defects created at room temperature, we have suggested that more stable light induced defects are created at longer illumination durations or at higher light intensities, shifting the peak value of the distribution of annealing activation energies from about 1 eV to 1.1 eV.

The growth parameters of the glow discharge a-Si:H are not definite: these parameters show considerable difference for the so called "device quality film" from one laboratory to the other. And also, light induced degradation of the a-Si:H films are studied using a variety of experimental conditions. Although, the nature of degradation is expected to be similar, these make it difficult to compare the observed light induced changes between the samples or with the properties of the sample. We have utilized multiple linear regression analysis to elucidate the dependence of distribution of annealing activation energies given in the literature on the light induced degradation parameters like continuous wave (cw) illumination intensity, illumination duration and illumination temperature. The importance of the present work becomes emphasised considering the difficulty in obtaining such time-consuming annealing measurements and the scarceness number of similar works in the literature. Results we have obtained are complementary with our previous studies and in a different way prove our suggested expectations [7,8].

2. Modelling and optimisation

2.1. Polynomial regression

An existence of a non-linear relationship among the variables involves investigating polynomial regression equations. kth order polynomial regression equation with only one regressor variable is as follows:

$$y_i = \beta_0 + \beta_1 x_i + \beta_2 x_i^2 + \cdots + \beta_k x_i^k + \varepsilon_i \quad i = 1, \ldots, n \tag{1}$$

By setting $x_{i1} = x_i, x_{i2} = x_i^2, \ldots, x_{ik} = x_i^k$, Eq. (1) may be represented as

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_k x_{ik} + \varepsilon_i \quad i = 1, \ldots, n \tag{2}$$

In this equation, y_i is the response variable, $x_{i1}, \ldots, x_{ik}$ are the regressor variables, $\beta_0, \ldots, \beta_k$ are the regression coefficients to be estimated, ϵ_i is an error term and n is the sample size. The usual method of estimation for the regression model is the ordinary least squares (OLS) [9]. Thus, the fitted OLS regression model is given by

$$\hat{y}_i = b_0 + b_1 x_{i1} + \cdots + b_k x_{ik} \quad i = 1, \ldots, n \tag{3}$$

Here, $\hat{y}_i$ is the predicted value using the multiple linear regression model, $b_0, \ldots, b_k$ are the predicted coefficients. $b_0, b_1, \ldots, b_k$ are the solution from minimizing the sum of the squares of the differences between the actual and fitted values of y, i.e.,

$$\sum_{i=1}^{n} (y_i - \hat{y}_i)^2 \tag{4}$$

A possible order of polynomial given in Eq. (1) can be determined by using backward elimination method [10]. This method begins with the model containing all regressors and higher order terms and then successively eliminates one at a time. At each iteration, a partial-F statistic is computed for each of the variables currently in the model. If the smallest partial-F value is smaller than or equal to F_α for some predefined α (say $\alpha = 0.05$),