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Thermal residual stresses in silicon thin film solar cells under operational cyclic thermal loading: A finite element analysis

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ABSTRACT

In manufacturing amorphous silicon solar cells, thin films are deposited at high temperatures (200–400 °C) on a thick substrate using sputtering and plasma enhanced chemical vapor deposition (PECVD) methods. Since the thin films and substrate have different thermal expansion coefficients, cooling the system from deposition temperature to room temperature induces thermal residual stresses in both the films and substrate. In addition, these stresses, especially those having been induced in the amorphous silicon layer can change the carrier mobility and band gap energy of the silicon and consequently affect the solar cell efficiency. In this paper, a 2D finite element model is proposed to calculate these thermal residual stresses. The model is verified by the available analytical results in the literature. Then using the model, the thermal residual stresses are studied in a commercial amorphous silicon thin film solar cell for different deposition temperatures, and subsequently, the simulation results are validated with experimental results. It is shown that for the deposition temperatures of 200 and 300 °C, the biaxial thermal stress reaches the values of −367 and −578 MPa, respectively, in the amorphous silicon layer. Finally, the model is utilized to study the cyclic thermal stresses arising in the solar cell installed in Tehran as a sample city during its operational time due to the ambient temperature changes and photovoltaic process. The results are reported for different months based on the minimum and maximum temperatures published during a year. It is demonstrated that the temperature changes can induce mean stress with stress amplitude of −526 and 60 MPa, respectively, in the amorphous silicon layer during June, for example. The calculated loading history can be used by the manufactures in thermal fatigue life assessment of the solar cell.

1. Introduction

Amorphous silicon thin film solar cells are fabricated by deposition of thin films on a thick substrate at temperatures higher than room temperature. Plasma enhanced chemical vapor deposition (PECVD) method is used to deposit the amorphous silicon layer while the substrate temperature is usually above 200 °C. Furthermore, the transparent conductive oxide (TCO) layer and back metal electrode are also usually deposited by sputtering method (Shih-Yung et al., 2011). These deposition processes lead to arising residual thermal stresses in the solar cells. Generally, the origin of stresses is due either to intrinsic stresses or mismatches of thermal expansion coefficients. The intrinsic stresses are due to the deposition process and their generating mechanism is not well specified (Hutchinson, 1996), and, hence, will be neglected here. In addition, upon cooling from the deposition temperature, a thermal stress field arises because of mismatches of thermal expansion coefficients between the thin films and the substrate (Hutchinson, 1996). These residual stresses are important to investigate, because they can change the carrier mobility as well as the band gap energy of the silicon which in turn affect the solar cell efficiency (Gleskova et al., 2006, 2009; Sun et al., 2007).

Up to date, many efforts have been devoted to derive analytical models to analyze thermal residual stresses in two and multilayers coating systems. For example, Stoney (1909) proposed a classical stress analysis which assumes the film thickness to be less than $\frac{1}{20}$ of the substrate thickness, and the induced stress is constant (Kim et al., 2000). Later, Timoshenko (1925) developed an analytical model for bi-metal strip thermostats which is based on the beam bending theory. This model preserves the strain continuity at the interface of the two metal layers. Next, Kim et al. (2000, 1999) and Gao et al. (2015) extended Timoshenko model to

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multilayers coating systems and compared their results with numerical solutions. While these models only consider the normal stresses, the 2D model proposed by Suhir (1988) captures the shear stress component in addition to the normal ones at the layer interfaces.

Besides analytical analyses, some numerical studies have also been done on 2D simulation of thermal stresses in a film–substrate composite (Haider et al., 2005; Han et al., 2009; Wright et al., 1994). These studies mainly focus on the effects of film thickness and deposition temperature on thermal stresses utilizing finite element method. Until recently, few works have focused on the simulation of residual stresses in the solar cells. For example, Lin et al. studied the residual stresses in a Copper Indium Gallium Selenide (CIGS) thin film solar cell after selenized annealing at 698 K for 20 min via experiments and numerical simulations (Lin et al., 2014).

The objective of this paper is to develop a 2D finite element model to study the thermal residual stresses in an amorphous silicon thin film solar cell during the fabrication process. The results are given for different deposition temperatures and compared with experimental results. Furthermore, the model is also utilized to study the cyclic thermal stresses arising in a solar cell installed in a sample city during its operational time and due to the ambient temperature changes.

2. Analytical approaches and finite element model

During manufacturing of a thin film–substrate composite (Fig. 1) and after the deposition of the thin film on the thick substrate ($d \ll D$), the composite is cooled from the deposition temperature to room temperature. During this process, the film and substrate tend to deform differently due to their thermal expansion coefficients mismatch. However, they are strained to match each other and remain attached; as a consequence, the thin film–substrate combination bends.

As discussed in the previous section, several researchers have tried to investigate the thermal stresses in the solar cell via employing theoretical techniques. A short list of the important outcomes of these efforts for biaxial stress is given in Table 1, where E_f, E_s, ν_f, and ν_s are the elastic moduli and Poisson ratios of the thin film and substrate, respectively. Also, the thermal expansion coefficients of the thin film and substrate are α_f and α_s, respectively. As shown in Fig. 1, d and D are also thickness of the thin film and substrate. The width of the thin film–substrate composite is shown as w. Moreover, T_d and T_r indicate the deposition and room temperatures (25 °C), respectively. Finally, it is noted that the mechanical properties are assumed isotropic both in the film and substrate.

On the other hand, the thermal stresses could also be studied by numerical simulations and then be verified via the available analytical results. For numerical simulations, the thin film–substrate

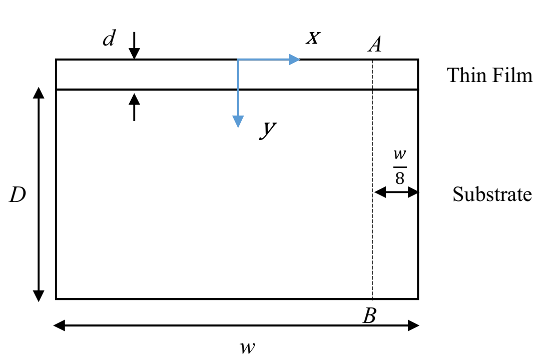

Fig. 1. Thin film–substrate composite.

Table 1
Biaxial stress relations in the thin film according to some analytical models (Gao et al., 2015; Stoney, 1909; Suhir, 1988; Timoshenko, 1925).

Analytical model	Biaxial stress σ_{rr}
Stoney (1909)	$\sigma_{rr} = \overline{E}_f(\alpha_s - \alpha_f)(T_r - T_d)$
Timoshenko (1925)	$\sigma_{rr}(z) = \frac{P}{wd} - \frac{M_f z}{I_f} \quad -\frac{d}{2} \leqslant z \leqslant +\frac{d}{2}$
	$P = \frac{2(\overline{E}_f I_f + \overline{E}_s I_s)}{\rho(d+D)}, \quad M_f = \frac{\overline{E}_f I_f}{\rho}$
	$I_f = \frac{1}{12} wd^3, \quad I_s = \frac{1}{12} wD^3$
	$\frac{1}{\rho} = \frac{(\alpha_s - \alpha_f)(T_r - T_d)}{\left(\frac{2(\overline{E}_f I_f + \overline{E}_s I_s)}{(d+D)w}\left(\frac{1}{\overline{E}_f I_f} + \frac{1}{\overline{E}_s I_s}\right) + \frac{d+D}{2}\right)}$
Suhir (1988)	$\sigma_{rr}(x,z) = \frac{P(x)}{wd} - \frac{M_f(x)z}{I_f} \quad -\frac{d}{2} \leqslant z \leqslant +\frac{d}{2}, I_f = \frac{1}{12} wd^3$
	$P(x) = \overline{E}_f dw X_0(x)(\alpha_s - \alpha_f)(T_r - T_d)$
	$M_f(x) = \frac{\overline{E}_f^2 d^4}{2\overline{E}_s D} w X_0(x)(\alpha_s - \alpha_f)(T_r - T_d)$
	$X_0(x) = 1 - \frac{Cosh(Kx)}{Cosh\left(K\frac{w}{2}\right)}, K = \sqrt{\frac{\lambda}{k}}$
	$k = \frac{2}{3}\left(\frac{1+\nu_f}{1-\nu_f}\frac{d}{\overline{E}_f} + \frac{1+\nu_s}{1-\nu_s}\frac{D}{\overline{E}_s}\right), \lambda = \frac{1}{\overline{E}_f d} + \frac{1}{\overline{E}_s D} + \frac{(D+d)^2}{(\overline{E}_f d^3 + \overline{E}_s D^3)}$
Gao et al. (2015)	$\sigma_{rr}(z) = \overline{E}_f[\varepsilon_r + K(z - z_r) - \alpha_f(T_r - T_d)] \quad D \leqslant z \leqslant D + d$
	$z_r = \frac{1}{2}\frac{(\overline{E}_s D^2 + \overline{E}_f((D+d)^2 - D^2))}{\overline{E}_f d + \overline{E}_s D}, \varepsilon_r = \frac{\overline{E}_s \alpha_s D + \overline{E}_f \alpha_f d}{\overline{E}_f d + \overline{E}_s D}(T_r - T_d)$
	$K = \frac{\frac{\overline{E}_s}{2}(\varepsilon_r - \alpha_s(T_r - T_d))D^2 + \frac{\overline{E}_f}{2}(\varepsilon_r - \alpha_f(T_r - T_d))((D+d)^2 - D^2)}{\left[\frac{\overline{E}_s}{2} z_r D^2 - \frac{\overline{E}_s}{3} D^3 + \frac{\overline{E}_f}{2} z_r((D+d)^2 - D^2) - \frac{\overline{E}_f}{3}((D+d)^3 - D^3)\right]}$

Note: $\overline{E}_s = \frac{E_s}{1-\nu_s}$, $\overline{E}_f = \frac{E_f}{1-\nu_f}$.

composite is presumed to undergo elastic deformation during temperature changes, and it is thin enough to consider the temperature to be uniform in the composite. In this study, COMSOL multiphysics software has been employed to simulate the thermal stresses via a 2D finite element model. For a more elaborated explanation, this model is composed of the 2D quadratic plane strain elements and the boundary conditions have been imposed on the corner points. To be more precise, the lower-left corner of the substrate is fixed in the x and y directions while the lower-right one is only fixed in the y direction. Actually, these constrains prevent the rigid-body motions, but they have little effect on the stress distribution.

3. Results and discussion

In this section, first, the proposed 2D finite element model is verified with the available theoretical results. It is shown that the proposed simulation approach is both accurate and efficient. The verified finite element model has then been employed to obtain the induced stresses in a commercial amorphous silicon thin film solar cell. Finally, as an application, the proposed finite element model has been employed to obtain the cyclic thermal stresses induced in the commercial amorphous silicon thin film solar cell under operating conditions in a sample city. These results can be of great importance in thermal life assessment of the solar cells.

3.1. Verification of the finite element model

In this subsection, the simulation results are compared and verified with the previously mentioned analytical models in Section 2. For this purpose, a silver thin film is supposed to be deposited on an aluminum substrate at temperature of 200 °C with the mechanical properties given in Table 2 (room temperature assumed to be 25 °C) (Antartis and Chasiotis, 2014; Gleskova et al., 2009; Hu et al., 2008; Takimoto et al., 2002). The substrate thickness is fixed at 100 μm, and the thickness of the Ag film is 0.1 and 1 μm in the finite element simulations. The width of the thin film–substrate composite is equal to 10 mm. Therefore, it is clear that the problem is multi-scale in nature (nano-sized film versus micro scale substrate with millimeter value for width of the composite) and hence