

Effects of Layer Thickness on the Residual Stresses of CIGS Solar Cells with Polyimide Substrate

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Abstract

In this paper, we investigate the effect of layer thickness on the residual stresses of copper indium gallium diselenide (CIGS) solar cells with polyimide substrate caused by CIGS layer deposition at 400°C and then cooling down to room temperature using the Finite Element Method (FEM). Moreover, we also examined the effect of layer thickness on residual stress of CIGS solar cells after cooling down to room temperature from the hotspot temperatures of 200°C, 300°C, and 400°C. Our simulated CIGS is composed of five layers: ZnO, CdS, CIGS, Mo, and PI substrate. We were able to quantify the effect of each layer's thickness and hotspot temperature on the average stresses of each layer for the CIGS solar cells. We found that the PI substrate layer has the most significant effect on the residual stress of CIGS solar cells. Our simulation results reveal that the stress type (tensile vs. compressive) and the magnitude of stress of the CIGS layer (main absorber layer) can be controlled by changing the thickness of the PI substrate while applying a heat to CIGS solar cells. Quantitative analysis of relationship between layer thickness and thermo-mechanical stress of thin film solar cells can help solar cell manufacturers design more robust and reliable solar cells. For example, fabricating PI layer thickness less than 17 μm can improve the performance of CIGS solar cells by nullifying the compressive residual stress in the CIGS absorber layer.

Keywords

Thin-Film Solar Cells, Residual Stress, Temperature, CIGS, Hotspot

1. Introduction

Copper indium gallium diselenide (CIGS) solar cells are one of the most widely

used flexible solar cells in the market. They are typically composed of Zinc Oxide as a front contact (ZnO), Cadmium Sulfide as a buffer layer (CdS), CIGS as an absorber layer (CIGS), and Molybdenum as a back contact (Mo). Soda-lime glass (SLG) is a material commonly used as a rigid substrate while stainless steel (SS) and polyimide (PI) are materials commonly used as flexible substrates. The typical range of thickness of the ZnO layer is 200 - 600 nm, 50 - 70 nm for CdS, 0.5 - 3 μm for CIGS, and 0.5 - 1 μm for Mo. For the substrate, SLG typically ranges from 2 - 5 mm, 25 - 200 μm for SS, and 12.5 - 75 μm for PI [1]. Generally, Mo is deposited by sputtering, CIGS by co-evaporation (p-type), CdS by chemical bath deposition (n-type), and ZnO by sputtering (n-type). High residual stress occurs due to the discrepancy of the thermal expansion coefficient between layers after CIGS deposition. The temperature of CIGS deposition is higher than the temperatures used for the deposition of other layers, which ranges from 400°C - 600°C [2]. The temperature of the CIGS deposition process is about 400°C - 500°C for the PI substrate, 520°C - 600°C for the SS substrate, and 400°C - 600°C for the SLG substrate. Lin *et al.* [3] investigated the residual stress of CIGS and Mo layers through Finite Element Method (FEM) simulations and experiments after depositing the CIGS on Mo at 698 K. Their structure is composed of three layers: PI substrate, Mo back contact, and a CIGS absorber layer. They reported that there exists compressive residual stress in both Mo and CIGS layers. Residual stress of the CIGS layer is strongly related to the thickness of the Mo contact layer. Garcia *et al.* [4] experimentally found that some tensile stress is advantageous for increasing the short circuit current of CIGS solar cells by nullifying the compressive residual stress of active layers induced during the fabrication process. Hotspots caused by partial shading can increase the temperature of the solar cells radically, causing damage to the cells [5] [6] [7]. They can generate additional residual stress in the cells when the cells return to normal temperatures after the partial shading (hotspot) disappears. Lee *et al.* [6] showed that the hotspots cause permanent damage in CIGS solar cells, identifying the formation of cracks and voids at the layer interfaces due to local heating. Nardone *et al.* [7] investigated the temperature increase of CIGS solar cells caused by partial shading through FEM simulations. Their simulation results showed that the temperature of CIGS cells could reach up to ~700 K after 600 seconds operation with 20% shading. Kim *et al.* [8] simulated the residual stress of active layers of CIGS solar cells by heating and then cooling the cells to room temperature. However, since their simulated solar cell is composed of only three active layers (ZnO, CdS, and CIGS), it is not possible to find out the effect of the Mo layer and substrate on the residual stress of CIGS solar cells.

In this paper, we investigated the effect of layer thickness on the residual stresses of CIGS thin film solar cells using FEM simulations caused by cooling to room temperature from CIGS deposition at 400°C as well as hotspot temperatures of 200°C, 300°C, and 400°C. We varied the thickness of the ZnO (200 - 600 nm), CdS (50 - 70 nm), CIGS (0.5 - 3 μm), Mo (0.5 - 1 μm), and PI (12.5 - 75 μm) layers for the simulations. Before simulating the residual stress of CIGS

cells due to a hotspot, we simulated the residual stress on the bottom three layers (PI, Mo, and CIGS) through depositing the CIGS layer at 400°C and cooling to room temperature. The residual stress after the CIGS deposition was used as initial stress for the hotspot simulation, which made our results more realistic. Quantitative analysis of the relationship between layer thickness and thermo-mechanical stress of thin film solar cells due to CIGS deposition and hotspots would be beneficial to the solar cell manufacturers for designing robust thin film solar cells.

2. Method

Simulation Procedure

The baseline model of a CIGS solar cell consists of an n-type ZnO (200 nm), n-type CdS (50 nm), p-type CIGS (0.5 μm), back contact Mo (0.5 μm), and PI substrate (75 μm). The p-type CIGS is the main PV layer. COMSOL Multiphysics software is used for finite element simulations because it can simulate thermal and stress analysis in the same framework. The detailed procedures of thermo-mechanical modeling and simulations of flexible solar cells can be found from our previous publication [8]. Theoretical equations to calculate thermal residual stress caused by temperature fluctuation are described as below.

$$\sigma = E\varepsilon \quad (1)$$

$$\varepsilon = \alpha(T - T_{ref}) \quad (2)$$

where σ : Thermal stress, E : Young's modulus, ε : Thermal strain, α : Thermal expansion coefficient, T : Temperature

Figure 1 shows the structure of the CIGS solar cell used for our simulations. The length of the solar cell was set to be 10 times larger than the thickness of the cell to prevent an edge effect from influencing overall stress.

Table 1 illustrates the properties of each layer for thermo-mechanical simulations. Most of the properties are obtained from published values. For all of our thermo-mechanical simulations, a 2D plane-stress assumption is used and each layer is assigned as a linear elastic material.

First, we simulated the effect of each layer's thickness for the bottom 3 layers (CIGS, Mo, and PI) on the residual stress of CIGS solar cells caused by cooling to room temperature from CIGS deposition at 400°C. Variations of each layer thickness of CIGS solar cells are described as below.

Table 1. Properties of each layer for thermos-mechanical simulation of CIGS solar cell.

	CIGS	CdS	ZnO	Mo	PI
Young's modulus (GPa)	83.6 [3]	46 [9]	173 [10]	133 [3]	9.1[3]
Density (g/cm ³)	5.9 [2]	4.8 [2]	5.6 [2]	10.2 [2]	1.5 [2]
Thermal expansion coefficient (10 ⁻⁶ K ⁻¹)	7.9 [3]	4.5 [2]	3.8 [2]	5.9 [3]	12 [3]

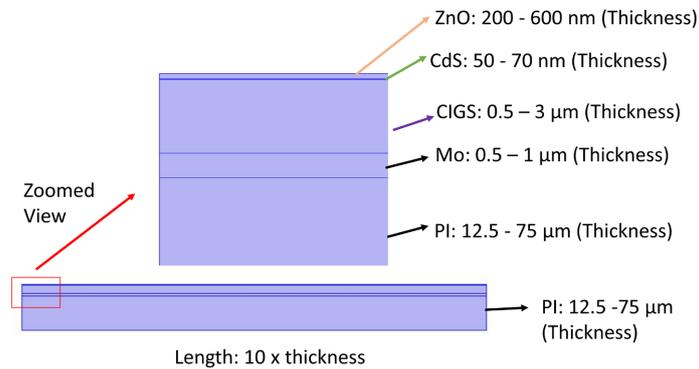


Figure 1. CIGS solar cell dimension.

- CIGS: 0.5 - 3 μm with 0.5 μm increments
- Mo: 0.5 - 1 μm with 0.1 μm increments
- PI: 12.5 - 75 μm at (12.5, 20, 40, 60, 75)

Second, we simulated the effect of each layer's thickness on the residual stress of CIGS solar cells caused by heating and then cooling to room temperature from a hotspot temperature of 400°C. Variations of each layer thickness of CIGS solar cells are described as below.

- ZnO: 200 - 600 nm with 100 nm increments
- CdS: 50 - 70 nm with 5 nm increments
- CIGS: 0.5 - 3 μm with 0.5 μm increments
- Mo: 0.5 - 1 μm with 0.1 μm increments
- PI: 12.5 - 75 μm at (12.5, 20, 40, 60, 75)

Then, we repeated the above simulations with different hotspot temperatures (200°C and 300°C) to analyze the effect of hotspot temperatures on the residual stress of CIGS solar cells. In order to get more realistic stress values caused by hotspots, we used the residual stress from the CIGS deposition at 400°C as an initial stress for the hotspot simulation. The maximum dimension of the simulated 2D CIGS solar cell is 79.67 μm by 796.7 μm. In general, the real size (diameter) of hot spot is larger than millimeters (mm) [11]. When we ran hotspot simulations, we assumed that the entire simulated CIGS cell undergoes hotspot since the dimension of the simulated cell is smaller than the general hotspot size (larger than mm), which represents the worst case scenario.

3. Results and Discussion

3.1. Effect of Layer Thickness on the Internal Stress Caused by CIGS Deposition

Figure 2 shows the stress distribution of a CIGS model consisting of PI, Mo and CIGS after depositing a CIGS layer at 400°C and cooling to room temperature. The overall dimension of the model is 76 × 760 μm consisting of 75 μm PI, 0.5 μm Mo, and 0.5 μm CIGS (Base model thickness). However, for a clearer visualization, **Figure 2** shows the stress distribution in a smaller area (5 × 6 μm). Negative values represent compressive stress while positive values represent

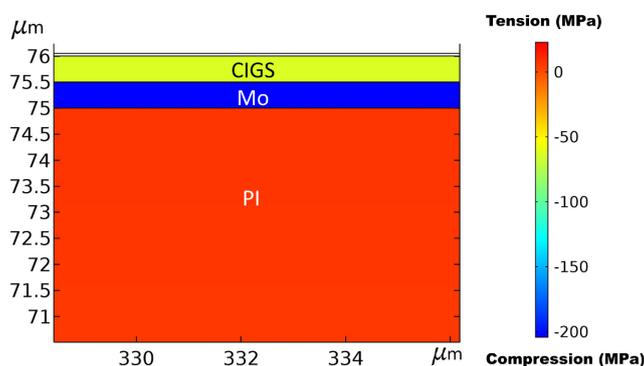


Figure 2. Stress distribution of a CIGS cell consisting of PI, Mo, and CIGS after depositing CIGS layer at 400°C and cooling down to room temperature. For a clear visualization, the stress distribution in a small area ($5 \times 6 \mu\text{m}$) is illustrated.

tensile stress. From the simulation results, it was found that the average stress of PI is 1.71 MPa (Tension), 197 MPa (Compression) for Mo, and 60 MPa (Compression) for CIGS. The magnitude of the simulated CIGS stress (60 MPa) is reasonably close to the experimental results (62 - 72 MPa) by Lin *et al.* [3]. Compared to Lin *et al.* [3], in this paper, we also tried to quantify the magnitude of residual stresses when CIGS solar cells undergo hotspot (partial shading) after the initial CIGS deposition process.

Figures 3(a)-(c) illustrate the effect of CIGS, Mo, and PI layer thickness on the residual stress after cooling to room temperature from a CIGS deposition at 400°C. In **Figures 3(a)-(c)**, it is difficult to identify the stress change of the PI layer due to change of each layer thickness, so we replotted the average stress of PI layer in **Figure 3(d)**. For **Figure 3(d)**, Logarithmic scale is used for x axis since the scale of PI thickness is different from that of CIGS and Mo.

Figure 3(a) and **Figure 3(b)** illustrate that the compressive stress of the CIGS and Mo layer decreases as the thickness of the CIGS and Mo layer increases. On the contrary, **Figure 3(c)** demonstrates that the compressive stress of the CIGS and Mo layer increases as the PI layer thickness increases. However, when the PI layer thickness is less than $\sim 17 \mu\text{m}$, the CIGS layer undergoes tensile stress. Salari *et al.* [12] observed that tensile stress is beneficial to improve the performance of organic solar cells. Moreover, as mentioned earlier, Garcia *et al.* [4] observed that the performance of CIGS solar cells was improved by applying tensile stress. Based on Salari *et al.* [11] and Garcia *et al.* [4], reducing PI layer thickness less than $17 \mu\text{m}$ can improve the performance of CIGS solar cells by nullifying the compressive residual stress in the CIGS absorber layer. Because of the fact that: 1) The thermal coefficients of CIGS and Mo are close to each other (5.9 and $7.9 \text{ E}10^{-6} \text{ K}^{-1}$), compared to that of PI layer ($12\text{E}10^{-6} \text{ K}^{-1}$) and 2) The thickness of the PI layer is significantly larger than those of CIGS and Mo combined, CIGS and Mo layers behave similarly competing against the PI layer. We can clearly observe that the effect of PI layer thickness ($12.5 - 75 \mu\text{m}$) is more significant than those of CIGS and Mo layer thickness ($0.5 - 3 \mu\text{m}$) to reduce the residual stress of CIGS solar cells as shown in **Figures 3(a)-(c)**.

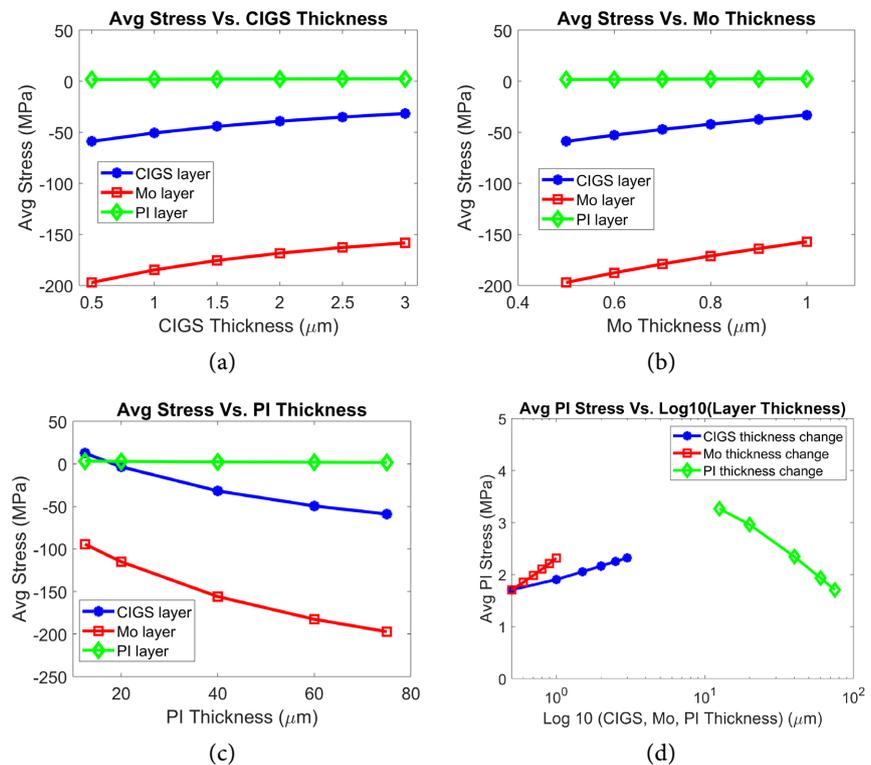


Figure 3. (a) Effect of CIGS layer thickness on the residual stress after CIGS deposition; (b) Effect of Mo layer thickness on the residual stress after CIGS deposition; (c) Effect of PI layer thickness on the residual stress; (d) Effect of each layer thickness on the residual stress of PI.

3.2. Effect of Layer Thickness on the Internal Stress of the PI Layer Caused by a Hotspot

First, we simulated the effect of layer thickness on the internal stress of the PI layer after heating and then cooling to room temperature from the hotspot temperatures of 200°C, 300°C, and 400°C. The dimensions of a baseline model are $76.25 \times 762.5 \mu\text{m}$ consisting of 75 μm PI, 0.5 μm Mo, 0.5 μm CIGS, 0.05 μm CdS, and 0.2 μm ZnO (Base model thickness). **Figures 4(a)-(d)** show that the PI layer goes through tensile stress when the CIGS cell is cooled down to a room temperature from a hotspot. Moreover, they confirm that a higher hotspot temperature produces a larger tensile stress in the PI layer. **Figure 4(a)** illustrates the effect of ZnO layer thickness on the average stress of the PI layer at different temperatures. It demonstrates a proportional relationship between PI stress and ZnO thickness. **Figure 4(b)** illustrates that CdS layer thickness ranging from 50 - 70 nm hardly influences the internal stress of the PI layer. Moreover, **Figure 4(c)** and **Figure 4(d)** show that the increase of both the CIGS and Mo layer thickness results in an increase of internal stress in the PI layer.

3.3. Effect of Layer Thickness on the Internal Stress of the Mo Layer Caused by a Hotspot

We simulated the effect of layer thickness on the internal stress of the Mo layer

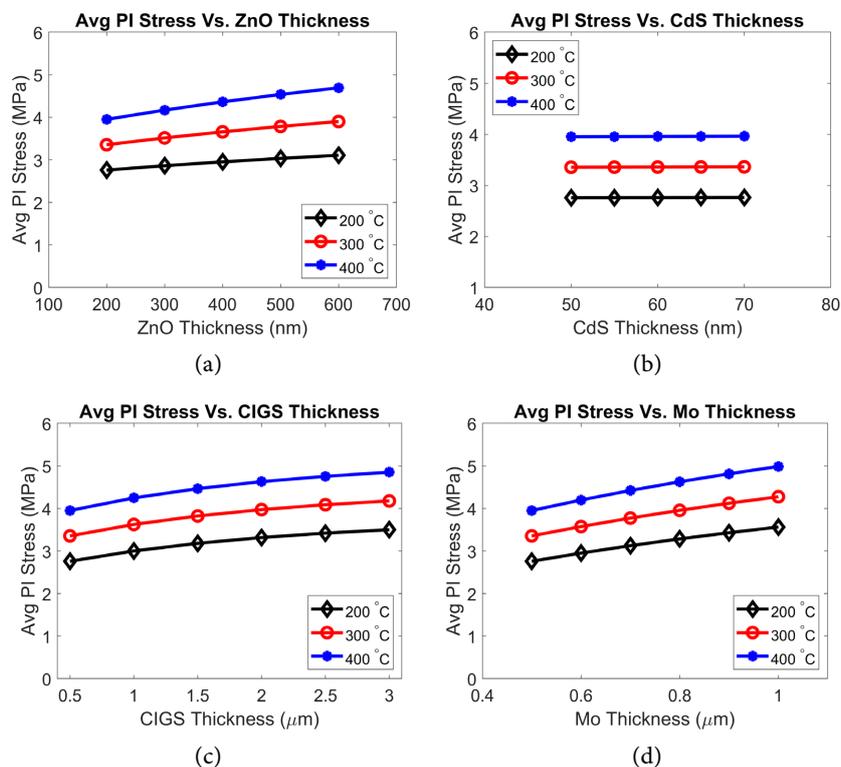


Figure 4. (a) The effect of ZnO layer thickness on average stress of PI layer due to different hotspot temperatures; (b) The effect of CdS layer thickness on average stress of PI layer due to different hotspot temperatures; (c) The effect of CIGS layer thickness on average stress of PI layer due to different hotspot temperatures; (d) The effect of Mo layer thickness on average stress of PI layer due to different hotspot temperatures.

after heating and then cooling to room temperature from the hotspot temperatures of 200°C, 300°C, and 400°C. **Figures 5(a)-(d)** show that the Mo layer goes through compressive stress ranging from 100 - 400 MPa when the CIGS cell is cooled down to room temperature, confirming that a higher hotspot temperature is more damaging to solar cells. **Figure 5(a)** shows the effect of ZnO layer thickness on the average stress of the Mo layer at different hotspot temperatures. It demonstrates that the increase of ZnO thickness results in a decrease of compressive stress in the Mo layer. **Figure 5(b)** shows that a CdS layer thickness ranging from 50 - 70 nm hardly influences the stress of the Mo layer. **Figure 5(c)** shows the increase of CIGS layer thickness reduces the stress of the Mo layer. In contrast, **Figure 5(d)** illustrates that the increase of PI thickness increases the stress of the Mo layer. In addition, it is observed that the effect of temperature is more significant at larger PI thicknesses for the stress of the Mo layer.

3.4. Effect of Layer Thickness on the Internal Stress of the CIGS Layer Caused by a Hotspot

Figures 6(a)-(d) show the effect of layer thickness and hotspot temperatures on the internal stress of the CIGS layer after cooling down to room temperature

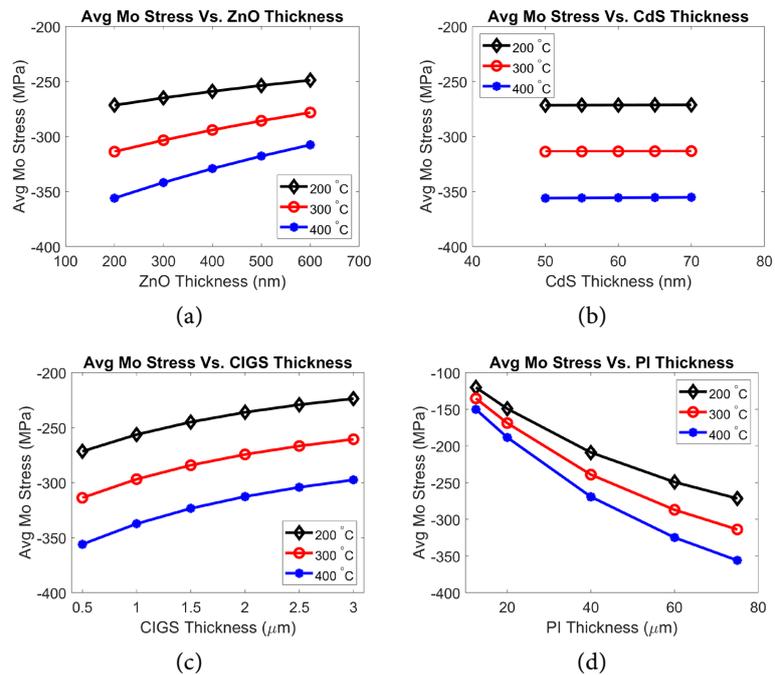


Figure 5. (a) The effect of ZnO layer thickness on average stress of Mo layer due to different hotspot temperatures; (b) The effect of CdS layer thickness on average stress of Mo layer due to different hotspot temperatures; (c) The effect of CIGS layer thickness on average stress of Mo layer due to different hotspot temperatures; (d) The effect of PI layer thickness on average stress of Mo layer due to different hotspot temperatures.

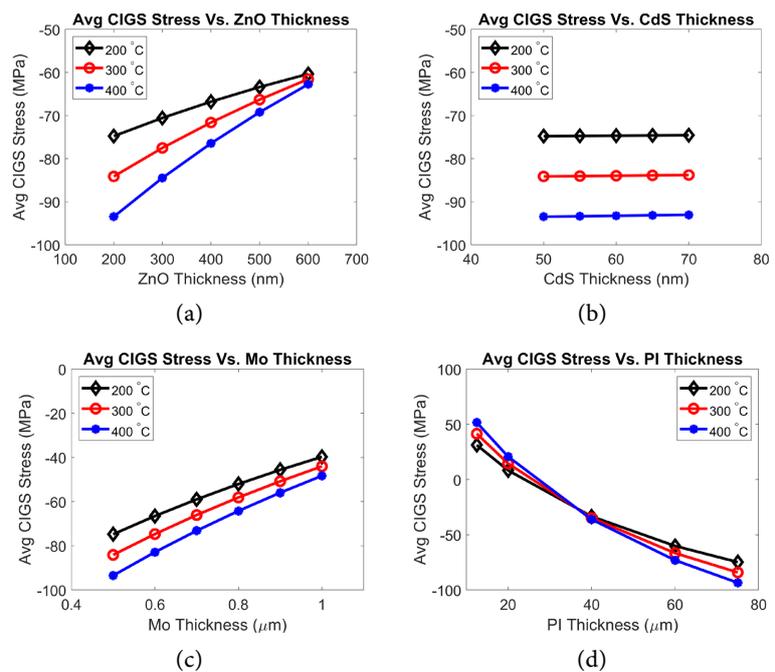


Figure 6. (a) The effect of ZnO layer thickness on average stress of CIGS layer due to different hotspot temperatures; (b) The effect of CdS layer thickness on average stress of CIGS layer due to different hotspot temperatures; (c) The effect of CIGS layer thickness on average stress of CIGS layer due to different hotspot temperatures; (d) The effect of PI layer thickness on average stress of CIGS layer due to different hotspot temperatures.

from a hotspot. Most of the time, the CIGS layer goes through compressive stress, but it undergoes tensile stress when the PI thickness is less than ~ 20 μm . Generally, the higher the hotspot temperature, the more damaging it is to the cell. **Figure 6(a)** shows that increasing the thickness of the ZnO layer mitigates the stress of the CIGS layer. Moreover, the effect of temperature diminishes as the ZnO thickness increases. **Figure 6(b)** shows that the thickness of CdS ranging from 50 - 70 nm has a negligible effect on the stress of the CIGS layer. **Figure 6(c)** illustrates that the stress of the CIGS layer decreases as the thickness of the Mo layer increases. On the contrary, **Figure 6(d)** demonstrates that the compressive stress of the CIGS layer increases as the PI layer thickness increases. However, it is interesting to see that when the PI layer thickness is less than ~ 20 μm , the CIGS layer undergoes tensile stress and the tensile stress decreases as the PI layer thickness increases. This finding reveals that manufacturers of CIGS solar cells can control the stress type (tensile vs. compressive) and the magnitude of the stress in the CIGS layer by manipulating PI thickness and applying heat to the CIGS cell (*i.e.* annealing).

3.5. Effect of Layer Thickness on the Internal Stress of the CdS Layer Caused by a Hotspot

We simulated the effect of layer thickness on the internal stress of the CdS layer after heating and then cooling to room temperature from the hotspot temperatures of 200°C, 300°C, and 400°C. **Figures 7(a)-(d)** show that the CdS layer goes through compressive stress ranging from ~ 10 - ~ 100 MPa when the CIGS cell is cooled down to room temperature from a hotspot. Again, they also confirm the general trend related to the temperature effect: The higher the hotspot temperature, the more damaging it is to the cell. **Figures 7(a)-(c)** show that the stress of the CdS layer decreases as the thickness of the ZnO, CIGS, and Mo layers increase. However, in **Figure 7(d)**, the stress of the CdS layer increases as the thickness of the PI layer increases.

3.6. Effect of Layer Thickness on the Internal Stress of the ZnO Layer Caused by a Hotspot

The effect of layer thickness on the internal stress of the ZnO layer after heating and cooling to room temperature from the hotspot temperatures of 200°C, 300°C, and 400°C were investigated. **Figures 8(a)-(d)** show that the ZnO layer goes through compressive stress ranging from ~ 100 - ~ 400 MPa when the CIGS cell is cooled down to room temperature from a hotspot. Again, they also confirm the general trend of the temperature effect: The higher the hotspot temperature, the more damaging it is to the cell. **Figure 8(a)** shows that CdS layer thickness ranging from 50 - 70 nm hardly changes the average stress of the ZnO layer. **Figure 8(b)** and **Figure 8(c)** show that as the thickness of the CIGS and Mo layer increases, the average stress of the ZnO layer decreases. However, **Figure 8(d)** illustrates that the increase of PI thickness results in an increase of the stress in the ZnO layer.

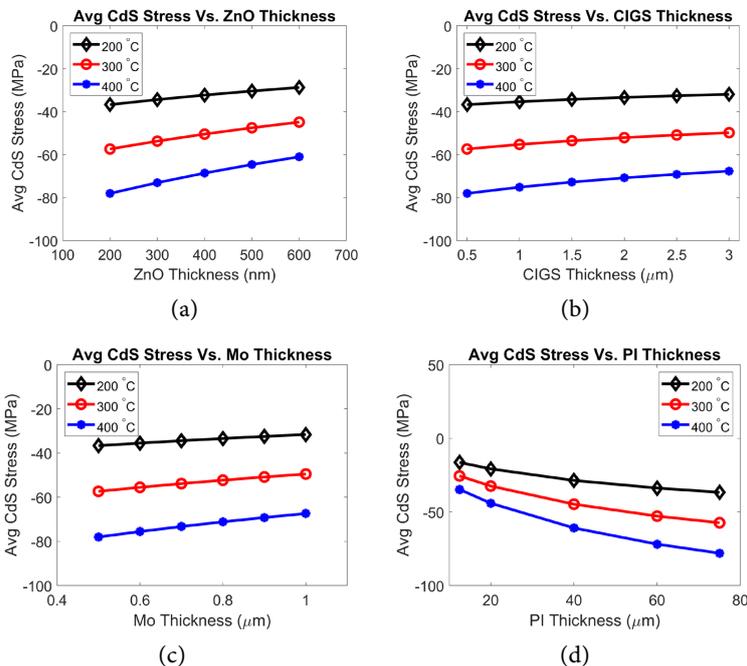


Figure 7. (a) The effect of ZnO layer thickness on average stress of CdS layer due to different hotspot temperatures; (b) The effect of CIGS layer thickness on average stress of CdS layer due to different hotspot temperatures; (c) The effect of Mo layer thickness on average stress of CdS layer due to different hotspot temperatures; (d) The effect of PI layer thickness on average stress of CdS layer due to different hotspot temperatures.

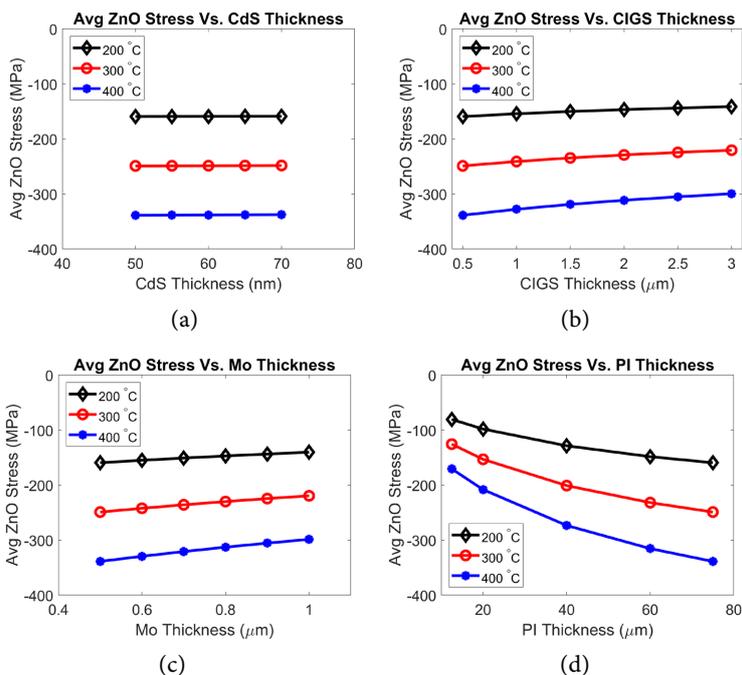


Figure 8. (a) The effect of CdS layer thickness on average stress of ZnO layer due to different hotspot temperatures; (b) The effect of CIGS layer thickness on average stress of ZnO layer due to different hotspot temperatures; (c) The effect of Mo layer thickness on average stress of ZnO layer due to different hotspot temperatures; (d) The effect of PI layer thickness on average stress of ZnO layer due to different hotspot temperatures.

4. Conclusions

High temperatures caused by CIGS deposition and hotspots can result in a significant thermal stress in a solar cell through thermal expansion mismatch between solar cell layers. We investigated the effect of layer thickness on the internal stress of CIGS solar cells with a PI substrate through heating and then cooling to room temperature from CIGS deposition at 400 °C as well as hotspot temperatures of 200 °C, 300 °C, and 400 °C with FEM simulations. We quantitatively analyzed the relationship between the layer thickness and internal stress caused by a CIGS deposition as well as hotspot. Unlike our previously published thermo-mechanical modeling of CIGS cells, since the proposed CIGS solar cell in this research is composed of ZnO, CdS, CIGS, Mo (back contact), and PI (substrate), we were able to quantify the effect of Mo and PI thickness on the internal stress of CIGS cells.

From the simulation results, we found that

1) The PI substrate layer has the most significant effect on the residual stress of CIGS solar cells since it has the largest thickness as well as the largest thermal expansion coefficient.

2) As the thickness of PI layer increases, the stresses of other layers increase.

3) Changes in the Mo, CIGS, and ZnO layers show competing effect against the PI layer but increases of thickness for those layers result in a general decrease of internal stresses.

4) The residual stress of the CIGS layer can be removed by changing the thickness of the PI substrate and applying heat to the CIGS cell. Especially, fabricating PI layer thickness less than 17 μm can improve the performance of CIGS solar cells by nullifying the compressive residual stress in the CIGS absorber layer.

5) Since the CdS layer ranges from 50 - 70 nm, it hardly changes the internal stress of the CIGS solar cell since the thickness variation is very small compared to other layers.

Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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