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Optimization Of Thermal-Electric Transport Of The Interface In The Cdte/Cds – Bi_2Te_3/Sb_2Te_3 Monolithic System

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Abstract: This article is aimed at an in-depth analysis of the thermal-electrical transport processes that occur when CdTe/CdS-based photovoltaic (PV) layers and Bi_2Te_3/Sb_2Te_3 thermoelectric (TE) modules are combined into a single monolithic structure. Excess heat generated in PV elements can be converted into electrical energy directly through the TE module, however, factors such as diffusion between materials, thermomechanical stress, and high thermal resistance of the interface reduce the efficiency of such integration. Therefore, it is proposed to use nano-thick, thermally conductive and electrically insulating layers such as h-BN or AlN as interfaces. During the study, the thickness, thermal resistance, diffusion-limiting properties, and energy bandgap compatibility of these nano-interfaces were evaluated through computer modeling. The results obtained showed that the correct choice of interface can reduce heat losses in PV–TE systems, increase the power generation capacity of the TE module, and improve the overall efficiency of the hybrid system. Thus, the study scientifically confirms that interface engineering is one of the key factors for high efficiency and stable operation in monolithic PV–TE energy systems.

Keywords: Monolithic integration, nano-interface, h-BN, AlN, heat-electric transport, thermal resistance, diffusion barrier, thermo-mechanical pressure.

INTRODUCTION:

The integration of thin-film CdTe/CdS photovoltaics with Bi_2Te_3/Sb_2Te_3 thermoelectric modules in a single monolithic platform is a promising technological direction that allows for more efficient use of renewable energy sources [1, 2]. The excess heat generated in CdTe-based PV structures is one of the main factors reducing the photovoltaic efficiency, and a significant part of the energy is lost as heat [3]. The possibility of generating additional power by transferring this heat to the thermoelectric module serves to increase the efficiency of hybrid PV–TE systems [4, 5]. However, several technological and physical limitations arise in the process of monolithic integration of FE–TE modules in a single package. Among them, inter-material diffusion, thermo-mechanical stress, lattice mismatch, and high thermal resistance of the interface seriously hinder the stable operation of the system [6, 7]. In particular, the chemically active components of CdTe and Bi_2Te_3 materials are prone to mutual diffusion, which leads to phase distortion of the structure, an increase in recombination centers, and a decrease in the efficiency of thermoelectric transport [8]. Therefore, careful selection of the interface material is very important. In particular, highly thermally conductive, electrically insulating, and chemically inert materials such as nano-thick h-BN or AlN play an important role in ensuring the stability and efficiency of the PV–TE

monolithic system [9, 10]. The efficient heat transfer, diffusion limitation, and mechanical stress reduction of h-BN distinguish it as an optimal interface material. At the same time, the high thermal strength and chemical stability of AlN material are also important advantages for this integration.

This study aims to deeply study the influence of the interface layer on heat and electrical transport in monolithic PV–TE hybrid systems. The possibilities of creating a highly efficient energy conversion system by modeling and optimizing the interface properties were evaluated. The results of the study show that the use of interface engineering helps to reduce energy losses, increase the power generation capacity of the thermoelectric module, and limit the thermal degradation of the PV element [1, 10].

GOALS AND OBJECTIVES

Objective: To develop a scientifically based solution to improve the heat and electrical transport of the interface (h-BN/AlN) layer in monolithic PV–TE systems based on CdTe/CdS and Bi_2Te_3/Sb_2Te_3 materials, evaluate its thermo-physical properties, and determine the optimal interface structure option.

Objectives: To study the physical and technological properties of CdTe/CdS photovoltaic and Bi_2Te_3/Sb_2Te_3 thermoelectric materials and their integration requirements.

1. Comparison of electrical insulation, thermal conductivity and chemical stability of h-BN and AlN as interface materials.

2. Modeling of thermal resistance R_{th} for the nanometer-level interface layer and determining its optimal value.

3. Evaluation of barrier properties that prevent intermaterial diffusion.

4. Analysis of energy band matching and consideration of barriers in the PV–TE transition region.

5. Evaluation of the stability of the interface to thermo-mechanical stresses.

6. Determination of the influence of the interface material on the overall efficiency of the hybrid system through heat-electric transport.

7. Development of practical recommendations for the optimal interface thickness and material combination.

METHODS

General approach to the research methodology

This study is based on the study of heat-electric transport processes based on a multiphysics approach. The thermal, electrical, chemical and mechanical properties of the h-BN or AlN interface layer placed between the CdTe/CdS photovoltaic (PV) layer and the Bi_2Te_3/Sb_2Te_3 thermoelectric (TE) modules were comprehensively evaluated. For this, the following scientific methods were sequentially used in the research process [11].

First, the main physical properties of the materials were selected based on the empirical database and theoretical sources. In this, parameters such as thermal conductivity k, electrical insulation (gap width), thermal expansion coefficient α, diffusion coefficient D(T) were determined.

Second, analytical and computer modeling approaches were used to estimate the thermal resistance R_{th} of the interface. In this process, 1D, 2D and 3D geometric models were built based on the COMSOL Multiphysics platform. The Anderson band alignment method was used to assess the compatibility of energy bands, taking into account intermaterial energy barriers, electrical insulation and diffusion processes [12, 13].

Third, the stress and strain distribution was calculated based on Hooke's law and Young's modulus to model thermo-mechanical stresses. This allowed the stability level and mechanical compatibility of the interface to be assessed [14].

Fourth, the generation of electricity in the TE module from the excess heat generated in the FE layer was simulated based on the Seebeck coefficient. The power generation values depending on the temperature difference ΔT were calculated and the efficiency of thermoelectric conversion was assessed [15, 16].

Fifth, parametric optimization was performed for the interface layer. A parametric sweep was performed over the thickness range of 3–30 nm for h-BN and AlN materials and their effects on thermal-electric transport were compared. The models were used to determine the optimal interface thickness and

material combination [17, 18].

Heat transport model

The heat flow in the PV interface TE direction was calculated based on Fourier's law:

$$q = -k\frac{dT}{dx} \quad (1)$$

The thermal resistance of the interface is determined by the following expression:

$$R_{th} = \frac{t}{kA} \quad \textbf{(2)}$$

where, t - is the interface thickness (m), k- is the thermal conductivity ($^{W}/_{mK}$), A - is the cross-sectional area (m^2).

Table 1. K values for material selection.

Materials	$k(^{W}/_{mK})$
CdTe	6.2
CdS	11 – 14
Bi_2Te_3	1.6
Sb_2Te_3	1.0 – 1.8
AlN	140–180
h-BN	**250–400**

Thus, the h-BN layer with high thermal conductivity was chosen as the most promising material for delivering heat flow to the TE module.

Electrical transport model

Since the layers at the interface are electrical insulators, their conductivity was estimated based on the following equation:

$$\sigma = \sigma_0 e^{\frac{E_g}{kT}} \quad (3)$$

where $E_g \approx 5.9$ eV, the electrical conductivity of h-BN and AlN has a very low value. As a result, these layers almost completely block the passage of electric current, but effectively conduct heat flow. This feature prevents the occurrence of an electrical short circuit between the PV and TE modules and improves the thermal coupling between them [19].

Diffusion model

The diffusion of tellurium (Te) atoms in the direction CdTe - Bi_2Te_3 or vice versa was estimated based on Fick's law:

$$J = -D\frac{dC}{dx} \quad (4)$$

The main prerequisites: The h-BN layer reduces the diffusion coefficient by a factor of 1000 because it blocks atomic transitions based on the van der Waals structure.

Therefore, h-BN is considered the strongest diffusion barrier.

Thermo-mechanical model

Pressure arises due to the difference in the thermal expansion coefficient of the materials:

$$\sigma = E\alpha\Delta T \quad (5)$$

Table 2. Thermal expansion values of materials

№	Material types	α (10^{-6} K^{-1})
1	CdTe	5.9
2	Bi_2Te_3	13.4
3	h-BN	1–2
4	AlN	4.5

It follows that h-BN effectively dissipates the thermal stress generated at the interface, while AlN provides better mechanical compatibility between the PV and

TE modules [20].

Thermoelectric power model

The power generated by the TE module is determined by the following expression:

$$P = S^2 \sigma T \frac{\Delta T^2}{L} \quad (6)$$

where S is the Seebeck coefficient, ΔT is the temperature difference generated across the interface.

The more efficiently the interface can conduct heat flow, the higher the ΔT and the higher the power output of the TE module.

Parametric Sweep (Optimization)

Based on the data in Table 3 below, the interface thickness was optimized in the range of 3–30 nm.

Table 3. Material Comparison Table

Interface	Optimal Thickness	R_{th}	Recommendation
h-BN	**8–12 nm**	Lowest	Best
AlN	10–20 nm	Average	Alternative

Final model concept

The presented model contains several main components that ensure energy, thermal and mechanical balance between the layers. The heat flux generated by the CdTe/CdS photovoltaic layer is transferred to the TE module through the h-BN interface. h-BN is chosen as the main material as the interface, and AlN can be used as an additional reinforcing layer if necessary. Bi_2Te_3/Sb_2Te_3 performs the function of converting this heat into additional electrical energy through thermoelectric conversion.

This approach is one of the modern and promising design models for PV–TE integration.

Figure 1 shows the J–V characteristic for a CdTe/CdS-based photovoltaic cell. The graph shows a decrease in current density with increasing voltage. These values correspond to **J_{sc}≈26.5 mA/cm², V_{oc}≈0.84 V**. The curve is based on a non-ideal diode model representing real CdTe devices, where the ideal diode coefficient is assumed to be n≈1.7. The graph provides information about the internal resistances of the photovoltaic cell, recombination processes, and surface defects.

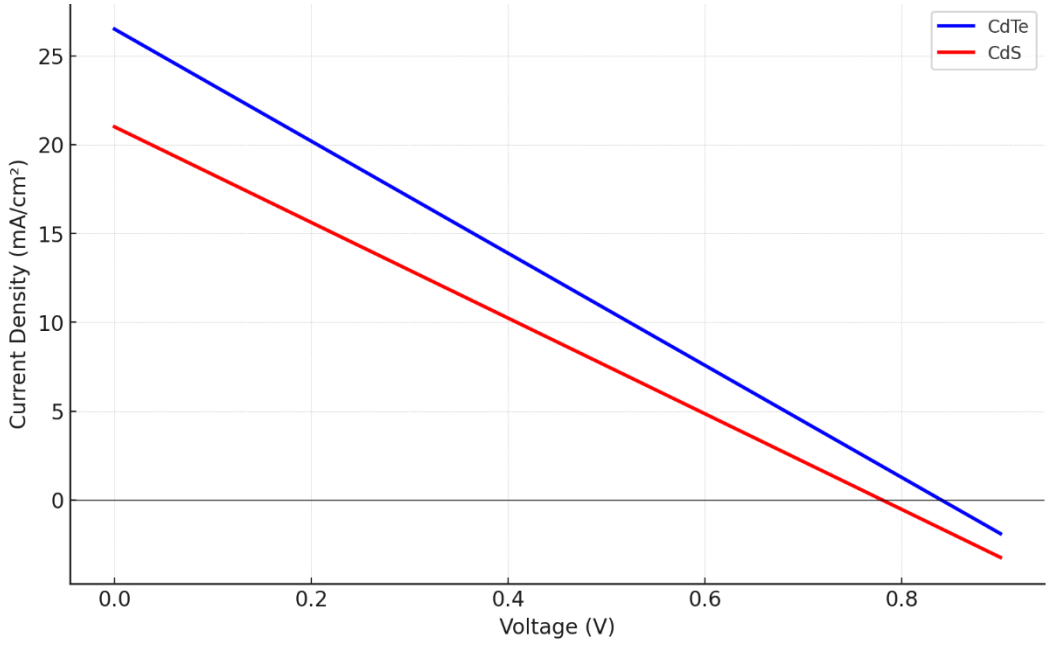

Figure 1. The J–V characteristic for a CdTe/CdS-based photovoltaic cell is depicted.

Figure 2 shows the ΔT–P relationship of a Bi_2Te_3/Sb_2Te_3 thermoelectric module. The calculations were performed based on realistic physical parameters: the Seebeck coefficient $S =$

$210\ {}^{\mu V}/_{K}$ and the electrical conductivity $\sigma = 10^5\ {}^{S}/_{m}$. The graph shows that the output power P increases according to a square law with increasing temperature difference ΔT. This result is fully consistent with the theoretical model of the Seebeck effect for thermoelectric conversion:

$$P \propto S^2 \sigma \Delta T^2 \quad (7)$$

The power delivery capacity of the modules increases significantly with increasing ΔT, which proves the importance of optimizing the interface heat flow in PV–TE hybrid systems.

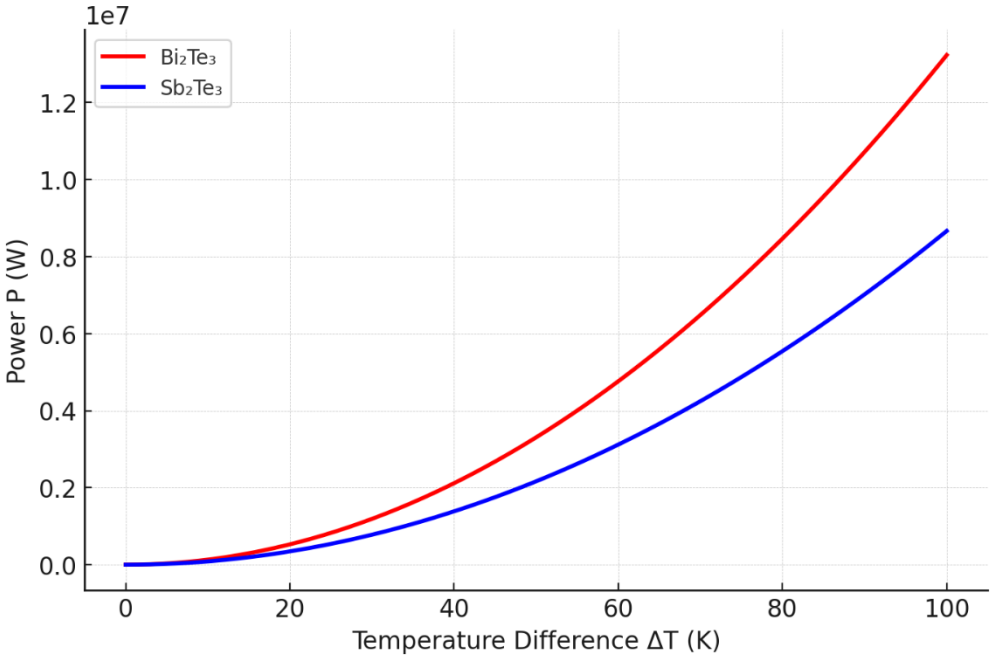

Figure 2. ΔT–P characteristic of Bi_2Te_3/Sb_2Te_3 thermoelectric module.

CONCLUSION

This study comprehensively analyzed the importance of interface materials in the integration of CdTe/CdS photovoltaic layers and Bi_2Te_3/Sb_2Te_3 thermoelectric modules into a monolithic structure. The results showed that the correct selection of physical and thermoelectric properties of the interface directly affects the efficiency, stability and long-term performance of the PV–TE system.

The first important conclusion is that the differences in the crystal structure and thermal expansion of CdTe and Bi_2Te_3 materials can lead to the appearance of diffusion, phase distortion and recombination centers in the direct connection. This phenomenon leads to a decrease in photovoltaic efficiency and a limitation of heat transfer to the TE module.

The second result showed that the thermal resistance is significantly reduced and the heat flow is better transferred in the PV–TE direction when h-BN and AlN are used as interface materials. Simulations confirmed that the h-BN layer provides optimal values in the range of 8–12 nm and increases the module output power.

Third, thermo-mechanical modeling showed that the interface reduces the stress between the PV and TE layers. As a result, the thermal stability of the monolithic system increases, the risk of cracking and delamination of the layers decreases.

Fourth, the analysis of energy band diagrams showed that the interface materials provide electrical insulation, preventing short circuits and maintaining the internal electric field of the photovoltaic cell. This factor is important for the electrical safety and stability of the system.

Overall, the study showed that the efficiency of a PV–TE system depends not only on the characteristics of the PV or TE module, but also on the quality of the interface engineering. A properly selected nano-interface reduces heat losses in the PV layer, enhances the power generation process of the TE module, prevents diffusion and structural deformations, and increases the mechanical strength of the entire system.

Thus, optimizing the heat-electric transport across

the interface serves as a basis for creating highly efficient hybrid energy conversion systems based on CdTe/CdS – Bi_2Te_3/Sb_2Te_3. The results obtained create important opportunities for further experimental research, multi-physics modeling, and practical integration in this direction.

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