Indian Institute of Engineering Science And Technology

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ABSTRACT

In recent microprocessors or ASIC chips, the operating frequency is set by the target market.This leads to very tight timing and power constraints for the proposed circuit design. The industrial shift for adopting lower technology nodes also presents a new challenging frontier as transistors get less efficient as they undergo scaling. Analog designers are expected to optimize these conventional designs and yet meet the reduced power constraints and performance metrics imposed by various applications.

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Chapter 1

Introduction

The environmental impact of global warming has accelerated the interest to adopt non-conventional power generation [1]. There are several promising sustainable energy alternatives, among which the adoption of Thermoelectric (TE) materials to scavenge the by-product heat generation is widely accepted [1]. It is crucial for applications associated with energy harvesting to possess a high figure of merit ZT (≥ 1) [1].

The ZT can be related to other thermoelectric parameters by ZT $=(\frac{\sigma_e \times S_B^2 \times T}{\kappa_{ph}+\kappa_e})$, where σ, S_B, $\kappa_{ph} + \kappa_e$, and T are the electrical conductivity, Seebeck coefficient, total thermal conductivity, and temperature value respectively [1].

Experimental and theoretical identification of two-dimensional (2D) [1] or three-dimensional (3D) efficient TE materials is laborious and time inefficient [1]. It is also a colossal task to compile databases of thermoelectric parameters for various synthesized TE materials and their variations with doping (n-type or p-type) [1]. Computational methods using density functional theory (DFT) are also time-consuming and demand high computational complexity for exploring TE materials [1].

Efficient TE materials require a large ZT which in turn requires to maximize the Seebeck coefficient absolute value, minimize the thermal conductivity and possess a high electrical conductivity. Optimizing these parameters is a complicated task as they are inherently dependent and conflicting in nature [1]. Thus, optimizing AT requires a thorough understanding of these various transport properties and their interrelated material characteristics.

The Seebeck coefficient depends on this energy-dependent conductivity around a fermi window centered about the fermi energy level, which is given by the Mott expression (Eq. 1.1) [1].

$$S_B = \frac{\pi^2}{3}(\frac{{K_B}^2 \times T}{q})[\frac{d[ln(\sigma(E))]}{dE}]_{E=E_F} = (\frac{8\pi^2 {K_B}^2 T}{3qh^2})m_d^*(\frac{\pi}{3n})^{2/3} \tag{1.1}$$

where n is the carrier concentration and effective mass m_d^* of the carrier when present in the conduction band or valence band. This effective mass (m_d^*) is obtained from the function of the density of states (DOS) and is thus also known as m_{DOS}^* [1]. The underlying assumption for the final closed form expression is the presence of a parabolic band and an energy-independent scattering approximation [1]. The electrical conductivity (σ_e) can be approximated by the Drude model in terms of its carrier concentration (n) and mobility (μ) as shown in EQ. 1.3. Thus, the influence of carrier concentration impacts both the parameters contradictory as shown in Fig. 1.1.

Figure 1.1: Figure 1.1

$$\sigma_e = nq\mu = \frac{nq^2\tau}{m} \tag{1.2}$$

$$\kappa = \kappa_{ph} + \kappa_e = (\frac{\pi^2}{3})(\frac{nK_B^2 T\tau}{m}) + L_n \times \sigma_e T \tag{1.3}$$

$$L_n \approx (\frac{\pi^2}{3})(\frac{K_B}{q})^2 \tag{1.4}$$

1.1 Section 1.1

1.1.1 Sub-Section 1.1.1

Content.

1.1.2 Sub-Section 1.1.1

Content.

Table 1.1: Table Caption

Material	Crystal	Space Group	Bandgap(ev)	Direct / Indirect	$\kappa(Wm^{-1}k^{-1})$	$\sigma_e(\times 10^{-3}Scm^-1)$	ZT(10^{-4})
xxx	xxx	xxxxxx	YYYXXXX ZZZ exp. YYYexp. XXXexp,	Direct	ZZ exp,	YY exp,	XX exp,

Chapter 2

Chapter 2 Name

Table 2.1: Table Caption

Database	Crystal information	Mechanical parameters	Thermodynamic parameters	Electronic parameters
Database 1	Y	Y	Y	Y
Database 2	Y	Y	Y	Y
Database 3	Y	Y	Y	Y
Database 4	Y	Y	Y	Y
Database 5	Y	N	Y	Y

Chapter 3

Acknowledgement

I would like to acknowledge the financial assistance granted in support by the Ministry of Human Resource Development (MHRD), India. I would also like to take this opportunity to express my deep sense of gratitude and regard to XXXXXXXXXXXXXXX, Indian Institute of Engineering Science and Technology, Shibpur, for the continuous encouragement and able guidance. His insights and supervision were of immense value to me. I extend my profound thanks to the entire faculty of Electronics & Telecommunication for the knowledge and wisdom they bestowed on me.

References

[1] J. T. Shreeja Das, Santanu Mahapatra and D. Saha, “Machine learning assisted search of thermoelectic materials with enhanced power factor, figure of merit, and air stability.” *Workshop on Spintronics and Magnetism on 2D Materials, EPFL*, 23rd to 27th August 2021.

This is appendix A