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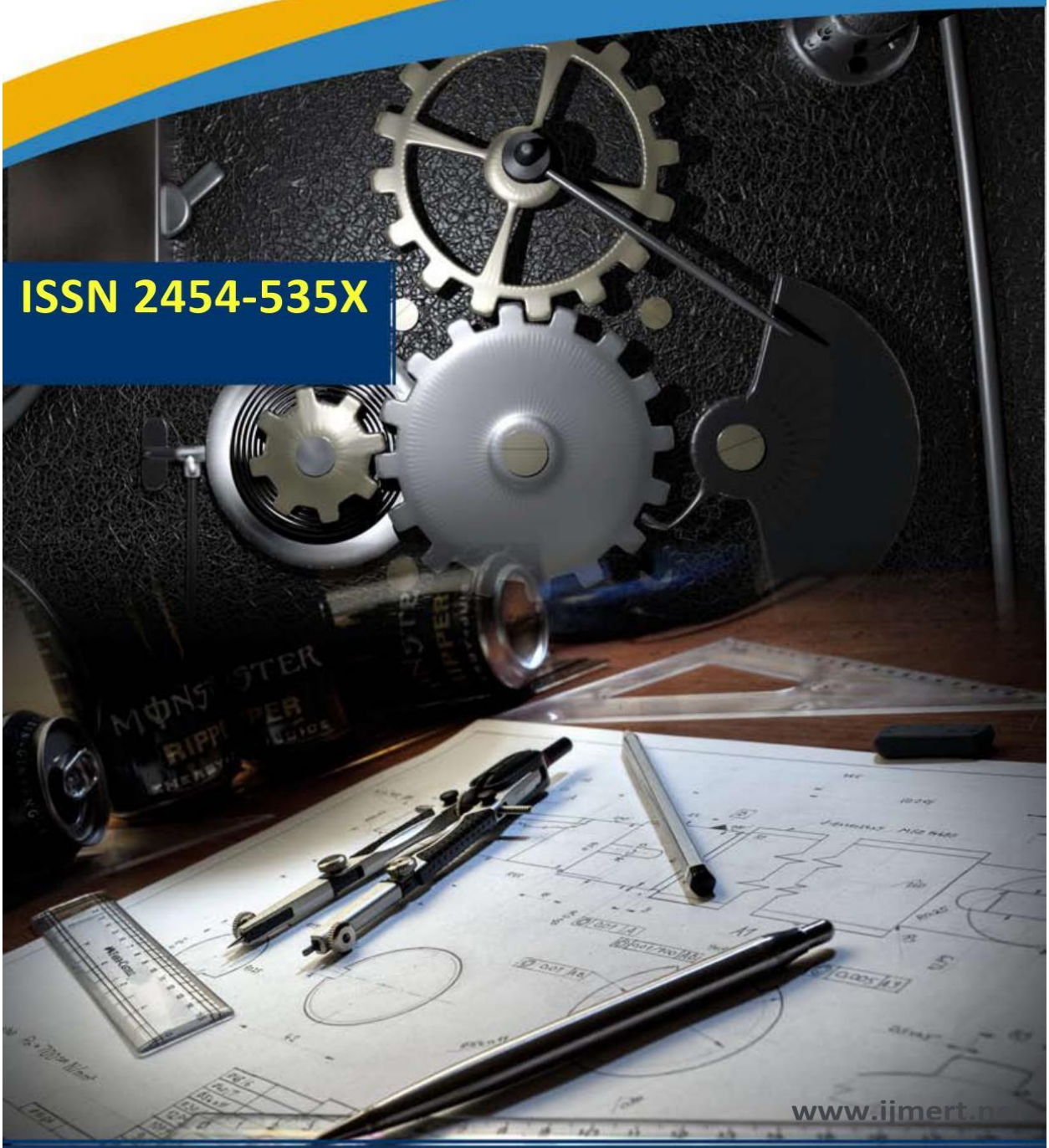

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The Comparison of Thermal Conductivity for Different Metals

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Table of Contents

Abstract

An important part of engineering properties, thermal conductivity consists of internal ability of material to transfer heat. It is a solid property in metals because of free electrons that help in proper thermal energy shift. When a material has low thermal conductivity, heat transfer takes place at a lower rate than a material with high thermal conductivity. For instance, metals can efficiently conduct heat with high thermal conductivity.

There have been a lot of studies conducted on electric conductivity of various materials, but there is a lack of research on thermal conductivity of various metals. This study is aimed to fill this gap by conducting a review of recent studies related to phonon and electron thermal conductivities of various metals because separating those

components is vital to understand the key mechanisms of heat transfer in metals and in various

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applications. It is inferred that phonon thermal conductivity is non-negligible in "transition-intermetallic-compounds (TICs)" and transition metals in comparison to noble metals because of high velocities of phonon group. In addition, the impact of coupling between phonon and electron on phonon conductivity in TICs is stronger than the coupling effect of nobles.
Keywords: thermal conductivity, heat transfer, electron, phonon, TICs, transition-intermetallic-compounds

1 Introduction

In any specific material, its thermal conductivity is related to the ability to conduct heat. Some elements present a low range of thermal conductivity when transferring the heat. In those cases, transferring heat takes place slowly. Generally, metals have high conductibility in terms of both heat and electricity. Hence, metals can display huge range of conductivity of heat. High conductivity of metals is emphasised by the aspect of having very high level of free electrons. Hence, heat conduction in the metals leads to electric conduction. Free electrons in them can move in the solid body freely and can transfer thermal energy at very high rate as compared to insulators. It is also worth noting that electrical conductors also show prime conductivity among the simplest metals. The level of thermal conductivity is similar to the electrical conductivity property. The electronic conduction and lattice are some of the important factors driving heat conduction rate which takes place in metals. The relation among thermal and electrical conductivity is assumed by "Wiedemann Franz law."

1.1 Background

Thermal conduction is categorized into different features, i.e., molecular vibrations in liquid and gaseous forms, lattice vibration of solids, as well as electrons in the metals. Metals have several processes of thermal conduction controlled by the collisions of molecules, electrons in gaseous form, and solid-state to process conduction related to lattice vibrations. Metals are best conductor of heat because of free electrons. Figure 1 illustrates factors responsible for metals' thermal conductivity.

Figure 1 – Factors responsible for thermal conductivity

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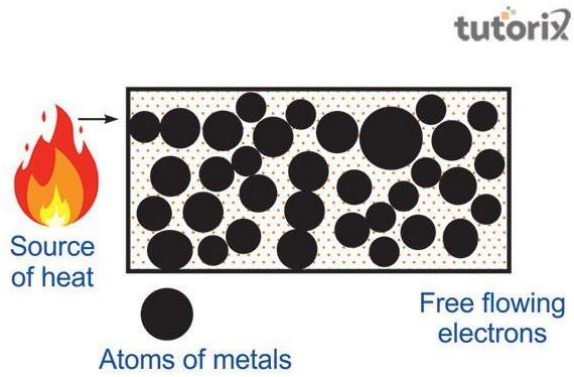
Vol. 15 Issue. 4, Dec 2023



Source – Tutorials Point

The free electrons in the material are the most vital factor playing a vital role in high metal conductivity. In the metal, the atoms can give out electrons that react chemically with several non-metals and are likely to form salts and oxides. Hence, the metal ions form cations. This bond makes metallic alloys and metal the best conductor of heat. The solids are likely to have several bonded electrons sharing valence electrons. A lot of conduction electrons can carry both electrical and heat charge with this aspect of electron sharing (Köbler, 2017). Hence, unlike electrons in covalent bonds, valence electrons in the metal can move without any barrier with lattice of metal and these electrons have heat without being restricted to atomic core.

In a lot of pure metals, the thermal conductivity of electron (κ_e) is supposed to be very large as compared to "thermal conductivity of phonon (κ_l). It is also evident that thermal conductivity of electron is relative to "electrical conductivity" or the "Wiedemann-Franz law" (Chester & Thellung, 1961). Hence, to estimate "electron thermal conductivity" in simple way, it is possible to measure electrical conductivity like "4-probe resistivity measurement" (Cahen et al., 1973) and "Wiedemann-Franz law" is employed for electron conductivity (Chester & Thellung, 1961). To further achieve "phonon thermal conductivity," it is possible to measure thermal conductivity and electron conductivity is calculated with electrical conductivity and difference can be associated with contribution to phonon (Makinson, 1938; Grüneisen & Reddemann, 1934; Kemp et al., 1955). Lorenz number should be fixed for applying the "Wiedemann-Franz law" which is considered as Sommerfeld value (Klemens & Williams, 1986). However, it is well regarded that Sommerfeld value relies on elastic scattering which is restricted to high or low temperature (Tritt, 2005).

International Journal of Mechanical Engineering Research and Technology
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www.ijmert.com
Vol. 10, Issue. 4, Dec 2023

1 Literature Reviews

Previous solutions were some of the attempts to find out the efficient thermal conductivity of varied materials. It was assumed that there is no thermal resistance among the stages in heterogenous materials. Later on, studies conducted on boundaries between solid and liquids found that a dip in temperature takes place when heat is flowing through a boundary among both stages and there is a need to include interfacial heat resistance. Pietrak & Wiśniewski (2015) review most valuable expressions to predict the right thermal resistance of composite items with volume and properties of essential stages.

Electronic cooling industries widely use thermal materials with solids of high heat conductivity and polymers. However, it is still important to predict proper heat conductivity of composites. Theoretical frameworks of thermal conductivity were mainly dependent on analogue between thermal and electric fields on composites. Xu et al. (2016) obtained current models using composite of conductor circuits and Laplace equation. By closely testing the former approach, it is found that there is a paradox. A statistical approach is used to solve the same. They first built a mesoscopic ensemble with microscopic conditions. The principle of least action was used to identify the thermal conductivities.

A lot of studies were conducted on technologies to store thermal energy as per "phase change materials (PCM)" due to their excellent control over thermal energy and their rise in effective use of energy. However, pure PCM cannot be used in some applications due to low heat conductivity like thermal control of clothes and devices. Cheng et al. (2021) conducted a review of recent advancements to improve thermal conductivity of PCM as per various nano-additives like "one-dimensional (1D), zero-dimensional (0D), 2-dimensional (2D), and three-dimensional (3D) nano-additives" apart from hybrid ones.

The "hexagonal boron nitride (h-BN)" is an ideal filler for polymers to make composite materials due to structural stability, high heat conductivity, and good anti-oxidant and mechanical properties. Several studies have found 2D with higher heat conductivity than bulk h-BM because of lower phonon to phonon scattering when reducing the material thickness.

Hence, 2D "boron nitride nanosheets (BNNS)" have been gaining prominence as they are applicable to design composite materials with best heat conductivity. Guerra et al. (2019) compared various synthesis methods used for BNNS as well as impact of BNNS dispersion on

ISSN 2454 – 535X
www.ijmert.com
Vol. 15 Issue. 4, Dec 2023

thermal conductivity of polymers.

Phase change technology for energy storage can fix contradiction of demand and supply of thermal energy to reduce power crisis. PCM has been used widely in thermal energy solutions because of significant stability of power output and high energy density. Wu et al. (2020) conducted a study on thermal conduction of phonons and morphology, thermal conductivity and preparation of composite PCMs. The mechanism used for phonon thermal conduction is recommended for "phonon-defect scattering, phonon-phonon scattering, and phonon-boundary scattering." Hence, they analysed microcosmic factors that may affect PCM thermal conductivity. They also reviewed recent developments of using 0D, 1D, 2D, and 3D structural additives.

1.1 Research Gap

A lot of theoretical analyses and experiments have been conducted to understand heat transfer in metals since the beginning of 20th century "(Makinson, 1938; Bidwell, 1940; Klemens, 1986; De Lang et al., 1978; Butler & Williams, 1978; Williams et al., 1981; Williams et al., 1982). These days, it has been observed that free electrons have played a dominant role in thermal transport of metals, while phonons are not contributing much. In a lot of applications, only total thermal conductivity is required. So, one cannot separate phonon and electron thermal conductivity. There has been a rise in interest when it comes to quantify conduction of temperature in metals, especially driven by recent technological advances in different processes. Hence, this study fills the gap by separating phonon and electron conductivity of metals, which enables researchers to conduct several theoretical and experimental studies.

1.2 Research Objective

- To predict mode-dependent phonon and electron thermal conductivity of various metals

2 Research Methodology

To fulfil the objectives of this study, secondary data has been collected from various relevant sources to find out recent developments in this field. Information has been collected from studies published in open-access journals to provide complete knowledge about the subject matter.

3 Analysis of Study

4

First of all, there is a need to estimate "phonon thermal conductivity" by keeping "phonon-phonon

International Journal of Mechanical Engineering Research and Technology
ISSN 2454 – 535X
www.ijmert.com
Vol. 10, Issue. 4, Dec 2023

scattering" in mind in theoretical perspective, when it comes to forecast mode-dependent electron and phonon thermal conductivity. Some of the previous efforts in this direction are "Klemens model (Leibfried & Ludwig, 1961), Leibfried and Schlömann (1954), and Slack (1973) equation". All of such analytical models only cover "phonon-phonon scattering" instead of "phonon-electron scattering" in metals (Wang & Ruan, 2016; Li et al., 2018). Klemens & Williams (1986) proposed "phonon-thermal conductivity" by adding the rate of "phonon-electron scattering" while assuming the interaction between free electrons and "long wavelength phonon modes" and found that there is 3 to 10 W/mK phonon thermal conductivity when taking pure metals.

An analytical expression of "phonon thermal conductivity" is developed by Stojanovic et al. (2010) for metal nano-structures while assuming isotropic properties of material, Debye approximation (Debye, 1912) and free electrons for phonons. Meanwhile, expressing "electron thermal conductivity" at high and low temperature was derived by Wilson (1937) for monovalent metals while assuming that interaction takes place only between electrons and longitudinal phonons. Makinson (1938) promoted thermal and electron conductivity expressed for both low and high temperatures while assuming the interaction between various polarization effects and electrons. These theoretical procedures advance the knowledge of thermal transport significantly. However, there will be significant uncertainty when using such models to obtain electron values and quantitative phonon conductivity.

Recent advancements in numerical approaches have predicted "phonon and thermal conductivity" in metals more accurately. For instance, phonon thermal conductivity is predicted using the molecular dynamic approach (Heino & Ristolainen, 2003). However, there is a significant problem with molecular dynamics, not just because of questionable accuracy of force fields, but also due to lack of empirical potential for majority of materials. One can extract phonon-electron coupling matrix by "first-principal method" and then achieving the mode-resolved phonon and electron transport properties with the combination of "Boltzmann transport equation" (Poncé et al., 2016; 2018; Giustino, 2017).

ISSN 2454 – 535X
www.ijmert.com
Vol. 15 Issue. 4, Dec 2023

Hence, this approach can be helpful to achieve the ideal "phonon thermal conductivity" with first-principles method to any metal. However, accurate results can only be achieved with very dense "q-mesh and k-mesh" for "Brillouin zone integration," which needs very high computational cost. There are only a few "first-principal calculations" conducted to predict metals' thermal conductivity in recent years (Li et al., 2018; Jain & McGaughey, 2016; Tong & Bao, 2018; Chen et al., 2019). These advancements play a vital role and one can finally achieve reliable and relative values of "phonon thermal conductivity" in metals. However, these simulations of first principles are scattered to only a few metals and data may not be compared directly because of change in simulations, such as Brillouin and pseudopotential zone integration. Hence, an in-depth analysis of conductivity in various metals is highly needed to get more generalized conclusions of metal heat conduction.

Tong et al. (2019) conducted a range of "first-principle calculations" for the prediction of mode-dependent phonon and electron thermal conductivity of various metals like "alkali-earth metals, noble metals, transition-intermetallic compounds (TICs), transition metals, and noble-intermetallic compounds (NICs)." It is possible to calculate the "phonon thermal conductivities" by considering both "phonon-electron (p-e) and phonon-phonon (p-p)" interactions and they have also discussed the impact of phonon electron scattering.

4.1. Phonon Thermal Conductivity

Equation (1) is used to calculate the "phonon thermal conductivity" tensor by combining the "Fourier's law and Boltzmann transport equation (BTE)" (Srivastava, 2022) –

$$\kappa_p^{\alpha\beta} = \sum_{\lambda} c_{v,\lambda} v_{\lambda}^{\alpha} v_{\lambda}^{\beta} \tau_{\lambda}^{p}, \quad (1)$$

Here, $\lambda = (\mathbf{q}, \nu)$ refers to the phonon mode with wave vector **q** and polarization ν, $c_{\nu,\lambda}$ is the volumetric heat, v_{λ}^{α} and v_{λ}^{β} means the α and β component of velocity vector of phonon group v_{λ}, and τ_{λ}^{p} refers to the "phonon relaxation time." The "Bose-Einstein statistics" is used to obtain the phonon volumetric-based heat as $c_{v,\lambda} = \frac{\hbar\omega_{\lambda}}{V}\frac{\partial n_{\lambda}}{\partial T}$ where n_{λ} is the function of "Bone-Einstein

International Journal of Mechanical Engineering Research and Technology
ISSN 2454 – 535X
www.ijmert.com
Vol. 10, Issue. 4, Dec 2023

distribution" and *V* refers to the primitive cell volume. It is possible to achieve the group volume by $v_{\lambda,\alpha} = \frac{\partial \omega_\lambda}{\partial \mathbf{q}}$. Matthiessen's rule is used to get the phonon relaxation time as $1/\tau_\lambda^p = 1/\tau_\lambda^{pp} + 1/\tau_\lambda^{pe}$, where $1/\tau_\lambda^{pp}$ refers to the p-p scattering associated with 3-phonon scattering element (Ziman, 2001) and $1/\tau_\lambda^{pe}$ refers to the rate of "p-e scattering" which is associated with electron phonon scattering element (Li et al., 2019). The "Ferni's Golden Rule (FGR)" results in the p-p scattering with 3-phonon scattering in Eq. (2).

$$\frac{1}{\tau_\lambda^{pp}} = \frac{\pi\hbar}{16N}\sum_{\lambda_1\lambda_2}\left|V_{\lambda\lambda_1\lambda_2}\right|^2 \left\{\left(n_{\lambda_1}+n_{\lambda_2}+1\right)\delta\left(\omega_\lambda-\omega_{\lambda_1}-\omega_{\lambda_2}\right)+\left(n_{\lambda_1}-n_{\lambda_2}\right)\right. \\ \left.\times\left[\delta\left(\omega_\lambda+\omega_{\lambda_1}-\omega_{\lambda_2}\right)-\delta\left(\omega_\lambda-\omega_{\lambda_1}+\omega_{\lambda_2}\right)\right]\right\}, \quad (2)$$

In Eq. (2), *N* refers to the number of phonon modes. Dirac delta function is denoted as δ. It is approximated by Lorentzian or Gaussian function (Giustino, 2017). The 3-phonon scattering is denoted as $V_{\lambda\lambda_1\lambda_2}$, which is associated with third order constants (Srivastava, 2022). The phonon electron scattering can also be calculated using FGR (Mahan, 2000) under the approximation of relaxation time.

$$\frac{1}{\tau_\lambda^{pe}} = \frac{2\pi}{\hbar}\sum_{\mathbf{k},i,j}\left|g^\lambda_{j\mathbf{k}+\mathbf{q},i\mathbf{k}}\right|^2\left(f_{i\mathbf{k}}-f_{j\mathbf{k}+\mathbf{q}}\right)\times\delta\left(\epsilon_{i\mathbf{k}}-\epsilon_{j\mathbf{k}+\mathbf{q}}+\hbar\omega_\lambda\right), \quad (3)$$

Here *g* refers to the electron phonon interaction element, *f* refers to the "Fermi-Dirac distribution", **k** refers to the vector of electron wave, *j* and *i* are the electron band indices, ϵ refers to the electronenergy, and ω is the frequency of phonon. Eq. (4) defines the electron phonon matrix describing event where electron is scattered to phonon mode –

$$g^\lambda_{j\mathbf{k}+\mathbf{q},i\mathbf{k}} = \sqrt{\frac{\hbar}{2\omega_\lambda}}\left\langle\psi_{j\mathbf{k}+\mathbf{q}}\left|\partial U_\lambda\right|\psi_{i\mathbf{k}}\right\rangle, \quad (4)$$

Electron Thermal Conductivity

Equations (5), (6) and (7) combine the Onsager and BTE relations to obtain the properties of electron transport (Mahan, 2000).

$$\sigma_{\alpha\beta} = -\frac{e^2 n_s}{V}\sum_{i\mathbf{k}}\frac{\partial f_{i\mathbf{k}}}{\partial\epsilon}v^\alpha_{i\mathbf{k}}v^\beta_{i\mathbf{k}}\tau_{i\mathbf{k}}, \quad (5)$$

$$[\sigma S] = -\frac{en_s}{V}\sum_{i\mathbf{k}}\left(\epsilon_{i\mathbf{k}}-\mu\right)\frac{\partial f_{i\mathbf{k}}}{\partial\epsilon}v^\alpha_{i\mathbf{k}}v^\beta_{i\mathbf{k}}\tau_{i\mathbf{k}}, \quad (6)$$

$$K_{\alpha\beta} = -\frac{n_s}{VT}\sum_{i\mathbf{k}}\left(\epsilon_{i\mathbf{k}}-\mu\right)^2\frac{\partial f_{i\mathbf{k}}}{\partial\epsilon}v^\alpha_{i\mathbf{k}}v^\beta_{i\mathbf{k}}\tau_{i\mathbf{k}}, \quad (7)$$

H ty" and $S_{\alpha\beta}$ refers to the 3x3 "Seebeck coefficient" tensors. The $K_{\alpha\beta}$ is associated with "electron thermal conductivity" $\kappa_e = K - S\sigma ST$ where *T* refers to temperature. In the above three equations, the summary is up to all the electrons counted with

International Journal of Mechanical Engineering Research and Technology
ISSN 2454 – 535X
www.ijmert.com
Vol. 15 Issue. 4, Dec 2023

"band index *i*" and "wave vector **k**".

4.2. Comparing Electron and Phonon Thermal Conductivity and Electrical Conductivity

Table 1 lists the comparison of total thermal conductivity and DFT forecasting of electrical conductivity with trial values at room temperature (Touloukian et al., 1970; Ho, 1975; White & Madelung, 1991; Tereda et al., 2002). With the implementation of "first principle calculations", the phonon κ_p and electron κ_e conductivity are achieved (Table 1). First of all, it is observed that predicted σ works well with tested data (Touloukian et al., 1970; Ho, 1975; White & Madelung, 1991; Tereda et al., 2002). The difference is ranging from 2 to 31 percent and most of them fall under 15 percent. Since there is association between band structure and electrical conductivity, the individual element of e-p scattering and Brillouin integration, proper agreement of σ estimated shows that band structure and coupling of e-p is reliable.

Material	σ ($\times 10^7\ \Omega^{-1}m^{-1}$)		κ_p (W/mK)	κ_e (W/mK)	κ_{total}^{DFT} (W/mK)	$\kappa_{total}^{Exp.}$ (W/mK)	$\frac{\kappa_p}{\kappa_{total}^{DFT}}$	$\frac{L}{L_0}$
	DFT	Exp.	DFT	DFT	DFT	Exp.	DFT, %	DFT
Ag	6.37	6.21	5.59	475.80	481.39	436.00	1.16	1.02
Au	3.50	4.50	2.72	264.94	267.66	318.00	1.02	1.03
Cu	5.17	5.78	17.61	360.90	378.52	402.00	4.65	0.96
Al	3.41	4.12	8.14	225.76	233.89	237.00	3.48	0.91
Mg	2.48	2.30	7.19	178.20	185.39	153.00	3.88	0.98
Pt	1.32	1.02	6.28	86.71	92.99	71.90	6.75	0.90
Pd	0.90	1.03	12.99	68.71	81.70	71.70	15.90	1.05
Ni	1.43	1.60	14.50	101.09	115.59	93.00	12.54	0.97
Ti	0.21	0.25	6.68	28.61	35.29	22.30	18.93	0.93
Co	1.15	1.67	12.20	70.72	82.92	99.00	14.71	0.84
Mn	0.08	0.07	3.28	5.05	8.33	7.80	39.38	0.84
NiAl	1.00	1.02	6.33	69.29	75.62	76.00	8.37	0.94
Ni_3Al	0.38	0.30	5.22	29.72	34.94	28.50	14.94	1.07
TiAl	0.11	0.13	4.57	7.80	12.37	11.50	36.94	0.95
FeAl	0.13	0.18	3.80	8.83	12.63	12.00	30.09	0.92
CoAl	0.55	0.71	4.83	44.48	49.31	37.00	9.80	1.10
Cu_3Au	1.74	1.85	1.89	126.27	128.15	157.20	1.47	0.99
CuAu	1.75	1.32	2.85	126.17	129.02	167.00	2.21	0.99

It is not easy to overlook the role of phonon played on absolute thermal conductivity of metals. In addition, κ_p pays a vital role in metal thermal conductivity because of loss of κ_e at nano-structure (Stojanovic, 2010). Hence, the calculation estimations refer to the need of "first-principle" investigation on the phonon transport.

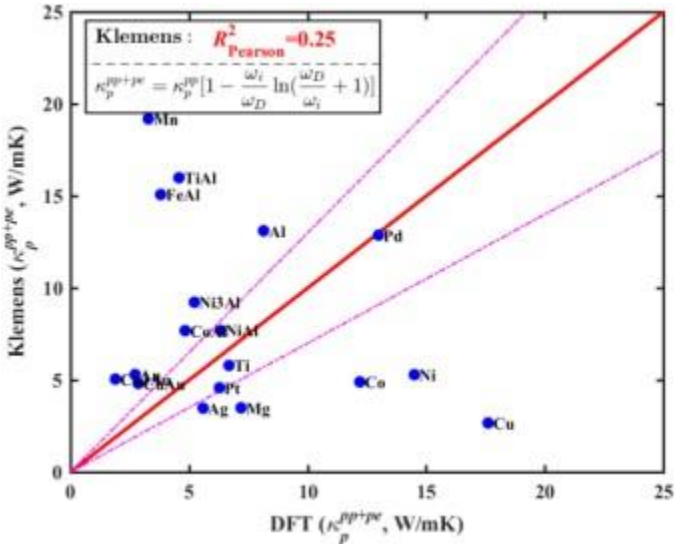
Table 1 – Comparison of Electron and Phonon Thermal Conductivity

Source –Tong et al. (2019)

International Journal of Mechanical Engineering Research and Technology
ISSN 2454 – 535X
www.ijmert.com
Vol. 10, Issue. 4, Dec 2023

Additionally, the estimated first principle κ_p^{pp+pe} is compared with estimations by Klemen's model and Figure 1 shows the comparison.

Figure 1 – Prediction of Phonon thermal predictions at 300K from "first principle calculation" and Klemen's model having both p-e and p-p scattering. The ± 30% error is represented by the dash line



Source – Tong et al. (2019)

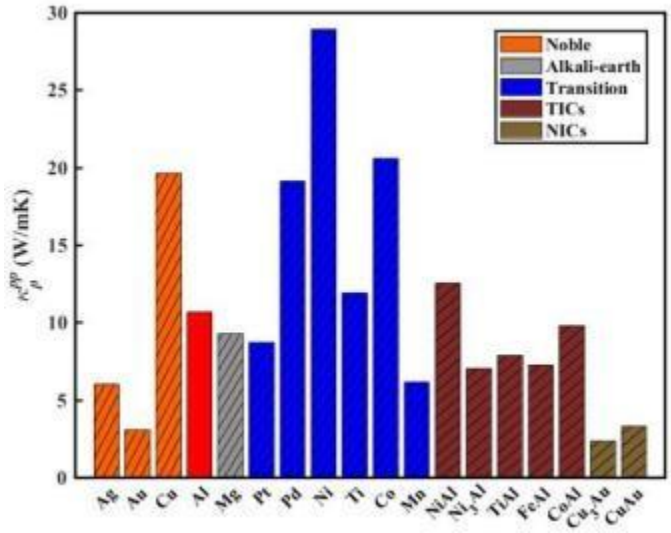
4.3. Adopting p-p scattering matrix for Phonon thermal conductivity

The calculations and equations mentioned above come up with relatively helpful data for phonon conductivity of metals. For further details on the phonon thermal conductivity, this study requires further analysis. Both phonon electron and phonon-phonon scattering affect phonon thermal conductivity. Hence, electron-phonon coupling can affect thermal conductivity by investigating "phonon-thermal conductivity" by considering only phonon-phonon scattering. Figure 2 illustrates the calculation of phonon conductivity using first principles at 300 K.

Though κ_p^{pt} is smaller than 10 W/mK in most of the metals, there are still a few exceptions like Pd, Cu, Co, and Ni. All of these elemental metals have small atomic masses. As Cu is relatively noble, other materials are transition metals. Phonon thermal conductivity is associated with bonding

International Journal of Mechanical Engineering Research and Technology
ISSN 2454 – 535X
www.ijmert.com
Vol. 15 Issue. 4, Dec 2023

strength, atomic mass, and anharmonicity of lattice. It goes without saying that the materials like Ti, Ni, Co, Mn, Pd, and Pt are known to have higher κ_p^{pl} than that of Ag, Au, and other noble metals as transition metals usually consist of stronger bond in comparison to others (Kittel, 2005).Figure 2 – Estimation of phonon thermal conductivity of alkali-earth, noble, transition, NICs, and TICs at 300 K while considering only p-p scattering



Source – Tong et al. (2019)

Some classical models of thermal conductivity were used widely to determine the metals' phonon conductivity (Slack, 1973). It is worth noting that calculation of first-principles with Grüneisen and Debye parameters is used in both Slack and Klemens model. It is indicated by Tong et al. (2019) that the Pearson correlation between theoretical and first-principles prediction is only 0.52 and 0.56 for Slack and Klemens model. It means such analytical models could not predict the phonon conductivity accurately. As these analytical models adopt the approximation by Debye and assumption of long wavelength is used in Klemens model, it is not that shocking (Klemens & Williams, 1986).

As compared to dielectrics and semiconductors, these models are not well suited for metals, mostly because they were developed originally for non-metallic items (Leibfried & Schlömann, 1954; Xie et al, 2019)." Earlier estimations of phonon conductivity with these metals are highly uncertain and care must be taken when using it (Stojanovic et al., 2010; Nath et al.,2017). Phonon electron scattering is a vital term in the process of phonon scattering and it should be considered strictly.

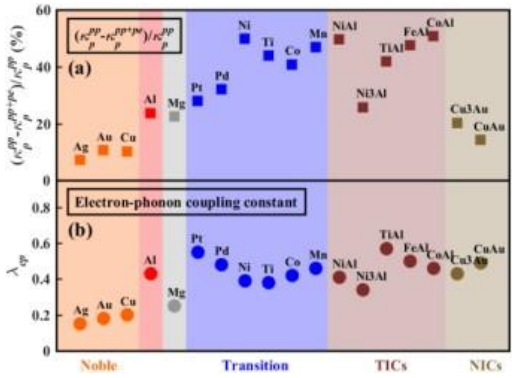
International Journal of Mechanical Engineering Research and Technology
ISSN 2454 – 535X
www.ijmert.com
Vol. 10, Issue. 4, Dec 2023

The term of phonon electron scattering has smaller role in phonon conductivity at medium range of temperature (Wang et al., 2016; Jain & McGaughey, 2016).

5 Results

As per the theoretical understanding and implementation of data (Figure 3), we have come to some findings. First of all, there is a stronger electron phonon coupling impact on transition metals than on noble ones. Secondly, if only one of the conditions are met by the material, the effect of electron phonon coupling is weaker. It suggests that optical phonon in Cu3Au and CuAu plays a vital role in electron phonon composition. In addition, the electron density of alkali-earth and Al act as free electron in density of states, which puts high density of electrons in the Fermi window. Hence, the effects of e-p coupling are stronger in Al and Mg than in noble metals with low density of electrons in the Fermi window. It is obvious that it is possible to measure absolute thermal conductivity and electrical conductivity in tests. However, it is not easy to measure phonon and electron conductivity individually.

Figure 3 – (a) Loss of phonon conductivity due to the effect of e-p coupling (b) Constant e-p coupling



Source – Tong et al. (2019)

The electron phonon scattering is very weak in electron transport for noble metals in comparison to their transition counterparts, making larger electrical conductivity than in transition metals (Table 1). For noble metals, electron conductivity is high and results in smaller thermal conductivity. In the intermetallic components and transition metals, it is easy to compare phonon

International Journal of Mechanical Engineering Research and Technology
ISSN 2454 – 535X
www.ijmert.com
Vol. 15 Issue. 4, Dec 2023

part of thermal conductivity. These factors can be combined in intermetallic compounds and transition metals. It goes without saying that their total thermal conductivity is low and phonon component is larger than in noble metals (Table 1). Metal structures were used widely with nano-scale dimension by developing nano-electronic devices. There is different thermal conductivity of nano-structures as compared to bulk values and size impact reduces because of phonon and electron scattering at surface level.

6 Conclusion

To conclude, it is observed that the predicted "first-principles" thermal conductivity values and electrical conductivity worked well in mode-dependent thermal conductivity of transition metals, noble metals, alkali-earth, TICs, and NICs at room temperature. The separation and quantification of phonon and electron is allowed by the first-principles data to contribute to thermal conductivity. It is observed that the impact of phonon and electron coupling in transition metals on phonon conductivity is stronger than that of noble metals, especially due to large coupling between electron and phonon. It is also observed that high electron conductivity is held by noble metals from 265 to 476 W/mK, especially because of weak e-p coupling.

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International Journal of Mechanical Engineering Research and Technology

ISSN 2454 – 535X
www.ijmert.com
Vol. 10, Issue. 4, Dec 2023

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