Thermoelectric properties of Graphite2H : Semi-classical

Boltzmann theory

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Abstract

Based on the calculated band structure,The electronic transport coefficients of Londsdaleite and Graphite2H were evaluated by using the semi-classical Boltzmann theory based on the calculated band structure,. The value of electrical conductivity for Londsdaleite and Graphite2H of about 1.4 x10 ^{7} (Ωms) $^{-1}$ and 0.67 x10 ^{19} (Ωms) $^{-1}$ at 300 K. The charge carrier concentration and the electrical conductivity linearly increases with increase of temperature in case of Graphite2H and is in agreement with the experimental work. Seebeck coefficients for Londsdaleite and Graphite2H is -2.3 x10 $^{-3}$ (V/K) at is -4.0 x10 $^{-5}$ (V/K) resp. at 600 K. As the temperature increases, the electronic thermal conductivity increases exponentially, in agreement with the experimental data. We have also calculated the power factor of Londsdaleite and Graphite2H at 300K as a function of chemical potentials between ±0.35μ (eV).

INTRODUCTION:

There is a great need to focus on finding new energy resources and materials that can convert sun's energy into electricity to enhance the production of electrical energy to meet with the present demand of energy. Thermoelectric materials can convert low grade heat into electricity, which can be a promising solution to it due to reasonable cost.1. Comprehensive research works on several materials were carried out to investigate and enhance the thermoelectric properties 2–10 . To investigate the thermoelectric properties of *Londsdaleite and Graphite2H,* we perform first-principles calculations using the density functional theory and the semi-classical Boltzmann theory as implemented in the BoltzTraP code.11

MATERIALS AND METHODS:

The *Londsdaleite and Graphite2H* have P63/mmc (hexagonal) space group, With band gap of 3.339 eV and 0.00eV resp.. The crystal structure of *Londsdaleite* is illustrated in Fig. 1

Fig. 1. The *Londsdaleite*

we have optimized the structure by minimization of the forces. To calculate the thermoelectric properties like carrier concentration (n), Seebeck coefficient (S), electrical conductivity (σ/τ) , electronic thermal conductivity (κ_e), at two constant temperatures 300K and 600 K , we have used the semi-classical Boltzmann theory as incorporated in BoltzTraP code11. The constant relaxation time approximation and the rigid band approximation were used in the calculations.11 BoltzTrap code depends on a well tested smoothed Fourier interpolation . The accuracy of this method has been well tested earlier, and the method actually turns out to be a good approximation.11,12 . High thermoelectric Efficiency materials possesses high electrical conductivity, large Seebeck coefficient, and low thermal conductivity.13

RESULTS AND DISCUSSION

Transport properties;

1. Electrical conductivity

Increase in the temperature of the materials increases the kinetic energy of the electrons resulting in an electric current. High mobility carriers are required in order to get the highest electrical conductivity, The electrical conductivity($\sigma = ne\ \mu$) is directly proportional

to the charge carriers density (n) and their mobility (μ), The charge carriers concentration of *Londsdaleite and Graphite2H* as a function of temperature is illustrated in Fig.2(a).

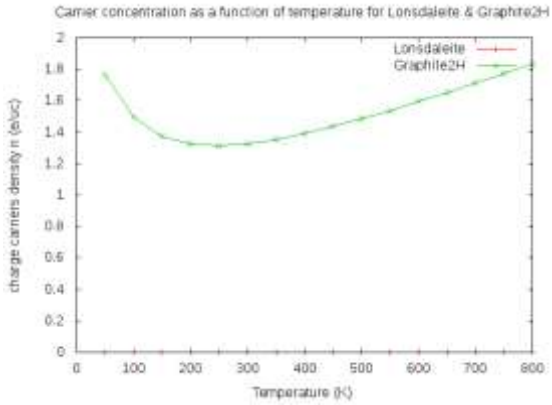


FIG. 2(a) The calculated carrier concentration as a function of temperature for *Londsdaleite and Graphite2H*.

It can be seen that the charge carrier concentration is linearly increasesing with increasing the temperature and is in agreement with the experimental work. Fig. 2(b) illustrates the electrical conductivity of *Londsdaleite and Graphite2H*

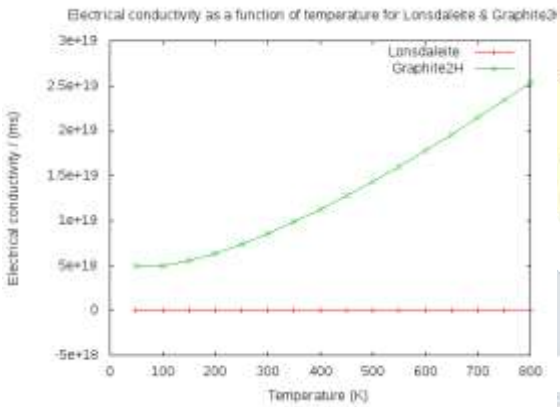


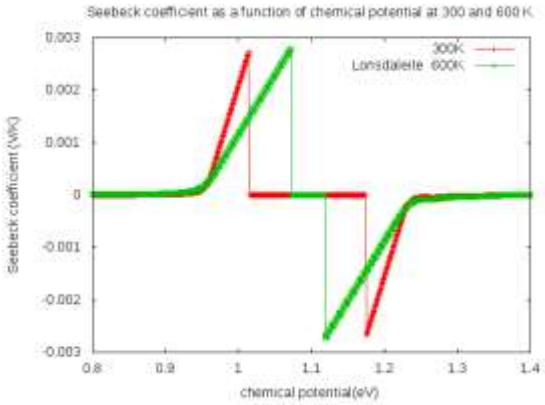
FIG. 2(b) The calculated electrical conductivity as a function of temperature for *Londsdaleite and Graphite2H*

as a function of temperatures. It can be seen that the electrical conductivity is increasesing linearly with increase in the temperatures .

The values of electrical conductivity of *Londsdaleite and Graphite2H* is about *1.4 x10 ^{7}(Ωms) $^{-1}$ and 0.67x10 ^{19} , 1.7 x10 ^{19} (Ωms) $^{-1}$ at 300 &600 K resp.*

2. Seebeck coefficient

Seebeck coefficient (S) or thermopower depends on the electronic structure of the materials. The sign of S indicates the type of dominant charge carrier, + S represents the p type materials, whereas - S for n-type materials. The Seebeck coefficients of *Londsdaleite and Graphite2H* vs chemical potential at 300K and 600K are presented in Figs. 3(a) and 3(b).



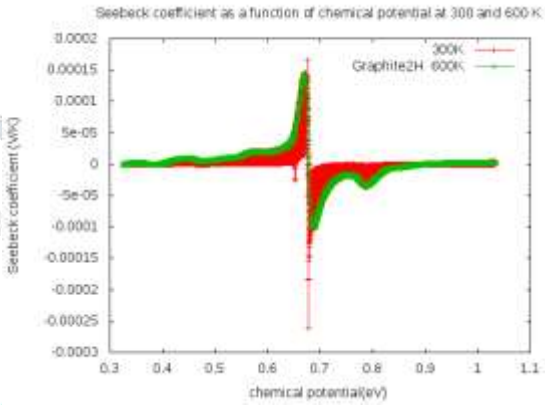


FIG. 3(a) and 3(b).. The calculated Seebeck coefficient as a function of chemical potential at two constant temperatures 300 and 600K for *Londsdaleite and Graphite2H*.

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It can be seen that in the vicinity of EF that the Seebeck coefficient shows two pronounced peaks for n-/p-type for the dominant charge carrier. *Seebeck coefficients for Londsdaleite and Graphite2H is -2.3 x 10 $^{-3}$ (V/K) and -4.0 x 10 $^{-5}$ (V/K) resp. at 600 K.*

3. Electronic thermal conductivity

The thermal conductivity (k = ke+ kl) consists of electronic and phonon contributions . Electrons and holes transporting heat for electronic and phonons traveling through the lattice are responsible for phonon part of thermal conductivity. BoltzTraP calculates only the electronic part. The electronic thermal conductivity for *Londsdaleite and Graphite2H* as a function of chemical potential for two different temperatures is plotted in Figs. 4(a) and 4(b).

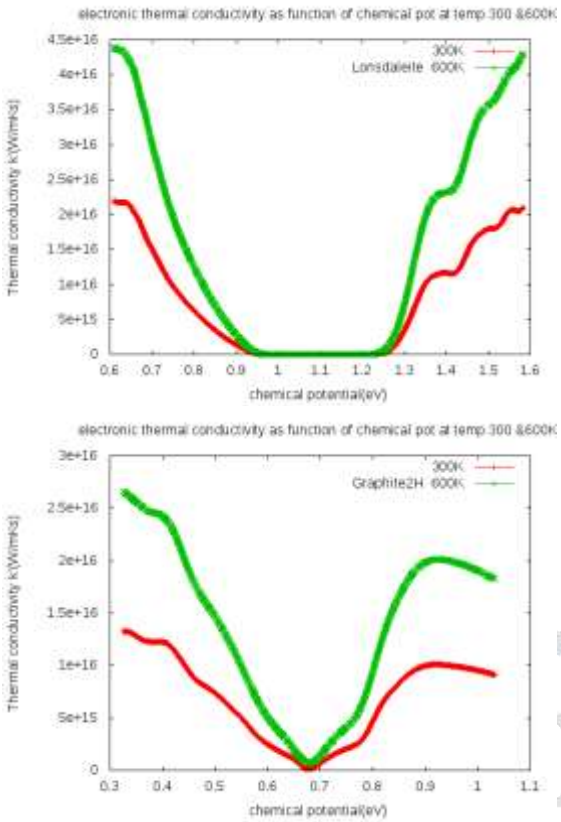

FIG. 4(a) and 4(b). The calculated electronic thermal conductivity as a function of chemical potential at two constant temperatures 300 and 600K for *Londsdaleite and Graphite2H*

The thermal electronic conductivity of *Londsdaleite and Graphite2H* as a function of temperature is plotted in Fig. 4(c)and (d)

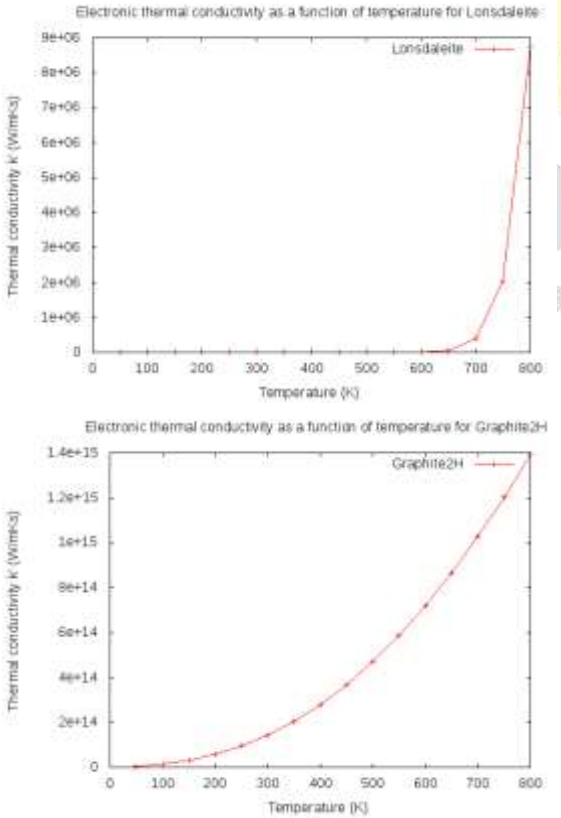

FIG. 4(c)and (d) The calculated electronic thermal conductivity as a function of temperature for *Londsdaleite and Graphite2H*

it can be seen that at low temperatures ke is zero, as temperature increases the ke increases exponentially in agreement with the experimental data .

The value of ke for *Londsdaleite and Graphite2H* of about 6.1×10^{5} W/(m K s) and 7.2×10^{16} W/(m Ks) resp. at temp 600K.

Conclusion:

For calculating the transport properties of the materials power factor plays significant role as it comes as a numerator in the figure of merit relation ($ZT = S^2\sigma T/\kappa$). We have calculated the power factor of *Londsdaleite and Graphite2H* at 300 and 600K as a function of chemical potential between ±0.35μ (eV). Calculated the power factor of *Londsdaleite and Graphite2H* at 600K is 74 (mW/mK ^{2}) and 2.7×10^{10} (mW/mK ^{2}) resp.

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