Journal of ELECTRONIC MATERIALS
DOI: 10.1007/s11664-016-4791-z
© 2016 The Minerals, Metals & Materials Society

Thermoelectric Properties of the Intermetallic Quasi-Two-Dimensional Layered Structure LiBe

A.H. RESHAK [1,2,3]

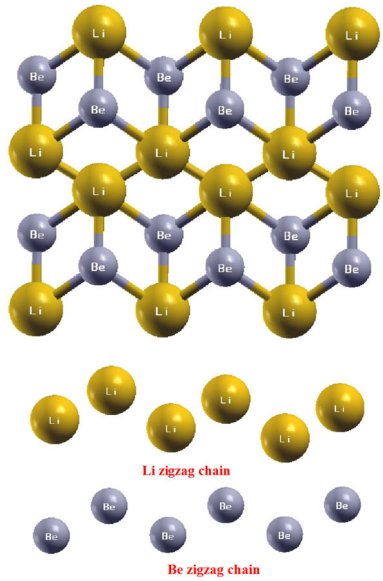
1.—New Technologies - Research Centre, University of West Bohemia, Univerzitni 8, 306 14 Pilsen, Czech Republic. 2.—Center of Excellence Geopolymer and Green Technology, School of Material Engineering, University Malaysia Perlis, 01007 Kangar, Perlis, Malaysia. 3.—e-mail: maalidph@yahoo.co.uk

The electronic transport coefficients of LiBe for the intermetallic quasi-two-dimensional layered structure are evaluated by means of the semi-classical Boltzmann theory and the rigid band model. It has been found that the charge carrier concentration is about -0.0026 e/uc at low temperature ($T = 50$ K), then it decreases with increase of temperature to reach -0.0028 e/uc at 250 K. Above this temperature the charge carriers concentration increases rapidly to reach -0.00228 e/uc at 600 K. The negative sign shows that LiBe exhibits n-type conduction at a certain value of chemical potential ($\mu = E_F$). The calculated electrical conductivity (σ/τ) at $\mu = E_F$ shows that at low temperatures (50 K) LiBe exhibits low σ/τ of about 1.318×10^{21} $(\Omega\ \mathrm{ms})^{-1}$, this value increases rapidly with an increase of temperature to be 1.389×10^{21} $(\Omega\ \mathrm{ms})^{-1}$ at 300 K. Above 300 K the σ/τ reach to the saturated value of about 1.389×10^{21} $(\Omega\ \mathrm{ms})^{-1}$. It has been found that LiBe possesses a thermo-power (S) of about -460 μV/K at 50 K, which decreases with increase of temperatures to reach -220 μV/K at around 350 K. Increasing the temperatures above 350 K lead to a decrease S to be -190 μV/K at 600 K. It is clear that at a certain value of chemical potential LiBe exhibits n-type conduction as it has negative S in the whole temperature range; this supports our previous observation about the charge carriers concentration. It is a remarkable finding that LiBe exhibits a large Seebeck coefficient, which is attributed to the non-zero density of states at the Fermi level. The electron thermal conductivity (κ_e/τ) increased linearly with the temperature, and we observed that at low temperature LiBe exhibits low κ_e/τ of about 0.2×10^{16} W/mKs at 50 K. A rapid increases in κ_e/τ occurs as a result of increasing the temperature to reach 2.1×10^{16} W/mKs at 600 K. The obtained values of the power factor ($S^2\sigma/\tau$) as function of temperature show that at low temperature (50 K) LiBe possesses a high $S^2\sigma/\tau$ of about 2.8×10^{10} mW/mK^2, and with increasing the temperature a rapid reduction in the $S^2\sigma/\tau$ occurs till 350 K to reach the value of about 0.5×10^{10} mW/mK^2. Above this temperature LiBe exhibits almost a stable $S^2\sigma/\tau$ of about 0.6×10^{10} mW/mK^2 at 600 K. Also, we have calculated the transport properties as a function of chemical potential at the vicinity of E_F (± 0.15 eV above and below E_F) for two different temperatures.

(Received April 4, 2016; accepted July 7, 2016)

Published online: 26 July 2016

In LiBe for the quasi-two-dimensional layered structure, the Li and Be atoms are packed in zig-zag layers along the y-axis. The Li and Be layers are puckered with square nets of Li and triangular nets of Be alternating with each others along the z-axis. Given that the LiBe system exhibits two-dimensional (2-D) doping behavior, it might be justifiable to study its transport properties; however, we would like to explore the unique transport behavior arising from its 2-D electronic structure.



Key words: Density functional theory, electronic structure, thermoelectric properties, *ab initio* calculation, thermoelectric power generation

INTRODUCTION

Finding new energy resources and novel promising materials that can convert heat into electricity to open a new direction for the ecologically friendly production of electrical energy is still a challenge for scientists. The search for novel materials with promising structural, optical, and thermoelectric properties is a very important topic of modern aspects in the domain of both science and technology. In recent years there has been a focus on thermoelectric materials, which are one of the promising alternative energy resources. Thermoelectric materials are novel power generators that can convert low grade heat into electricity, which appears to be a promising solution due to their friendly environmental use and reasonable cost.[1] In order to improve the thermoelectric performance of intermetallic compounds, two main routes are taken: the search for new active materials and the optimization of already known thermoelectric materials. Recently, there has been considerable interest in the physical properties of the compounds formed by the light elements such as lithium and beryllium, the lightest known metals, which are immiscible under normal conditions.[2] The interaction between light elemental metallic solids such as Li and Be has been studied with a view to unravel bonding trends and formation of dimmers.[3–5] The binding energy curves have been calculated for $2\sigma^+$ and 2π states of LiBe, LiMg, and LiCa using the density functional theory (*DFT*).[6] Feng et al.[7] have used the *VASP* code within *PBE* − *GGA* to investigate the emergent reduction of electronic state dimensionality in dense ordered Li-Be alloys; they calculate the static-lattice internal energies of both Be-Li ordered alloys and the elements at given densities. It has been found that the density of states of LiBe show a remarkable step-like feature at the bottom of the valence bands, which is a typical characteristic of a quasi 2-D electronic structure.[7] They reported that at 80 GPa, LiBe is stable and expected to be accessible to experimental synthesis in view of the substantially negative heats of formation. Using first-principles calculations, the electronic, vibrational, and superconducting properties of the LiBe alloy in the $P2_1/m$ structure under pressure are investigated; it has been found that $P2_1/m$ LiBe is

dynamically stable at 80 GPa.[2] A density functional theory calculation is performed by Ling et al.[8] to study the equilibrium geometry and the electronic properties of Be_n and $LiBe_n$ clusters. The electric dipole, potential energy, and electronic transition moment functions are calculated from highly correlated *MRCI* electronic wave-functions for low lying doublet and quartet states of the simplest heteronuclear metal diatomic, LiBe, and the isoelectronic ion Be_2^+. The *MRCI* values for the equilibrium bond length is about 2.619 Å, which agrees well with the experimental value (2.59 Å).[8] The ground state of LiBe is calculated and found to be bound by 0.31 eV.[9] Recently *ab initio* calculations were performed using the *CRYSTAL* package within the local density approximation (*LDA*) and gradient approximation (*GGA*) to study the structural electronic properties of, for instance, the bulk modulus, lattice parameters, and pressure derivative of the bulk modulus of LiBe.[10]

From the above, it is clear that there exist a number of band structure calculations for the LiBe compound using different methods based on non-full potential methods. To the best of our knowledge, no comprehensive work of either experimental data or first principles calculations on the thermoelectric properties of LiBe for the intermetallic quasi-two-dimensional layered structure have appeared in the literature. Given that the LiBe system exhibits two-dimensional (2-D) doping behavior, it might be justifiable to study its transport properties; however, we would like to explore the unique transport behavior arising from its 2-D electronic structure. Therefore,as a natural extension to our previous theoretical work[11] and the previous theoretical and experimental works on the structural properties, a detailed depiction of the thermoelectric properties of LiBe using the full potential method and the semi-classical Boltzmann theory as implemented in the BoltzTraP code[12] is timely and would bring us important insights in understanding the origin of the thermoelectric properties of LiBe. Being a metallic compound, LiBe has non-zero density of states at the Fermi level, which leads to unusual transport properties and, hence, a large Seebeck coefficient. Therefore, we addressed comprehensive theoretical calculations based on the density functional theory within the full-potential augmented plane wave plus local orbitals approach (FPLAPW + lo) to calculate the electronic band structure and the density of states at the Fermi level, and, hence, the thermoelectric properties utilizing the BoltzTraP code. The FPLAPW + lo method has proven to be one of the most accurate methods for the computation of the electronic structure of solids within DFT.[13–15]

DETAILS OF CALCULATIONS

LiBe is an intermetallic quasi-two-dimensional layered structure (Fig. 1) and crystallizes in a monoclinic space group $P2_1/m$ with two formula units per unit cell.[7] The Li and Be atoms are packed in zig-zag layers along the y-axis (Fig. 1b and c). In LiBe the quasi-two-dimensional layered structure,[7] the Li and Be layers, are puckered with square nets of Li and triangular nets of Be alternating with each other along the z-axis (Fig. 1a). The lattice constants are a = 1.898 Å, b = 3.204 Å, and c = 4.041 Å, the unit cell contains four atoms.[7] In the unit cell, the Li atom is situated at (0.49797, 0.75000, 0.12165) and Be is at (0.19160, 0.75000, 0.60034) with $\alpha = \gamma = 90°$ and $\beta = 80.50°$.[7] Based on the electronic band structure calculations, the thermoelectric properties of the LiBe are obtained utilizing the semi-classical Boltzmann theory as implemented in the BoltzTraP code.[12] Simulations of the transport properties is a transition from first- to second-principles methods. The first-principles method used here is an all-electron full potential linear augmented plane wave method whereas the second-principles is BoltzTraP code,[12] which solves the semi-classical Bloch-Boltzmann transport equations.[12] Transport properties were obtained from the ground state within the limits of Boltzmann theory[16–18] and the constant relaxation time approximation as implemented in the BoltzTraP code.[12] In short, BoltzTraP performs a Fourier expansion of the quantum chemical band energies. This allows us to obtain the electronic group velocity v and inverse mass tensor, as the first and second derivatives of the bands with respect to k. Applying v and to the semiclassical Boltzmann equations, the transport tensors can be evaluated.

The ground state properties of a LiBe compound are calculated using the all-electron full potential linear augmented plane wave (FPLAPW + lo) method as implemented in Wien2k code.[19] The geometry of LiBe is relaxed by minimizing the forces acting on each atom, the relaxation is performed within the gradient approximation (*PBE* – *GGA*).[20] We assume that the structure is totally relaxed when the forces on each atom reach values less than (1 mRy/a.u.). The resulting relaxed geometry is used to calculate the ground state properties of LiBe and; hence, the thermoelectric properties using the recently modified Becke–Johnson potential (mBJ),[21] which optimizes the corresponding potential for electronic band structure calculations. To solve the Kohn–Sham equations, a base of linear *APW's* is used. In the muffin-tin (*MT*) spheres the potential and charge density are expanded in spherical harmonics with $l_{max} = 8$ and nonspherical components up to $l_{max} = 6$. In the interstitial region the potential and the charge density are represented by Fourier series. Self-consistency is obtained using 200 $\vec{k}$ points in the irreducible Brillouin zone (*IBZ*). The self-consistent calculations converge since the total energy of the system is stable within 10^{-5} Ry. The transport coefficients are calculated using 12000 $\vec{k}$ points in the *IBZ*.

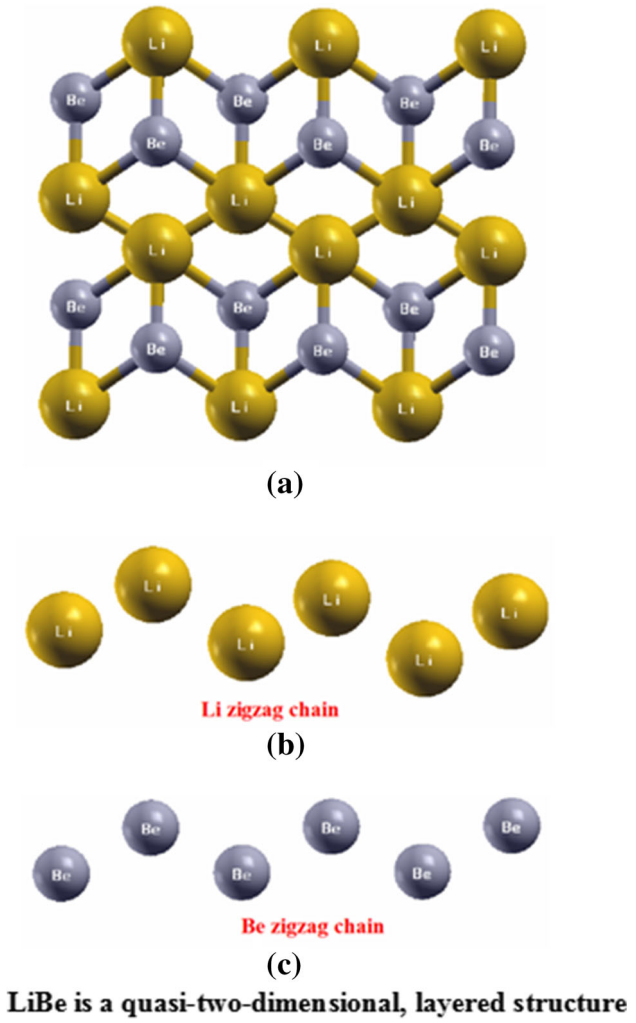


Fig. 1. (a) Fragment of the crystal structure of intermetallic LiBe (a quasi-two-dimensional, layered structure); (b) Li zigzag chain; (c) Be zigzag chain.

RESULTS AND DISCUSSION

Salient Features of the Electronic Band Structures

In this section we will recall the main features of the electronic band structure and the total density of states (*TDOS*) of the monoclinic LiBe (Fig. 2).[11] The *TDOS* (Fig. 2) exhibit that the lower valence bands (*VBs*) that show striking step-function-like singularity, which agrees well with the previous results.[7] The observed sharp step-function-like is suggestive of a van Hove singularity of a 2-D electronic structure, which is unusual for a compound of two metallic elements.[7,22] The electronic band structure is calculated along the high symmetry directions $\Gamma \rightarrow Y \rightarrow C \rightarrow Z \rightarrow \Gamma \rightarrow B \rightarrow D$ using the *mBJ* approach. It has been found that there are three bands that cross the Fermi level (E_F) indicating the metallic nature of LiBe. Our calculated electronic band structure shows reasonable agreement with that obtained by Galav et al.[10] The similar features are also observed by Xu et al.[2] at 80 GPa in monoclinic LiBe. Our calculation shows that the top of the valence band is about 5.0 eV above E_F in reasonable agreement with previous results.[10] The 1 *s* states of Li and Be lie deep below the bands shown in Fig. 2. The four visible *VBs* in Fig. 2 are dominated by the 2*s* states of Li and Be. It is clear that the four *VBs* are parabolic at the Γ point along the $\Gamma - Y$ direction. This would imply high mobility and small effective mass for the carriers belonging to these bands. However, the presence of carriers with large mobility is required for obtaining a higher electrical conductivity (σ). The thermoelectric power factor ($S^2\sigma/\tau$) is indirectly related to the effective mass through $\sigma = ne\eta$, where n and η are the carriers' density and their mobility.[23] The mobility of electrons and holes are defined as $\eta_e = e\tau_e/m_e^*$ and $\eta_h = p\tau_h/m_h^*$, where m_e^* and m_h^* are the electrons and holes effect masses.[23] Therefore, $S^2\sigma/\tau$ can be improved, if the effective mass decreases, because the gain in the Seebeck coefficient is larger than the decrease in η.[24] The main factors to determine the transport properties are the effective charge carrier's mass, the Seebeck coefficient, and electrical conductivity of materials. The electron mobility characterizes how quickly an electron can move through a metal or semiconductor. Due to the electronic structure of LiBe (a two-dimensional layered structure), the unusual valence electronic density of states,[7] the high density of states at the Fermi level $N(E_F) = 9.6$ (states/Ry/cell),[11] and the strong Li-Li and Be-Be bonds, this material is expected to be a good thermoelectric material at the investigated pressure's range.

Transport Properties

Electrical Conductivity

The kinetic energy of the electrons increases with increasing the temperature, which causes to immigration of the electrons from the hot to the cold end, resulting in an electric current. Increasing the temperature leads to an increase in the carrier's mobility favoring enhancement of the electrical conductivity according to the formula ($\sigma = ne\eta$). The total mobility is a sum of the electron's mobility $\eta_e = e\tau_e/m_e^*$ and the hole's mobility $\eta_h = p\tau_h/m_h^*$, where η_e and η_h are inversely proportional to m_e^* and m_h^*. Therefore, materials with small m_e^* and m_h^* possess high electron and hole mobility. The total charge carriers concentration is defined as the difference between the holes and the electrons concentration.

Figure 3a exhibits the charge carriers concentration (n) as a function of temperature at a certain value of the chemical potential ($\mu = E_F = 0.5134$ eV). It has been found that the charge carriers concentration of LiBe is about -0.0026 e/uc at low temperature

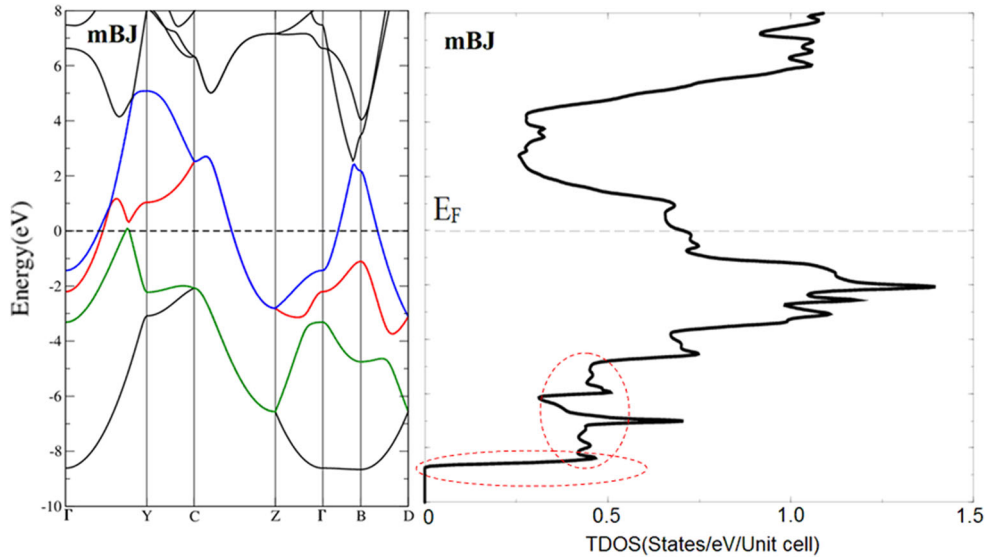


Fig. 2. The calculated electronic band structure of intermetallic LiBe using mBJ. The high symmetry directions are Γ (0.0 0.0 0.0) → *Y* (0.5 0.0 0.0) → *C* (0.5 0.5 0.0) → *Z* (0.0 0.5 0.0) → Γ(0.0 0.0 0.0) → *B* (0.0 0.0. 0.5) → *D* (0.0 0.5 0.5), the red and blue colors just to highlight the bands which cross the Fermi level. The calculated density of states (States/eV/unit cell), and the density of states of LiBe show a remarkable step-like feature at the bottom of the valence (around −8.0 eV), which is a typical characteristic of a quasi 2-D electronic structure.[7] After the step-like feature, the DOS stay roughly constant up to −4.0 eV.

(T = 50 K), then it reaches −0.0028 e/uc at 250 K. Above 250 K, n increases rapidly to reach −0.00228 e/uc at 600 K. It is clear that n exhibits an exponential relation with the temperature at the temperature range between 50 K and 600 K.

In Fig. 3b the electronic band structure of LiBe in the energy region between 0.15 and −0.15 eV is plotted together with the carrier concentrations at two constant temperatures (300 and 600) K. The difference between chemical potential and Fermi energy ($\mu - E_F$) is positive for valence bands and negative for the conduction bands. Therefore, LiBe possesses n-/p-types conductions in the $\mu - E_F$ confined between ∓ 0.15 eV, the region where LiBe is expected to give maximum efficiency.

The electrical conductivity (σ/τ) as a function of temperature at a certain value of the chemical potential ($\mu = E_F = 0.5134$ eV) is illustrated in Fig. 3c. It has been found that at low temperatures (50 K) the LiBe exhibits a low σ/τ of about 1.318×10^{21} $(\Omega\ \mathrm{ms})^{-1}$, this value increases rapidly with a rise in temperature up to 300 K to be around 1.385×10^{21} $(\Omega\ \mathrm{ms})^{-1}$. Above 300 K we can see that σ/τ reaches to the saturated value of about 1.389×10^{21} $(\Omega\ \mathrm{ms})^{-1}$.

In Fig. 3d we plot σ/τ as a function of chemical potential ($\mu - E_F$) at the vicinity of E_F (±0.15 eV above and below E_F) for two constant temperatures (300 and 600) K. The critical points of $\mu - E_F$ for σ/τ in the p-type and n-type regions are +0.15 and −0.15 (eV). It is clear that at the vicinity of E_F (above and below E_F), σ/τ as a function of $\mu - E_F$, shows the same trends and values at 300 K and 600 K. A maximum value of about 1.45×10^{21} $(\Omega\ \mathrm{ms})^{-1}$ for σ/τ is achieved at $\mu - E_F = 0.04$ (eV).

Thermo-Power

The thermo-power or Seebeck coefficient (S) is related to the electronic structure of the materials. The sign of S indicates the type of dominant charge carriers, S with positive sign represent the p-type materials, whereas n-type materials have negative S. Figure 3e shows the temperature dependences of S at a certain value of the chemical potential ($\mu = E_F = 0.5134$ eV). It is clear that LiBe exhibits n-type conductions for ($\mu = E_F = 0.5134$ eV) as it has a negative S in the whole temperature range. We observed that LiBe possesses S of about −460 μV/K at 50 K. Then it decreases with a rise of the temperature to reach −220 μV/K at around 350 K. Raising the temperatures above 350 K leads to a decreasek of S to be −190 μV/K at around 600 K.

In Fig. 3f we have plotted S as a function of $\mu - E_F$ in the vicinity of E_F for $\mu - E_F = \pm 0.15$ eV at 300 K and 600 K. It has been found that LiBe exhibits the highest S value for p-type conductions at ($\mu - E_F = +0.07$ eV), which is about 395 μV/K at 300 K and 495 μV/K at 600 K. Whereas for n-type conductions, it is about −400 μV/K at 300 K and −680 μV/K for 600 K at ($\mu - E_F = -0.15$ eV). The critical points of S for the p-type and n-type are +0.15 and −0.15 eV;, the range where the materials are expected to exhibit good thermoelectric properties. It is clear that the non-zero density of states at E_F, $N(E_F)$ lead to unusual transport properties and, hence, large Seebeck coefficients. Similar behavior was observed in Co_2MnAl and Co_2MnSn compounds.[25] Therefore, the bands which cross E_F are responsible for the transport properties of the

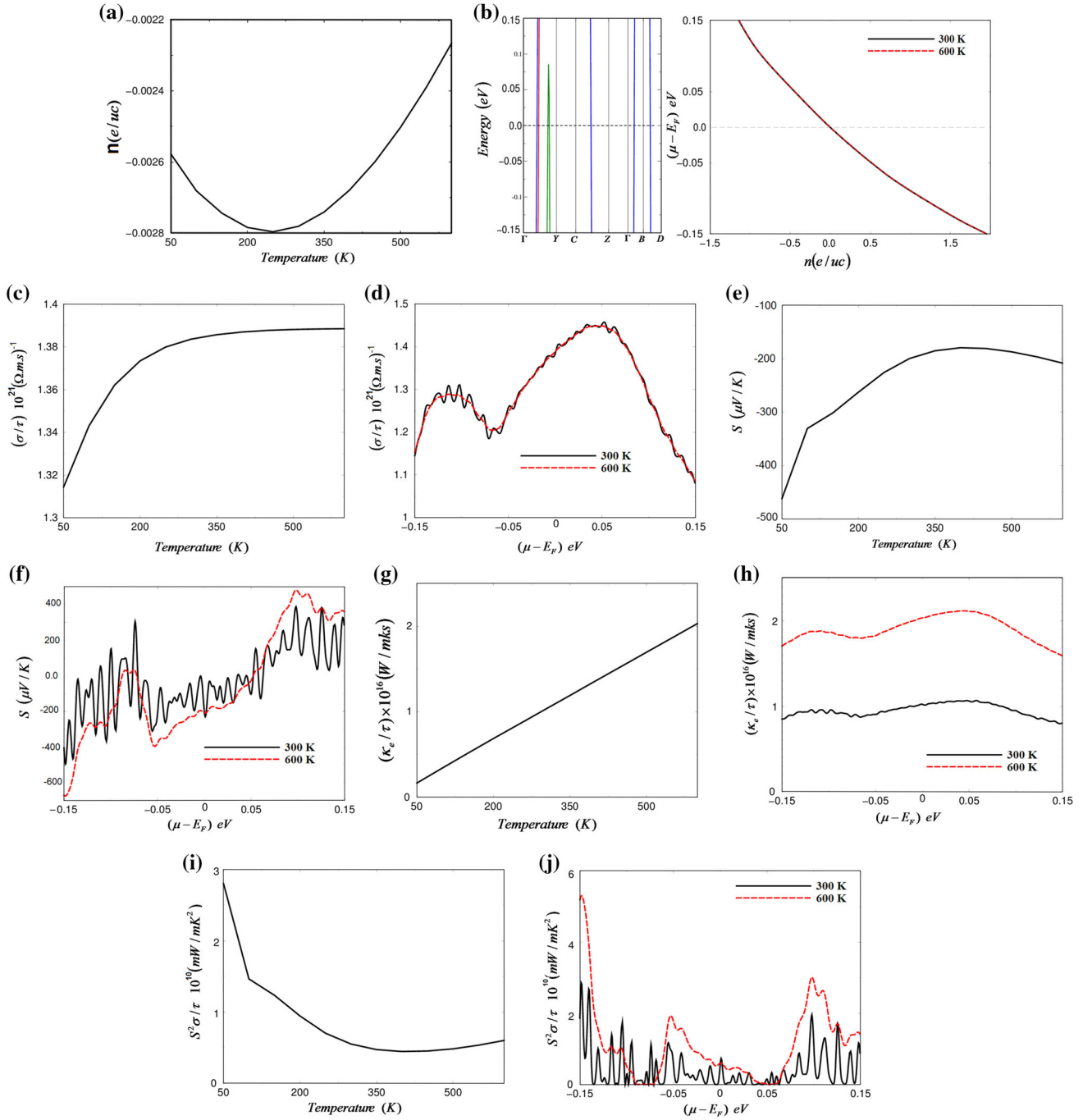


Fig. 3. The transport properties of the intermetallic LiBe; (a) carrier concentration as a function of temperature at a certain value of the chemical potential μ = 0.5134 eV; (b) Band structure of LiBe at the energy range between −0.15 and +0.15 eV together with the calculated number of carrier concentrations at two constant temperatures (300 and 600) K and in the $\mu - E_F$ range between ±0.15 eV; (c) Electrical conductivity as a function of temperature at a certain value of the chemical potential μ = 0.5134 eV; (d) Electrical conductivity as a function of chemical potential for two constant temperatures at the vicinity of E_F in the $\mu - E_F$ range between ±0.15 eV; (e) Seebeck coefficient as a function of temperature at a certain value of the chemical potential μ = 0.5134 eV; (f) Seebeck coefficient as a function of chemical potential for two constant temperatures at the vicinity of E_F in the $\mu - E_F$ range between ±0.15 eV; (g) Electronic thermal conductivity as a function of temperature at a certain value of the chemical potential μ = 0.5134 eV; (h) Electronic thermal conductivity as a function of chemical potential for two constant temperatures at the vicinity of E_F in the $\mu - E_F$ range between ± 0.15 eV; (i) power factor as a function of temperature at a certain value of the chemical potential μ = 0.5134 eV; (j) power factor as a function of chemical potential for two constant temperatures at the vicinity of E_F in the $\mu - E_F$ range between ±0.15 eV.

compound, and those bands which are not crossing E_F will contribute negligibly to the transport properties.[26]

Electron Thermal Conductivity

In order to maintain the temperature gradient, materials with low thermal conductivity are required for designing efficient thermoelectric devices. In general thermal conductivity consists of two parts ($\kappa = \kappa_{e+}\kappa_l$), the first is the electron thermal conductivity contribution (electrons transporting heat) (κ_e) and the second is the lattice vibration (κ_l) (phonons traveling through the lattice). The BoltzTraP code calculates only k_e.[12] Figure 3g exhibits the calculated κ_e/τ of LiBe as a function of temperature at a certain value of chemical potential ($\mu = E_F = 0.5134$ eV). Following this figure one can see that κ_e/τ increases linearly with the temperature. At low temperatures LiBe exhibits low κ_e/τ of about 0.2×10^{16} W/mKs at 50 K. A rapid increases in κ_e/τ occurs with raising the temperatures to reach 2.1×10^{16} W/mKs at 600 K.

Furthermore, the κ_e/τ of LiBe as a function of chemical potential in the vicinity of E_F for $\mu - E_F = \pm 0.15$ eV at two different temperatures is presented in Fig. 3h. It is clear that in the chemical potential between ∓ 0.15 eV, LiBe exhibits a low κ_e/τ value at 300 K in comparison to a κ_e/τ value at 600 K. Therefore, at $\mu - E_F = \pm 0.15$ eV, LiBe is expected to give its maximum efficiency at 300 K due to the low value of κ_e/τ at 300 K.

We should emphasize that the thermal conductivity of any material is dependent on the motion of the free electrons and the molecular vibrations. For metals (our case) the thermal conductivity is mainly a function of the motion of free electrons, which implies that the k_e contribution is dominant. As the temperature increases, the molecular vibrations increase (in turn increasing the mean free path of molecules). So, they obstruct the flow of free electrons, thus reducing κ_l. In high-purity metals, the electron mechanism of heat transport is much more efficient than the phonon contribution, because electrons are not as easily scattered as phonons and have higher velocities. Furthermore, metals are extremely good conductors of heat, because of a relatively large number of free electrons that exist in participating in thermal conduction. Since free electrons are responsible for both electrical and thermal conduction in pure metals, theoretical treatments suggest that the two conductivities should be related according to the Wiedemann–Franz law ($L = \kappa/\sigma T$) where σ is the electrical conductivity, T is the absolute temperature, and L is a constant. The theoretical value of L, 2.44×10^{-8} ΩW/K^2, should be independent of temperature and the same for all metals if the heat energy is transported entirely by free electrons.[27] Therefore, as we have mentioned above that the BoltzTraP code calculates only the electron thermal conductivity (k_e) and, we noticed that k_e increases with increasing the temperature (Fig. 3h).

Power Factor

The power factor is defined as ($P = S^2\sigma/\tau$), where (S) is the Seebeck coefficient (thermo-power) and (σ/τ) is the electrical conductivity. With the aid of the existing information about S and σ/τ, we have calculated $P = S^2\sigma/\tau$. The obtained values of $P = S^2\sigma/\tau$ as function of temperature at a certain value of the chemical potential are illustrated in Fig. 3i. At low temperature (50 K), LiBe possesses a high $S^2\sigma/\tau$ of about 2.8×10^{10} mW/mK^2, with raising the temperature, a rapid reduction in the $S^2\sigma/\tau$ occurs up to 350 K to reach the value of about 0.5×10^{10} mW/mK^2. Above this temperature LiBe exhibits almost stable $S^2\sigma/\tau$, it reaches the value of about 0.6×10^{10} mW/mK^2 at 600 K.

In Fig. 3j we have presented the calculated $S^2\sigma/\tau$ of LiBe at 300 and 600 K as a function of chemical potential at the vicinity of E_F for $\mu - E_F = \pm 0.15$ eV. At E_F the power factor exhibits low value and beyond that $S^2\sigma/\tau$ increases rapidly to form a pronounced peak. The power factor of LiBe exhibits high peaks at around -0.15 (eV) for both temperatures. The highest $S^2\sigma/\tau$ occurs at 600 K. It is interesting to highlight that $S^2\sigma/\tau$ is a very important quantity for calculating the transport properties of the materials, because it is a numerator in the figure of merit relation ($ZT = S^2\sigma T/\kappa$).

CONCLUSIONS

Based on the semi-classical Boltzmann theory and the rigid band model, the electronic transport coefficients of LiBe are evaluated. The all-electron full potential linear augmented plane wave (FPLAPW + lo) method in a scalar relativistic version as embodied in the Wien2k code within *mBJ* approach is used to obtain accurately calculated electronic structures. A charge carrier concentration (n) of about -0.0026 e/uc is achieved at low temperature ($T = 50$ K), then it decreases with increasing temperature to be -0.0028 e/uc at 250 K. Above this temperature n increases rapidly to reach -0.00228 e/uc at 600 K. The negative sign shows that LiBe exhibits n-type conduction for a certain value of the chemical potential ($\mu = E_F = 0.5134$ eV). The electrical conductivity (σ/τ) as a function of temperatures exhibit that at low temperatures (50 K) LiBe possesses low σ/τ of about 1.318×10^{21} (Ω ms)$^{-1}$, this value increases rapidly with raising the temperature till 300 K (1.389×10^{21} (Ω ms)$^{-1}$). Above 300 K the σ/τ reaches the saturated value, which is about 1.389×10^{21} (Ω ms)$^{-1}$. It has been found that LiBe possesses a thermo-power (S) of about -460 μV/K at 50 K, which decreases with increasing the temperature to reach -220 μV/K at around 350 K. Increasing the temperature above 350 K leads to decreased S to -190 μV/K at around 600 K. It is clear that at a

certain value of the chemical potential ($\mu = E_F = 0.5134$ eV), LiBe exhibits n-type conduction as it has a negative S in the whole temperatures range. The electronic thermal conductivity κ_e/τ is linearly increases with the temperature. We observe that LiBe exhibits low κ_e/τ of about 0.2×10^{16} W/mKs at 50 K. A rapid increase in κ_e/τ occurs when we increase the temperature to reach 2.0×10^{16} W/mKs at 600 K. The obtained values of the power factor ($S^2\sigma/\tau$) as function of temperature shows that LiBe possesses high $S^2\sigma/\tau$ of about 2.8×10^{10} mW/mK^2 at 50 K, with increasing the temperature, a rapid reduction in $S^2\sigma/\tau$ values occur till 350 K to reach the value of about 0.5×10^{10} mW/mK^2. Above this temperature LiBe exhibits almost a stable $S^2\sigma/\tau$ of about 0.6×10^{10} mW/mK^2 at 600 K. A remarkable finding is that LiBe exhibits a large Seebeck coefficient, which is attributed to the non-zero density of states at the Fermi level.

ACKNOWLEDGEMENT

The result was developed within the CENTEM project, Reg. No. CZ.1.05/2.1.00/03.0088, cofunded by the ERDF as part of the Ministry of Education, Youth and Sports OP RDI programme and, in the follow-up sustainability stage, supported through CENTEM PLUS (LO1402) by financial means from the Ministry of Education, Youth and Sports under the National Sustainability Programme I. Computational resources were provided by MetaCentrum (LM2010005) and CERIT-SC (CZ.1.05/3.2.00/08.0144) infrastructures.

REFERENCES

1. H. Wang, W. Chu, and H. Jin, *Comput. Mater. Sci.* 60, 224 (2012).
2. Y. Xu, C. Chen, and B. Wu, *Solid State Commun.* 152, 151 (2012).
3. G. Das and A.C. Wahl, *Phys. Rev. A* 4, 825 (1971).
4. W.H. Fink, *J. Chem. Phys.* 57, 1822 (1972).
5. J. Pascale and J. Vandeplanque, *J. Chem. Phys.* 60, 2278 (1974).
6. R.O. Jones, *J. Chem. Phys.* 72, 3197 (1980).
7. J. Feng, R.G. Hennig, N.W. Ashcroft, and R. Hoffmann, *Nat. Lett.* 451, 445 (2008).
8. L.X. Ling, H.Z. Jiang, W.X. Ming, and L.Y. Hua, *Chin. Phys. B* 17, 3687 (2008).
9. I. Fischer, V.E. Bondybey, P. Rosmus, and H.-J. Werner, *Chem. Phys.* 151, 295 (1991).
10. K.L. Galav, U. Paliwal, and K.B. Joshi, *Comput. Mater. Sci.* 69, 267 (2013).
11. A.H. Reshak, *Indian J. Phys.* (2015). doi:10.1007/s12648-015-0682-z.
12. G.K.H. Madsen and D.J. Singh, *Comput. Phys. Commun.* 175, 67 (2006).
13. Y. Saeed, S. Nazir, A. Shaukat, and A.H. Reshak, *J. Magn. Magn. Mater.* 322, 3214 (2010).
14. H.S. Saini, M. Singh, A.H. Reshak, and M.K. Kashyap, *J. Magn. Magn. Mater.* 331, 1 (2013).
15. K.J. Plucinski, I.V. Kityk, J. Kasperczyk, and B. Sahraoui, *Semicond. Sci. Technol.* 16, 467 (2001).
16. P.B. Allen, *Quantum Theory of Real Materials*, ed. J.R. Chelikowsky and S.G. Louie (Boston: Kluwer, 1996), p. 219.
17. J.M. Ziman, *Electrons and Phonons* (Oxford: Clarendon, 2001).
18. C.M. Hurd, *The Hall Effect in Metals and Alloys* (New York: Plenum, 1972).
19. P. Blaha, K. Schwarz, G.K.H. Madsen, D. Kvasnicka, and J. Luitz, *WIEN2k: An Augmented Plane Wave Plus Local Orbitals Program for Calculating Crystal Properties* (Austria: Vienna University of Technology, 2001).
20. J.P. Perdew, S. Burke, and M. Ernzerhof, *Phys. Rev. Lett.* 77, 3865 (1996).
21. F. Tran and P. Blaha, *Phys. Rev. Lett.* 102, 226401 (2009).
22. A.N. Kolmogorov and S. Curtarolo, *Phys. Rev. B* 73, 180501 (2006).
23. W. Shi, J. Chen, J. Xi, D. Wang, and Z. Shuai, *Chem. Mater.* 26, 2669 (2014).
24. W. Wunderlich, H. Ohta, and K. Koumotoa, *J. Phys. B Condens. Matter* 404, 2202 (2009).
25. J. Kübler, A.R. Williams, and C.B. Sommers, *Phys. Rev. B* 28, 1745 (1983).
26. S. Sharma and S.K. Pandey, *J. Phys. Condens. Matter* 26, 215501 (2014).
27. Chapter 17/Thermal Properties. http://www.ehu.eus/estibalizapinaniz/Transparencias/Thermal_Properties.pdf. Accessed on 27 June 2016.