First Principles Study of structural, electronic and thermoelectric properties of Mo_2ScAlC_2

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ABSTRACT

In this study, the structural, electronic and thermoelectric properties of belong to MAX phase, Mo_2ScAlC_2 are investigated by within the framework of the density-functional theory (DFT) using the plane-wave pseudopotential approach and Boltzmann transport theory as implemented within the MedeA-VASP package. We have computed the structural parameters and electronic band structure of Mo_2ScAlC_2. All results are in agreement with the available experimental data and other theoretical calculations. We also calculated Seebeck coefficient, electrical conductivity, and electronic thermal conductivity and discussed in detail.

1. INTRODUCTION

MAX phases constitute a class of nanolaminated ternary carbides and nitrides, described by the general formula, $M_{n+1}AX_n$ (n =1, 2, 3, etc) where M is a transition metal, A is an A–group element, and X is usually C or N. MAX phases adopt the hexagonal P63/mmc structure in which M and X atoms form octahedral edge-sharing building blocks interleaved by A-atomic layers. This structure is highly anisotropic and catalytic for the combination of metallic and ceramic characteristics in MAX phases [4]. Al- element contain in MAX phases have been reported bay Anasori and Dahlqvist [3] such as Mo_2TiAlC_2 and $Mo_2Ti_2AlC_3$. Furthermore, very recently Mo_2ScAlC_2 was synthesized by heating the mixture of elemental powders of Mo, Sc, Al and graphite at 1700°C [5].

Thermoelectric materials can directly convert waste heat into electricity using the Seebeck effect. The efficiency of thermoelectric materials is directly linked to the figure-of-merit (ZT) of the semiconductors (n and p, respectively) composing the module. This figure of merit (ZT) [6,7] is given by

$$ZT = \frac{S^2\sigma}{\kappa}T$$

where T is the temperature, *S* the Seebeck coefficient, σ and κ the electrical and thermal conductivity respectively. Thus, we understanding that high thermoelectric performance is found in materials with high Seebeck coefficient and electrical conductivity but with low thermal conductivity. In the present study, we aim to explore the electronic and thermoelectric properties of Mo_2ScAlC_2.

2. METHOD

The calculations have been performed using the augmented plane-wave pseudopotential approach to the density functional theory (DFT) implemented in Vienna Ab-initio Simulation Package (VASP)[8–11] and Boltzmann transport theory as implemented within the MedeA-VASP [12] package. We have used the exchange-correlation potential within the Generalized Gradient Approximation (GGA) of Perdew, Burke, and Ernzerhof [13]. The wave functions are expanded in the plane waves up to a kinetic-energy cutoff of 450 eV. The k-point is sampled according to the Monkhorst–Pack scheme [11], which yields 17 × 17 × 2 k-points, in the irreducible edge of Brillouin zone. The total energy is converged numerically to less than 1.10^{-8} eV/unit. After structural optimization, calculated forces are converged to less than 0.01 eV/Å.

3. RESULTS AND DISCUSSION

Mo_2ScAlC_2 crystallizes in a hexagonal structure with the space group of P63/mmc. The crystal structure of Mo_2ScAlC_2 is represented in Figure 1. The unit cell of Mo_2ScAlC_2 contains 12 atoms and two formula units (Z = 2). Table 1 lists the calculated lattice constants (a and c), unit cell volume together with total energy The theoretical results are in good agreement with the experimental values.

Table 1. Calculated lattice parameters (a, b ve c, in Å), volume (V_0 in Å3/f.u.), and total energy (E_0 in eV)

Material	Space Group	a	c	V_0	E_0	Reference
Mo_2ScAlC_2	$P6_3/mcm$	3.05	19.06	153.85	-104.99	Present
		3.03	18.77	149.61	-	Ref. [1]
		3.05	19.06	153.82	-	Ref. [2]

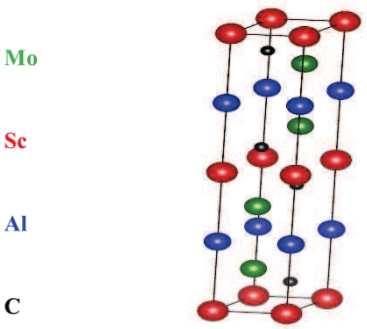

Figure 1. The unit cell of the Mo_2ScAlC_2

In order to get some insight on the electronic properties of materials, we have to calculate the band structure. Specially, the band gap's is very critical for the design of electronic materials. The band structure for high symmetry points in the first Brillouin zone are shown in Figure 2. We see that Mo_2ScAlC_2 compound there is no any band gap at Fermi energy level (E_F) for. The band structures clearly show that it has metallic behavior.

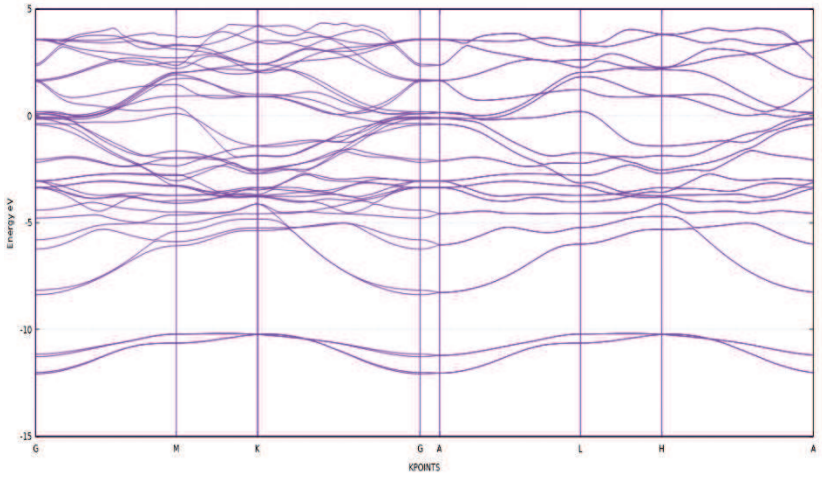

Figure 2. The Band structure of the Mo_2ScAlC

ZT value in thermoelectric materials is a measure of efficiency. For this reason, thermal conductivity, Seebeck coefficient and electrical conductivity which are effective on ZT value are calculated. The calculated plots for the Seebeck coefficient of Mo_2ScAlC_2 at different temperatures are presented in Figure 3. At same time, the electrical conductivity and electronic thermal conductivity are shown in Figure 4 and Figure 5, respectively.

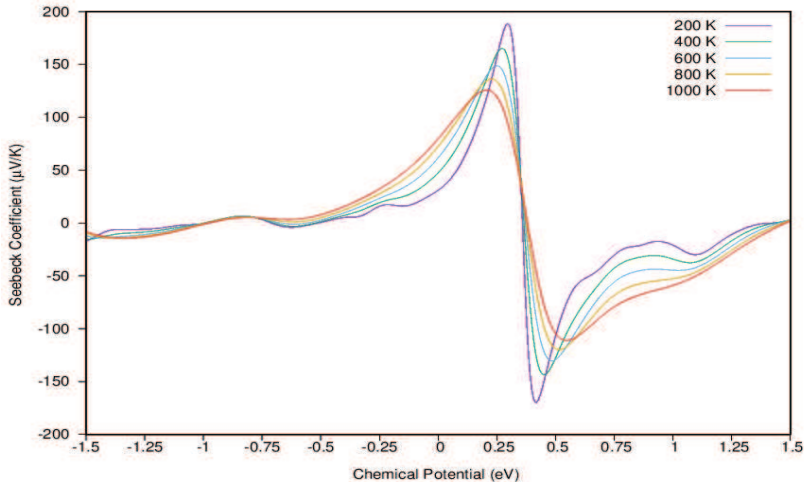

Figure 3. Calculated Seebeck coefficient as a function chemical potential.

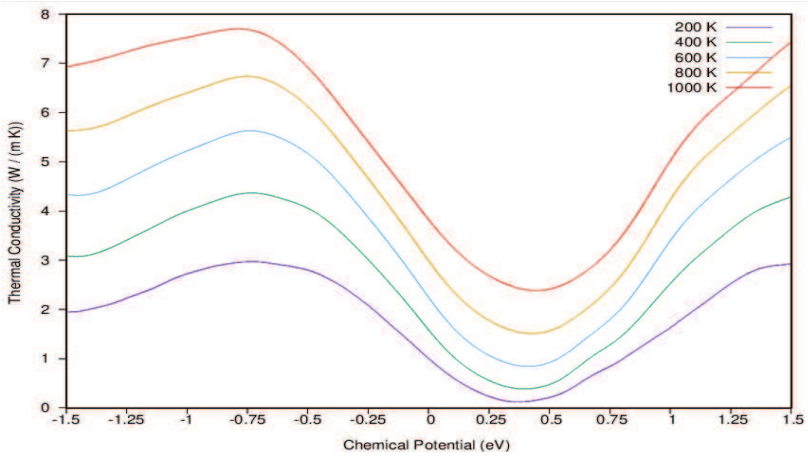

Figure 4. Calculated electronic thermal conductivity as a function chemical potential.

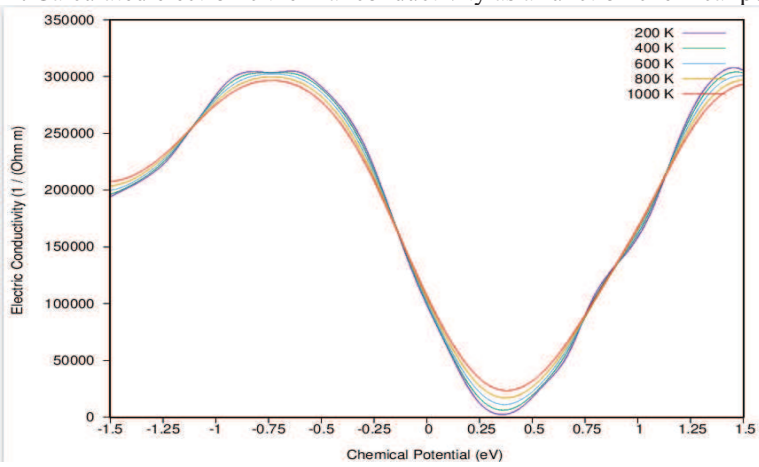

Figure 5. Calculated electric conductivity as a function chemical potential.

3. CONCLUSION

In this study, the structural, electronic, and thermoelectric properties of Mo_2ScAlC_2 have been calculated via ab initio methods. The calculated lattice parameters are in good agreement with the experimental values. The Seebeck coefficient, electronic thermal conductivity, and electric conductivity of Mo_2ScAlC_2 have been tabulated, however, there is no any experimental or theoretical results for the comparison of these results. The band structure of Mo_2ScAlC_2 exhibit metallic character.

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