FIRST-PRINCIPLES CALCULATIONS OF STRUCTURAL, ELASTIC, ELECTRONIC AND TRANSPORT PROPERTIES OF VANADIUM-DOPED ZIRCONIUM LEAD CARBIDE MAX PHASE

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DEDICATION

This thesis is dedicated to my wife Mary, Benedict my son and my daughter Esther for their love, prayers, and patience, throughout the Ph.D. journey. They have been a source of inspiration. Remembering my late parents Mr. Bai Summanuwa and Mrs. Kush'da Bai both of blessed memory; may their souls rest in peace with the Lord; their prayers and love have taught me to be sincere and courageous in life. I missed their company and will forever remain indebted to them.

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ABSTRACT

First-principles calculations have been used to systematically investigate the structural, electronic, elastic, thermodynamic, and transport properties of Zr_2PbC MAX phase and its alloys. The V-based alloys $(V_xZr_{1-x})_2PbC$, $0 \leq x \leq 1$ were synthesized by substituting V on the M-site of the MAX phase at a concentration of 0.25, 0.50, 0.75, and 1.00 respectively. Within the density functional theory (DFT), density functional perturbation theory (DFPT), and Boltzmann transport theory, the generalized gradient approximation (GGA: PBE, PBEsol, PW91), the local density approximation (LDA: PZ) exchange-correlation functionals, and the plane-wave pseudopotential method were used. The examined materials crystallized into a hexagonal shape of space group P63/mmc in relaxed and optimized configurations. The calculated electronic bands and density of states show that the studied MAX phases are conductors. The elastic constants show that all studied materials are mechanically stable based on the Born stability criteria for hexagonal crystals, and structurally stable based on the total minimum energy of the relaxed structures. The 100 % replacement of the Zr atoms shows a significant increase in the Seebeck coefficient and the thermoelectric figure of merit of the terminal MAX phase (V_2PbC). Structurally all the studied materials are hard, brittle, and of high directional anisotropy. Calculated properties have been compared with available experimental data and are in good agreement. All four alloys show a significant increase in the electronic, elastic and thermodynamic properties with a decrease in the lattice parameters as the V concentration increases. The terminal alloy V_2PbC has a lower total energy compared to the Zr_2PbC. The transport properties have been calculated in a temperature range of 200 to 800 K by applying GGA (PBE). For the material at 800 K, a rapid decrease in the thermal conductivity with a slow decrease in electrical conductivity leads to an increase in the figure of merit.

ABSTRAK

Pengiraan prinsip pertama telah digunakan untuk menyiasat secara sistematik sifat struktur, elektronik, elastik, termodinamik dan pengangkutan bagi fasa Zr_2PbC MAX dan aloinya. Aloi berasaskan V $(V_xZr_{1-x})_2PbC$, $0 \leq x \leq 1$ telah disintesis dengan menggantikan V pada tapak-M fasa MAX pada kepekatan 0.25, 0.50, 0.75, dan 1.00 masing-masing. Dalam teori fungsian ketumpatan (DFT), teori usikan fungsian ketumpatan (DFPT), dan teori pengangkutan Boltzmann, penghampiran kecerunan umum (GGA: PBE, PBEsol, PW91), penghampiran ketumpatan tempatan (LDA: PZ) fungsian korelasi pertukaran, dan kaedah pseudo-keupayaan gelombang satah telah digunakan. Bahan yang diperiksa menghablur menjadi bentuk heksagon kumpulan ruang P63/mmc dalam konfigurasi santai dan teroptimum. Jalur elektronik yang dikira dan ketumpatan keadaan menunjukkan bahawa fasa MAX yang dikaji adalah konduktor. Pemalar anjal menunjukkan semua bahan yang dikaji adalah stabil secara mekanikal berdasarkan kriteria kestabilan Born untuk kristal heksagon, dan stabil secara struktur berdasarkan jumlah tenaga minimum struktur santai. Penggantian 100% atom Zr menunjukkan peningkatan ketara dalam pekali Seebeck dan angka merit termoelektrik fasa MAX terminal (V_2PbC). Secara struktur semua bahan yang dikaji adalah keras, rapuh, dan anisotropi berarah tinggi dalam arah yang sama. Sifat yang dikira telah dibandingkan dengan data experimen sedia ada dan berada dalam persetujuan yang baik. Keempat-empat aloi menunjukkan peningkatan ketara dalam sifat elektronik, elastik dan termodinamik dengan penurunan dalam parameter kekisi apabila kepekatan V meningkat. Aloi terminal V_2PbC mempunyai jumlah tenaga minimum berbanding dengan Zr_2PbC. Sifat pengangkutan telah dikira dalam julat suhu 200 hingga 800 K dengan menggunakan GGA (PBE). Untuk bahan pada 800 K, penurunan pesat dalam kekonduksian haba dengan penurunan perlahan dalam kekonduksian elektrik membawa kepada peningkatan dalam angka merit.

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LIST OF ABBREVIATIONS

DFT	Density functional theory
GGA	Generalized gradient approximation
LDA	Local density approximation
PBE	Perdew Burke Ernzerhof
ecut	Cut-off kinetic energy
QE	Quantum Espresso
pw	Plane-wave
CB	Conduction band
VB	Valence band
a.m.u.	Atomic mass unit
DFPT	density-functional perturbation theory
K-S	Kohn-Sham
H-K	Hohenberg-Kohn
TDOS	Total density of states
PDOS	Partial density of states
CRTA	Constant Relaxation Time Approximation

LIST OF SYMBOLS

Å	Angstrom
σ_τ	Electrical conductivity
τ	Time
σ	Stress tensor
ϵ	Strain tensor
C_{ij}	Elastic constant tensor
ε_0	Ground state energy
ε_{XC}	Exchange correlation energy
eV	Electron volt
P	Pressure
S_τ	Seebeck coefficient
ε_f	Chemical potential
k_0	Thermal conductivity
k_B	Boltzmann constant
F	Free energy
M	Molecular weight
N_A	Avogadro number
ZT	Figure of merit
BTP2	BoltzTraP2
Ψ	Many electrons wave function
ψ	Single-electron wave function
v	Velocity
Ry	Rydberg
H_v	Vicker's hardness
Γ	Gamma
n	Density
n	Number of atoms
θ_D	Debye temperature
C_v	Heat capacity at constant volume
b	Energy bands
S	Entropy
T	Temperature
K	Kelvin

v_l	Longitudinal sound velocity
v_t	Transverse sound velocity
v_m	Mean sound velocity
N_A	Avogadro number

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CHAPTER 1

INTRODUCTION

1.1 Research Background

The growing interest and demand for high-efficiency clean energy sources are critical to developing renewable energy instruments which will alleviate and resolve the energy issue of the world's ever-expanding population [1]–[4] Traditional energy sources are either depleting or endangering the environment [5]–[7]. The majority of materials developed for thermoelectric generators nowadays are bandgap materials, which are prone to wear and tear at high temperatures[8]–[10].

Thermoelectric materials are a kind of new energy material that can directly convert heat energy into electric energy, and vice versa without needing any other energy conversion via the Seebeck effect of solid materials. Improving the thermoelectric performances of existing thermoelectric materials and exploring new thermoelectric materials with excellent performance are eternal research topics in the thermoelectricity field performance of thermoelectric materials can be evaluated by the figure of merit $ZT = (S_\tau^2 \sigma_\tau / k_{el})T$, where S_τ is the Seebeck coefficient, σ_τ is the electrical conductivity, k_{el} is the thermal conductivity and T is the temperature [11]. These three parameters for fundamental physical properties of solid are, however, dependent upon each other as a function of the carrier concentration. In particular, S_τ and σ_τ generally vary reciprocally, making a dramatic improvement in the power factor, $S_\tau^2 \sigma_\tau$, difficult. Accordingly, semiconducting alloys and compounds with high carrier mobilities have been intensively studied as thermoelectric materials, e.g., Bi_2Te_3[12], PbTe[13], and Si–Ge[14] alloys. A highly covalent character of these materials appears to be responsible for their high mobilities. The efficiency of thermoelectric energy conversion also improves with increasing temperature differences over which the thermoelectric device operates. In recent years, the MAX phases and their derived MXene phases have gradually received the attention of

researchers as promising thermoelectric materials due to their unique microstructures and properties [15].

The term MAX phases (also called nanolaminates because of their layered structures, which consist of hexagonal carbide or nitride blocks $M_{n+1}X_n$ refers to ternary nitrides and carbides classified into families of $M_{n+1}AX_n$ ($n = 1$ to 3) with over 150 different structures that have been widely studied over the last two and a half decades [16]–[25]. They have a layered structure and a distinct set of features bridging the gap between metals and ceramics characteristics [26]–[29]. The group crystallizes to the hexagonal shape of the $P6_3/mmc$ space group, with M representing the early transition d metals like Cr, Hf, Zr, Ta, Nb, Mo, Ti, and V. The A is the p elements from group 12 to16 in the periodic table such as Al, Sn, P, Ge, S, In and Si, while the X is nitrogen (N) and, or carbon (C)[30]–[33].

Due to the metal like characteristics they are categorized as good thermal and electrical conductors, plastically deformable at room temperature, damage tolerant, resistant to thermal shock, and relatively soft whereas as ceramics materials, they are often distinguished by high temperature elastic and mechanical properties, as well as superior corrosion resistance [34]–[38]. They are a new class of materials that have intrigued the academic and commercial interests of many since their reappearance in the 1990s [39], [40]. Several MAX phases, emanating from the integer $n = 1$ also known as the 211 MAX phases with examples like Zr_2PbC, Cr_2AlC[41], Cr_2GaC, Hf_2InC, Hf_2SC, Mn_2GaC[42], Mo_2GaC, Nb_2AlC, Nb_2AsC[43]–[46], have been synthesized. Others are the 312 MAX phases with $n = 2$ like Ti_3AlC_2, Ti_3GeC_2, Ti_3SnC_2, Ta_3AlC_2, Ti_3ZnC_2, Zr_3AlC_2, and the 413 MAX phases with $n = 3$ like Ti_4GaC_3, Ti_4SiC_3, Ti_4GeC_3, Nb_4AlC_3, Ta_4AlC_3[47], $(Mo,V)_4AlC_3$ are some examples of the various classes of MAX phases to mention just a few that have been synthesized and studied theoretically and experimentally to date[43], [48]–[52].

The well-known potential applications of MAX phase materials include high-temperature applications in the aviation and automobile industries[28] [53], protective and bond-coatings for gas turbines, accident-tolerant fuel cladding in nuclear power plants, solar receivers in concentrated solar power systems, and

electrical contacts for catalysis [37], [50], and joining material[28]. The robustness of the compounds to external forces also called their mechanical stability is a property to ensure its sustainability in any application[54]. Stability and hardness are crucial for industrial applications[54], [55].

The pursuit of advanced technologically high-impact qualities, as well as the opportunity to develop materials with new functionalities, has spurred interest in MAX phases formed by substitution or replacement on the M, A, or X sublattices [41], [46], [56]–[62]. The ability to alloy MAX complexes not only helps to improve their properties but also helps to lower the total energy that would otherwise be metastable in their pure condition [63]. There have been quite a number of both theoretical and experimental research aimed at investigating the different ground and elevated state properties like the structural, electronic, thermodynamic, optical, and transport properties of MAX families of compounds [41], [46], [56]–[58].

According to the literature, the majority of studies on bulk Zr_2PbC focus on the effect of pressure and temperature changes on the properties. While several accessible publications on Zr_2PbC and selected literature on similar crystals have explored the effects of substituting different atoms on the M, A, and X sites on the properties of Zr_2PbC and other selected MAX phases [59]–[62], [64]. The majority of the study has concentrated on the structural, electrical, elastic, and thermodynamic properties of the pure and alloy of Zr_2PbC MAX phase. A handful of such works available on the parent Zr_2PbC MAX phase, and the selected literature on similar nanolaminates have, however, studied the effects of substituting different elements like Mn [65], Cr, Mo [66] [19], Ti, V, Mn, Fe, Mo [67] on the M-site; Sn, Bi, Sb[68], Bi[69], and Pb[70] on the A-site., and C, N [46], respectively, on the X site to investigate the properties.

1.2 Problem Statement

The current state of research on thermoelectric materials limits their engineering uses in thermoelectric devices. Discovering novel thermoelectric materials are continual research areas that need closer attention [71]. MAX phases and their MXene phase counterparts have all it takes to be the alternative thermoelectric materials due to their enormous high-temperature adaptability, and structural and mechanical stability. To harness the thermoelectric potentials in MAX phases, relevant substitution elements of the early transition metals like vanadium V on the M site will enhance the thermoelectric figure of merit by maximizing the Seebeck coefficient, electrical conductivity, and minimizing the electronic thermal conductivity to meet the ever-expanding global energy challenges. Several MAX phases, most notably Ti_3SiC_2 [72], [73], Cr_2AlC, Nb_2AlC [74], Ti_3AlC_2 [75], have been found to possess very low Seebeck coefficients[76], [77]. Previous works of literature on Zr_2PbC[24], [78], Ti_2AlC, V_2AlC, Cr_2AlC, and Nb_2AlC [74] [74], and other MAX phases have focussed mostly on the use of different substitution elements on the M, A, and X-site which has raised the hope to investigate the thermoelectric properties of MAX phases.

Therefore, this has motivated expansive research in the past decade toward the development of novel thermoelectric MAX phases. However, despite many recent studies of these MAX phases several of their physical properties like the Seebeck coefficient issue have not been encouraging due to low values [72], [73][74][75]. This work aims at enhancing the electrical, elastic, thermodynamic, and thermoelectric properties of the parent Zr_2PbC MAX phase using V as a replacement element to enhance the Seebeck coefficient, and electrical conductivity and simultaneously lower the electronic thermal conductivity. Understanding these fundamental properties is of great importance for thermoelectric performance and future technological applications.

1.3 Research Objectives

This thesis investigates the properties of the parent Zr_2PbC MAX phase by employing V as the substituting element on the M-site at a concentration of $(V_xZr_{1-x})_2PbC$, $0.25 \leq x \leq 1.00$, using GGA and LDA exchange functionals, respectively. The specific objectives are to:

(a) Determine the structural, electronic, elastic, and thermoelectric properties of Zr_2PbC MAX phase.

(b) Evaluate the structural and electronic properties of $(V_xZr_{1-x})_2PbC$.

(c) Compute the elastic properties of $(V_xZr_{1-x})_2PbC$

(d) Calculate the thermoelectric coefficients of $(V_xZr_{1-x})_2PbC$ using GGA XC functional within a temperature range of 200 to 800 K.

1.4 Scope of Research

The structural, electronic, elastic, thermodynamic, and transport properties of $(V_xZr_{1-x})_2PbC$, $0 \leq x \leq 1$, MAX phase have been investigated using the density functional theory (DFT)[79] plane-wave method, density functional perturbation theory(DFPT) [80], and Boltzmann transport theory (BTE) [81], [82], respectively. The GGA (PBE, PBEsol, PW91) [83], and LDA(PZ) [84] exchange functionals, respectively have been used to study the structural, electronic, elastic, and thermodynamic properties of the bulk Zr_2PbC, the V-containing MAX phase using an average converged k-mesh of 14 × 14 ×14 and cut-off energy of 500 Ry. While thermoelectric properties: Seebeck, power factor, electrical and thermal conductivities have been calculated using GGA(PBE) using cut-off energy of 500 Ry and a dense k-mesh of 30 × 30 × 30 within a temperature of 200 to 800 K.

1.5 Significance of Study

Thermoelectricity has recently gained recognition due to its capacity to transform waste heat into energy while emitting no toxic toxins. The rebirth of research into thermoelectric materials began in the early 1990s [15]. Thermoelectric materials are environmentally friendly for power generation and refrigeration, thus providing a solution for energy crisis and pollution; however, the thermoelectric conversion efficiency is low and mainly limited by the performance of thermoelectric materials. New concepts and technologies were applied recently to enhance ZT, but accompanied difficulties need to be solved. There is still a long way between high thermoelectric performance and high thermoelectric conversion efficiency. Building a device that could reach the theoretical efficiency is not a trivial pursuit, but a huge development project by itself considering the tremendous practical challenges involved, suitable low resistance hot side, and cold side metal contacts, optimizing assembly of modules, etc. The development of thermoelectric materials and devices needs connected efforts involving physicists, chemists, materials scientists, and theory scientists[11].

This work is an effort to enhance the thermoelectric coefficients and other properties of Zr_2PbC by substituting the Zr atoms with V atoms. research on MAX phases has intrigued the interest of many people and continues to do so due to their unusual hybrid metal/ceramic capabilities coming from their structure and atomic arrangement, and they are being evaluated for several applications[85], [86]. The simplicity with which MAX phases may be machined to high tolerance is also a key factor to consider when designing tools for dry drilling concrete surfaces in civil engineering tasks. This may bring the materials close to the market. Other applications include electrodes, free-cutting elements[26], exhaust gas filters for automobiles, corrosion-resistant materials, surface coatings materials, and microelectronics[87].

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LIST OF PUBLICATIONS

1. S. T. Ahams, A. Shaari, R. Ahmed, N. F. Abdul Pattah, M. C. Idris & B. U. Haq. (2021) Ab initio Study of the Structure, Elastic, and Electronic Properties of $Ti_3(Al_{1-n}Si_n)C_2$ Layered Ternary Compounds. *Scientific Reports.* https://doi.org/10.1038/s41598-021-84466-5

2. S. T. Ahams*, A. Shaari, R. Ahmed, N. F. Abdul Pattah, M. C. Idris, B. U Haq. (2021) Theoretical investigation of Zr_2PbC, $(V_{0.25}Zr_{0.75})_2PbC$, $(V_{0.5}Zr_{0.5})_2PbC$, $V_{0.75}Zr_{0.25})_2PbC$, and V_2PbC MAX phases: A DFT based study. *Materials Today Communications* **27** 102397. https://doi.org/10.1016/j.mtcomm.2021.102397.

3. S. T. Ahams*, A. Shaari, R. Ahmed, N. F. Abdul Pattah, M. C. Idris, B. U Haq. (2021) A DFT investigation of the structural, mechanical, thermodynamic, and electronic properties of Zr_2PbC MAX phase. *Solid State Technology* 64(2)4863-4874.

4. S. T. Ahams, A. Shaari, R. Ahmed, N. F. Abdul Pattah, M. C. Idris. (2020) Ab-initio Calculations of the Structural and Electronic Properties of Zr_2AC . *Proceedings of Science and Mathematics*, **1**, 41-4641.