



A study on the vibrational frequencies, elastic properties and sound velocities of vanadium spinel oxides AV_2O_4 ($A = Mn, Fe$ and Zn) short-range non-Coulomb potential theoretical model

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Abstract. Owing to the fact of the AB_2O_4 spinel oxide's chemical and thermal stability, and other intriguing properties make them suitable candidate materials for many applications, including chemical looping and catalytic reactions. To do our investigations, a short-range non-Coulomb potential theoretical model is used to calculate the zone-centre, elastic constants, infrared phonon mode frequencies, Raman phonon mode frequencies, velocities of the sound wave along the highly symmetric three crystallographic-axes and Debye temperature of the vanadium spinel oxides AV_2O_4 ($A = Mn, Fe$ and Zn). The preliminary results of our calculations show that the interaction in the second neighbour ($V-O$) is much stronger than the interaction of the first neighbour ($A-O$). Moreover, from the analysis of the obtained results of elastic constants, the nature of the studied vanadium spinels are found to be ductile.

Keywords. Vanadium spinels; elastic constants; non-Coulomb interaction potential; vibrational modes; Debye temperature.

1. Introduction

Recently, the geometrically frustrated materials have attracted great interest among the theoretical and experimental researchers due to their interesting properties, such as suitable bandgap values, which make them ideal for electronic and spintronic applications.

The vanadium spinels are a member of the family of frustrated materials. The vanadium compounds AV_2O_4 ($A = Mn, Fe$ and Zn) having closed packed face-centred cubic structure crystallize at normal conditions with space group $Fd\bar{3}m$ (# 227). There are 56 atoms in the conventional cell of the AV_2O_4 cubic spinels, occupying the following Wyckoff sites: at 32e (u, u, u) position oxygen 32-atoms, 8 A-type atoms at 8a (1/8, 1/8, 1/8) and 16 B-type atoms at 16c (1/2, 1/2, 1/2). The primitive cell contains 14 atoms. The crystal structure of AV_2O_4 is depicted in figure 1. Cubic spinels show 39 optical

normal modes which are described by the following irreducible representation:

$$\Gamma = A_{1g}(R) + E_g(R) + F_{1g} + 3F_{2g}(R) + 2A_{2u} + 2E_u + 5F_{1u}(IR) + 2F_{2u}, \quad (1)$$

where (IR) represents infrared and (R) represents Raman active vibrational species. AV_2O_4 spinels undergo structural and magnetic transitions at various temperatures [1]. Recently, Wheeler *et al* [2] predicted that MgV_2O_4 goes through a structural transition from cubic structure to tetragonal one, and magnetic transition from paramagnetic state to antiferromagnetic one at 51 and 42 K temperatures, respectively. Due to the electron–electron correlations, the vanadium spinels AV_2O_4 behave like Mott insulators. Using the density functional theory, Kaur *et al* [3] stated that the inclusion of spin–orbit coupling is necessary to explain the semiconducting behaviour of CoV_2O_4 . Very recently, Li

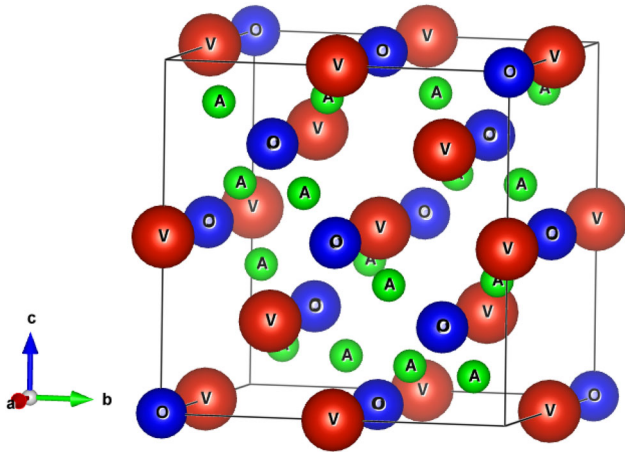


Figure 1. Crystal structure of AV_2O_4 ($A = \text{Mn, Fe and Zn}$).

et al [4] calculated the bulk modulus and cell volume of AV_2O_4 ($A = \text{Mg, Mn, Fe, Co, Zn}$) using density functional theory. Myung-Whun *et al* [5] measured the single-crystal infrared active phonon modes of MnV_2O_4 at 300 K using infrared ellipsometry. Jung *et al* [6] measured the infrared active phonon modes for the cubic and tetragonal phases of ZnV_2O_4 by reflectivity measurement. Rabia [7] measured the zone-centre infrared active phonon modes for ZnV_2O_4 at 1.0 GPa. Luan [8] measured the elastic constants for the three vanadium spinels: MnV_2O_4 , FeV_2O_4 and ZnV_2O_4 using resonant ultrasound spectroscopy (RUS). Although some other investigations are also reported in the literature, there is room for further investigations to expose their scope.

In this study, we perform computational investigations on the elastic properties, vibrational frequencies and sound velocities of vanadium spineloxides AV_2O_4 ($A = \text{Mn, Fe and Zn}$) within the theoretical model of short-range non-Coulomb interaction model potential.

2. Computational methodology

The present study was performed through the short-range non-Coulomb interaction potential model. In this approach, potential energy (ϕ^N) expanding through Taylor's series, for studied compounds, can be expressed by the following model [9,10]:

$$\phi^N = \sum_{\text{lmn}} \left[\frac{1}{r} \left(\frac{d\phi^N}{dr} \right) \Big|_{r=|r_k|} \left\{ r_{\text{lmn}}^o (S_{\text{lmn}} - S_o) + \frac{1}{2} |S_{\text{lmn}} - S_o|^2 \right\} + \frac{1}{2} \left\{ \frac{1}{r} \frac{d}{dr} \left(\frac{1}{r} \frac{d\phi^N}{dr} \right) \Big|_{r=|r_k|} \left\{ r_{\text{lmn}}^o \cdot (S_{\text{lmn}} - S_o) \right\}^2 \right\}, \quad (2)$$

where S_o and S_{lmn} represent central ion distance and its nearest neighbour ions distances from their normal positions, respectively, whereas r_{lmn} stands for position coordinates of the neighbouring ions at their equilibrium states.

However, l , m and n describe direction cosines of the lines formed by joining the central ion and nearest neighbouring ions. And $|r_k|$ is used to represent the distance of the nearest neighbouring ion. In this study, we have taken into account the potential model of the non-Coulombic interaction between central and its three nearest neighbouring ions, respectively, which gives out the following expression:

$$\frac{e^2}{V} A_k = \frac{d^2 \phi^N}{dr^2} \Big|_{r=|r_k|}, \quad (3)$$

where A_k is supposed to be force constant of bond stretching, which is derived by taking second-order derivative of the potential energy (ϕ^N) expressed in equation (1). However, force constant B_k for the bond bending is expressed by taking the first-order derivative of ϕ^N :

$$\frac{e^2}{V} B_k = \frac{1}{r} \frac{d\phi^N}{dr} \Big|_{r=|r_k|}, \quad (4)$$

where k mentioned in equations (3 and 4) represents first, second and third neighbouring ions, i.e., $k = 1$.

3. Results and discussion

3.1 Interatomic interactions and zone-centre phonons

In this study, we have considered the interatomic interactions of up to three nearest neighbouring ions. The corresponding three interactions of bond stretching represented by A_1, A_2, A_3 , and interactions of bond bending represented by B_1, B_2, B_3 , between the atoms A–O, V–O and O–O, respectively, were computed. The simulated unit cells of the compounds under this study were found with 14 atoms per unit cell and hence the dynamical matrix of the order of (42×42) is obtained. Then by solving this dynamical matrix at the zone-centre, we get different analytical expressions for fundamental modes. For the studied compounds, the LO-TO of F_{1u} modes are not available in the literature and thus it is not possible to calculate the effective dynamical charge. Therefore, long-range Coulomb interaction is not included in this study. In the case of MnV_2O_4 and ZnV_2O_4 spinels, we have used the experimental values of four infrared modes F_{1u} [5,6] and the experimental values of the elastic constants C_{11} and C_{12} [8] to calculate the three bond-stretching and three bond bending interactions. Due to the unavailability of experimental data for the zone-centre phonon modes for FeV_2O_4 , we have used the experimental values of the elastic constants C_{11} , C_{12} and C_{44} [8] to calculate the three bond-stretching interactions. On the other hand, to find out the bond bending interactions of the FeV_2O_4 , it was assumed that its bond bending interaction will be equal to average values of the related bond-bending interactions of the MnV_2O_4 and ZnV_2O_4 spinels, as the Fe atom is between the Mn and Zn atoms in the periodic table. The adopted assumption was found to be quite reasonable.

Table 1. Calculated force constants (in kdyn cm^{-1}) for the vanadium spinels AV_2O_4 ($A = \text{Mn, Fe and Zn}$).

Force parameters	Internal coordinates	MnV_2O_4	FeV_2O_4	ZnV_2O_4
A_1	A–O	74.46	81.59	96.78
B_1	A–O	3.16	3.67	4.27
A_2	V–O	135.31	141.89	149.13
B_2	V–O	2.71	3.52	3.91
A_3	O–O	25.37	23.43	19.39
B_3	O–O	0.62	0.48	0.41

The calculated force parameters for vanadium spinels AV_2O_4 ($A = \text{Mn, Zn and Fe}$) are listed in table 1. Then the calculated bond bending and bond stretching force parameters of the studied vanadium spinels were used to calculate Raman phonon modes and infrared (active and inactive) phonon modes of the MnV_2O_4 , FeV_2O_4 and ZnV_2O_4 . The obtained results of our calculations along with available experimental data are provided in tables 2 and 3. From the analysis of the data, we found that the results obtained by the proposed model are comparable to the available experimental values [5,6] for MnV_2O_4 and ZnV_2O_4 . However, experimental data are not available in the literature for comparison with FeV_2O_4 .

3.2 Elastic constants and their related properties

To calculate elastic properties, the calculations of the elastic constants are important. To determine elastic properties, three elastic constants only, named C_{11} , C_{12} and C_{44} , are sufficient for the complete description of the elastic-related properties of a cubic-structured material. In the present study, we have calculated the above three elastic constants for the studied vanadium spinels AV_2O_4 ($A = \text{Mn, Zn and Fe}$) by using the methodology available in the references [9,10]. The obtained results of studied vanadium spinels are tabulated in table 4 along with the previously measured and calculated data. From table 4, the following results can be drawn:

(i) The calculated elastic constants verify the Born's stability criteria for cubic systems [11]:

$$\begin{aligned} (C_{11} - C_{12}) > 0, \quad C_{12} < B < C_{11}, \\ (C_{11} + 2C_{12}) > 0, \quad C_{44} > 0. \end{aligned} \quad (5)$$

Table 2. Calculated zone-centre Raman active and inactive phonon modes (in cm^{-1}) for the vanadium spinels AV_2O_4 ($A = \text{Mn, Fe and Zn}$).

System	A_{1g}	E_g	$F_{2g}(1)$	$F_{2g}(2)$	$F_{2g}(3)$	F_{1g}
MnV_2O_4	652	426	613	523	178	439
FeV_2O_4	659	435	628	531	186	444
ZnV_2O_4	678	452	638	543	201	456

These results clearly show that the studied vanadium spinels AV_2O_4 ($A = \text{Mn, Zn and Fe}$) are mechanically stable.

(ii) C_{12} and C_{44} are smaller than C_{11} , indicating that the studied vanadium spinels are more resistant to the linear compressional deformation as compared to the shear one [12,13].

(iii) The elastic constant C_{44} characterizes the resistance of a solid to shearing stress along the (100) plane [13,14]. One notes that the C_{44} value decreases in the sequence $\text{ZnV}_2\text{O}_4 \rightarrow \text{FeV}_2\text{O}_4 \rightarrow \text{MnV}_2\text{O}_4$, indicating that the resistance to the shape change (shear deformation) decreases in the same order.

(iv) The calculated values of the single elastic constants for MnV_2O_4 and MnV_2O_4 are in fairly good agreement with previous measured data [8], whereas those of MnV_2O_4 deviate from the experimental data [8]. This may be due to the fact that the single crystal used for the measurement was not pure.

(v) Bulk modulus (B) of a solid characterizes its resistance against the variation of its volume by an externally applied pressure. By using Voigt, Reuss and Hill approximations, the polycrystalline elastic constants, such as bulk modulus (B) and shear modulus (G) are calculated from the single crystal elastic constant approach described in literature [15–18]. For cubic systems, the bulk modulus (B) can also be computed by using the following relation:

$$B = B_H = B_V = B_R = (C_{11} + 2C_{12})/3, \quad (6)$$

where B_V , B_R and B_H stand for the Voigt, Reuss and Hill bulk moduli, respectively. The obtained results for B are listed in table 4. The calculated bulk moduli for MnV_2O_4 and FeV_2O_4 are in good agreement with the experimental results [8]. The calculated B values of the three considered compounds are in very good agreement with previous theoretical calculations [4]. It is clear from the data that the calculated bulk moduli results are decreased in the following order: $\text{ZnV}_2\text{O}_4 > \text{FeV}_2\text{O}_4 > \text{MnV}_2\text{O}_4$.

The shear modulus of a solid represents its resistance against reversible deformation due to shearing strain and it is more relevant to the hardness of the material. The Voigt (G_V), Reuss (G_R) and Hill (G_H) shear moduli were

Table 3. Calculated frequencies of the zone-centre infrared active and inactive phonon modes (in cm^{-1}) for vanadium spinels AV_2O_4 (A = Mn, Zn and Fe) along with available experimental data [5,6].

System	$F_{1u}(1)$	$F_{1u}(2)$	$F_{1u}(3)$	$F_{1u}(4)$	$A_{2u}(1)$	$A_{2u}(2)$	$E_u(1)$	$E_u(2)$	$F_{2u}(1)$	$F_{2u}(2)$
MnV₂O₄										
This work	588	438	341	161	856	513	889	347	778	268
Expt. [5]	581	427	344	168						
FeV₂O₄										
This work	546	311	212	201	778	438	713	313	688	228
ZnV₂O₄										
This work	557	321	233	189	710	479	823	338	725	251
Expt. [6]	547	311	234	190						

Table 4. Calculated elastic constants (C_{11} , C_{12} and C_{44} , in GPa), bulk modulus (B , in GPa), shear modulus (G , in GPa), Young's modulus (Y , in GPa), Poisson's ratio (σ , dimensionless) anisotropy factors (A^Z and A^U) for the vanadium spinels AV_2O_4 (A = Mn, Zn and Fe) along with the available experimental and theoretical results for comparison.

	C_{11}	C_{12}	C_{44}	B	G_H	Y	σ	A^Z	A^U	
MnV₂O₄										
Present	221.81	151.36	78.91	174.8	57.32	90.09	0.4056	2.148	0.7755	
Expt. [8]	215.70	149.22	74.22	171.4						
Other [4]				170.2						
FeV₂O₄										
Present	228.38	154.03	74.74	178.8	56.42		0.4028	2.072	0.6192	
Expt. [8]	249.91	217.65	72.86	228.4						
Other [4]				168.2						
ZnV₂O₄										
Present	237.23	159.74	72.32	185.6	56.18		0.4024	2.061	0.5068	
Expt. [8]	138.95	56.83	41.06	84.2						
Other [4]				192.5						

calculated using single-crystal elastic constants using the following relationships:

$$\begin{aligned} G_V &= (C_{11} - C_{12} + 3C_{44})/5; \\ 5/G_R &= 1/(C_{11} - C_{12}) + 3/C_{44}; \\ G_H &= (G_R + G_V)/2. \end{aligned} \quad (7)$$

The obtained results of the shear moduli, from our calculations, related to the spinels compounds studied in this paper are listed in table 4. Shear modulus decreases in the sequence: $\text{MnV}_2\text{O}_4 > \text{FeV}_2\text{O}_4 > \text{ZnV}_2\text{O}_4$, which is opposite to the variation trend of the bulk modulus, suggesting that the hardness of these compounds decreases in the following sequence: $\text{MnV}_2\text{O}_4 \rightarrow \text{FeV}_2\text{O}_4 \rightarrow \text{ZnV}_2\text{O}_4$. The Young modulus (Y) describes the resistance offered by a solid against external uniaxial tension. It was noted that if Young modulus results are higher, it indicates that material is stiffer

[19]. The Young's modulus is calculated using a single elastic constants approach using the following relation:

$$Y = \frac{(C_{11} + 2C_{12})(C_{11} - C_{12})}{C_{11} + C_{12}}. \quad (8)$$

The Poisson's ratio (σ) measures the strength of expansion or contraction of a material in the direction perpendicular to the direction of compression or stretching. Moreover, it is used to understand the nature of the material's bonding. In this regard, typical values of Poisson's ratio for metallic, ionic and covalent materials are 0.33, 0.25 and 0.1, respectively [14]. The Poisson's ratio can be calculated through the following expression:

$$\sigma = \frac{C_{12}}{C_{11} + C_{12}}. \quad (9)$$

The calculated results are summarized in table 4. No experimental or theoretical data are available for comparison purposes. The calculated values of σ for MnV_2O_4 , FeV_2O_4 and ZnV_2O_4 are 0.4056, 0.4028 and 0.4024, respectively. These results show that the metal bond is dominant in the explored compounds.

Pugh's empirical criterion [20,21] is a measure of the ductile or brittle nature of a solid. According to this criterion, the B/G ratio is greater (lower) than 1.75 for a ductile (brittle) material. The calculated value of B/G is equal to 3.049 for MnV_2O_4 , 3.169 for FeV_2O_4 and 3.304 for ZnV_2O_4 , indicating the ductile nature of the studied materials. Besides this, Cauchy pressure measured by a relation $(C_{12} - C_{44})$ also points out the brittle and ductile nature of materials [13,22,23]. Negative (positive) values of the Cauchy pressure show correspondingly the brittle (ductile) nature of the materials. As the calculated Cauchy pressure values are equal to 72.45 GPa for MnV_2O_4 , 79.29 GPa for FeV_2O_4 and 87.42 GPa for ZnV_2O_4 , confirming the ductile nature of the studied materials.

The knowledge of the elastic anisotropy of the materials is also important because its proper evaluation provides information about the creation of the micro-cracks in materials [24,25]. In this study, four different criteria were employed to evaluate the extent of the elastic anisotropy for the given compounds.

(i) Zener anisotropy is given by:

$$A^Z = \frac{2C_{44}}{C_{11} - C_{12}} \quad (10)$$

(ii) Universal anisotropy is defined as follows [26]:

$$A^U = \frac{5G_V}{G_R} + \frac{B_V}{B_R} - 6 \quad (11)$$

(iii) Three dimensional (3D) representation of Young's modulus (Y) depend upon the crystallographic directions.

(iv) Shear modulus anisotropy for an elastically isotropic material, $A^Z = 1$ and $A^U = 0$. Hence, any deviation in A^Z and A^U values from their critical values indicates the presence of the elastic anisotropy in the studied crystalline materials. Our calculated results of the A^Z and A^U (see table 4) show that the title compounds have a noticeable elastic anisotropy and their elastic anisotropy was found to be decreased in the sequence: $MnV_2O_4 \rightarrow FeV_2O_4 \rightarrow ZnV_2O_4$. 3D representation of the directional dependent E is a very useful way to visualize the extent of the elastic anisotropy. 3D-closed surface representing crystallographic directions dependent E for the cubic system can be expressed by using the following relation:

$$\frac{1}{E} = (l_1^4 + l_2^4)s_{11} + l_3^4s_{33} + l_1^2l_2^2(2s_{12} + s_{66}) + l_3^2(1 - l_3^2)(2s_{13} + s_{44}), \quad (12)$$

where l_1 , l_2 and l_3 are representing directional cosines with respect to the axes, x , y and z respectively, and s_{ij} denotes

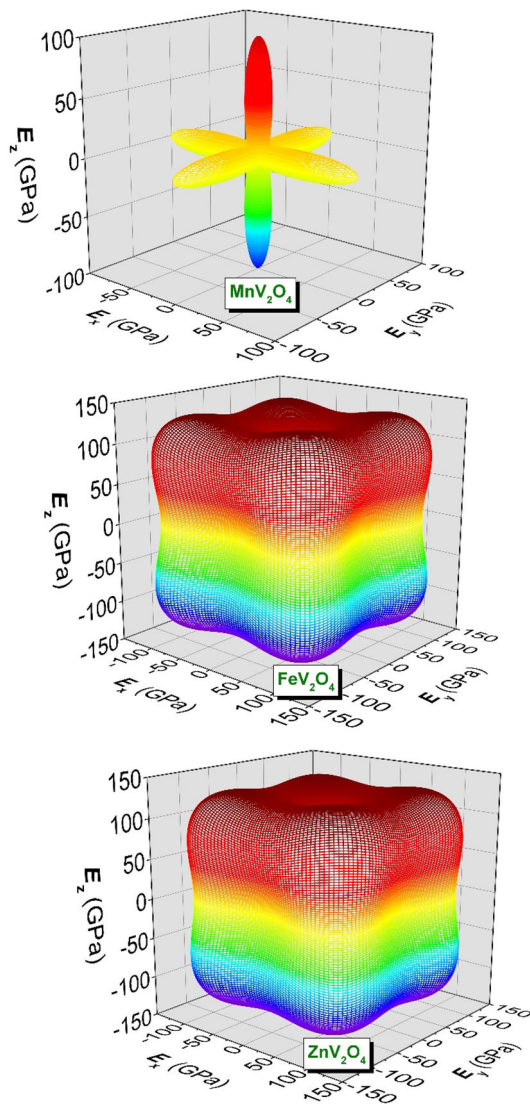


Figure 2. 3D representation of the crystallographic direction dependence of Young's modulus Y for MnV_2O_4 , FeV_2O_4 and ZnV_2O_4 compounds.

Table 5. Calculated isotropic elastic wave velocities (in $m\ s^{-1}$) and Debye temperature (T_D , in K) for the vanadium spinels AV_2O_4 ($A = Mn, Fe$ and Zn).

Compound	V_L	V_T	V_m	T_D
MnV_2O_4	7139	3410	4213	635
FeV_2O_4	7003	3300	4129	608
ZnV_2O_4	6796	3156	3867	558

the generalized form of the elastic compliance constants. For an isotropic material, the obtained 3D-closed surface, represented for the crystallographic directions dependent E , is found to be in the spherical shape. Any deviation from the spherical shape reveals its extent for the elastic anisotropy.

Table 6. Calculated acoustic wave velocities (in m s^{-1}) propagating along the [100], [110] and [111] crystallographic directions for the vanadium spinels MnV_2O_4 , FeV_2O_4 and ZnV_2O_4 .

Propagation direction	Velocity expression	MnV_2O_4	FeV_2O_4	ZnV_2O_4
[100]	$v_L = \sqrt{C_{11}/\rho}$	6708	6640	6486
	$v_T = \sqrt{C_{44}/\rho}$	4001	3798	3581
[110]	$v_L = \sqrt{(C_{11} + C_{12} + 2C_{44})/2\rho}$	7338	7167	6929
	$v_T = \sqrt{C_{44}/\rho}$	4001	3798	3581
	$v_{T\perp} = \sqrt{(C_{11} - C_{12})/2\rho}$	2673	2679	2621
[111]	$v'_L = \sqrt{(C_{11} + 2C_{12} + 4C_{44})/3\rho}$	7537	7455	7071
	$v'_T = \sqrt{(C_{11} - C_{12} + C_{44})/3\rho}$	3178	3097	2976

The expressions of the acoustic wave velocities in the aforementioned crystallographic directions. ρ is the mass density; L and T stands for longitudinal and transverse polarizations of the acoustic wave.

3D-closed surfaces for E , as shown in figure 2 for the title compounds, are noticeably different from spherical shapes, revealing the presence of strong characteristics of the elastic anisotropy for the considered compounds. The interatomic forces are not centrosymmetric for the cubic crystal in case the elastic constants C_{11} and C_{44} are different ($C_{11} \neq C_{44}$). The elastic moduli of the studied vanadium spinels are directional dependent since $C_{11} \neq C_{44}$ (see table 4).

The anisotropy of shear modulus can be characterized through the difference between the shear moduli along the [100], $G_{100} = C_{44}$, and [110], $G_{110} = (C_{11} - C_{12})/2$, crystallographic directions. For a cubic system, the crystal is isotropic if $G_{100} = G_{110}$. It is observed that G_{100} (G_{110}) is equal to 78.91 (35.23) GPa for MnV_2O_4 , 72.86 (37.18) GPa for FeV_2O_4 and 72.32 (38.75) GPa for ZnV_2O_4 . These results reveal that G_{100} is different from G_{110} ($G_{100} \neq G_{110}$), suggesting that the shear modulus of the explored compounds is anisotropic. The calculated value of the average shear modulus $G' = (G_{100} + G_{110})/2$ is approximately equal to the calculated shear modulus G of each studied compounds.

Debye temperature (T_D) is also important for many of the physical fundamental parameters, for example, melting temperature, specific heat, etc. [27]. T_D can be calculated using the results of bulk modulus and shear modulus through the following relations [28,29]:

$$\begin{aligned}
 T_D &= \frac{h}{k_B} \left[\frac{3n \rho N_A}{4\pi M} \right]^{1/3} V_m, \\
 V_m &= \left[\frac{1}{3} (2V_T^{-3} + V_L^{-3}) \right]^{-1/3}, \quad V_L = \left(\frac{3B + 4G}{3\rho} \right)^{1/2}, \\
 V_T &= \left(\frac{G}{\rho} \right)^{1/2}
 \end{aligned}
 \tag{13}$$

where h is Plank's constant, k_B is Boltzmann's constant, n the number of atoms in a molecule, N_A the Avogadro number, ρ the mass density and M the molecular weight is used. Similarly, V_m , V_L and V_T are used for the average

sound velocity, average longitudinal sound velocity and average transverse sound velocity, respectively. Calculated values of the Debye temperature (T_D) and average sound wave velocities (V_m , V_L and V_T) for the three studied compounds are reported in table 5. There are no experimental or theoretical data available for comparison. The calculated results show that T_D decreases in the sequence: $\text{MnV}_2\text{O}_4 > \text{FeV}_2\text{O}_4 > \text{ZnV}_2\text{O}_4$.

Thermal conductivity and some other fundamental properties are related to the directional sound wave velocities. Therefore, velocities of the propagation of the sound waves in the crystallographic directions of the [100], [110] and [111] were calculated using a relation obtained from the resolution of the Cristoffel equation [30]. The obtained results (table 6) are showing that the transverse velocity is smaller than the longitudinal acoustic velocity. The sound wave velocities decrease in the same sequence as the calculated elastic constants, because they are proportional to the corresponding square root of the elastic constants (see the relations in table 6).

4. Conclusions

In this study, we have calculated the frequencies of the zone-centre, infrared and Raman active and inactive modes, single and polycrystalline elastic constants, elastic wave velocities and Debye temperature for the vanadium spinels MnV_2O_4 , FeV_2O_4 and ZnV_2O_4 by employing potential model based on short-range non-Coulomb interaction up to the three nearest neighbours. Our calculations showed that the interaction in the second neighbour (V–O) were much more stronger than the interaction of the first neighbour (A–O). Moreover, from the analysis of the obtained results of elastic constants, the nature of the studied vanadium spinels were found to be ductile. Our obtained results were analysed, discussed and also compared with the available theoretical and experimental results. Good concordance of the obtained results with literature showed the success of the suggested model.

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