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Elastic and Thermal Properties of Silicon Compounds from First-Principles Calculations

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Abstract: The structural and elastic properties of V-Si (V_3Si, VSi_2, V_5Si_3, and V_6Si_5) compounds are studied by using first-principles method. The calculated equilibrium lattice parameters and formation enthalpy are in good agreement with the available experimental data and other theoretical results. The calculated results indicate that the V-Si compounds are mechanically stable. Elastic properties including bulk modulus, shear modulus, Young's modulus, and Poisson's ratio are also obtained. The elastic anisotropies of V-Si compounds are investigated via the three-dimensional (3D) figures of directional dependences of reciprocals of Young's modulus. Finally, based on the quasi-harmonic Debye model, the internal energy, Helmholtz free energy, entropy, heat capacity, thermal expansion coefficient, Grüneisen parameter, and Debye temperature of V-Si compounds have been calculated.

Keywords: Elastic; Thermal Properties; Vanadium-Silicides.

1 Introduction

Due to the potential chemical and physical properties, transition metal silicides draw much interest in high-temperature applications [1]. According to the V-Si binary phase diagram, there are four binary silicide compounds (A15-V_3Si, C40-VSi_2, D8m-V_5Si_3, and V_6Si_5 with an orthorhombic structure) [2]. The V-Si compounds have been studied for many years. For V_5Si_3, there are three phases with W_5Si_3-prototype, Mn_5Si_3-prototype, and Cr_5B_3-prototype, where the W_5Si_3-prototype phase is a stable structure [3]. We just study the W_5Si_3-prototype V_5Si_3. In order to obtain the structural and mechanical properties of the V-Si compounds, a number of works have been reported. Carcia and Barsch measured the pressure derivatives of the single-crystal elastic constants of V_3Si at 77 and 298 K [4]. Zhang et al. investigated the thermodynamic stability of V_6Si_5 [5]. Zhang et al. also optimised thermodynamic modeling of the V-Si compounds by experiments [6]. The structural and electronic properties (electronic band structures and density of states) of V_3Si, VSi_2, V_5Si_3, and V_6Si_5 have been investigated by using density functional calculations [7].

However, other studies have also studied the elastic constants of V-Si compounds using ultrasonic measurements [8]. In theoretical studies, elastic constants and the directional dependences of Young's modulus have not been discussed adequately but are important. In this work, we performed first-principles calculations for the elastic properties of V_3Si, VSi_2, V_5Si_3, and V_6Si_5 consisting of elastic constants, bulk modulus, Young's modulus, shear modulus, Poisson's ratio, and directional dependences of Young's modulus. Based on the quasi-harmonic Debye model, Debye temperature, Grüneisen parameter, heat capacity, and thermal expansion coefficient of V_3Si, VSi_2, V_5Si_3, and V_6Si_5 compounds are also investigated.

2 Method

The first-principles calculations are performed by using the plane wave method, as implemented in the CASTEP code [9], which has been shown to obtain the reliable results for the structural properties of various solids [10]. For structural property calculations, the exchange correlation potential is described in the generalised gradient approximation (GGA) using the Perdew–Burke–Ernzerhof (PBE) functional [11]. Vanderbilt-type ultrasoft pseudopotentials (USPPs) [12] are employed to describe the electron–ion interactions. Two parameters that affect the accuracy of calculations are the kinetic energy cutoff that determines the number of plane waves in the expansion and the number of special *k* points used for the Brillouin zone (BZ) integration. We performed convergence with respect to BZ

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sampling and the size of the basis set. Converged results are achieved with special k-points mesh $10\times10\times10$ for V_3Si, $8\times8\times8$ for VSi_2, $5\times5\times4$ for V_5Si_3, and V_6Si_5, respectively. The size of the basis set is given by cutoff energy equal to 500 eV.

3 Results and Discussion

3.1 Structural Properties

In this article, the initial crystal structures are based on the experimental crystallographic data of V-Si compounds, and the lattice parameters of these compounds are optimised by using first-principle calculations. The crystal structures of V-Si compounds are shown in Figure 1. The optimised lattice parameters are listed in Table 1, where the available experimental data and other theoretical results are included. For V_3Si, the calculated lattice parameters by the GGA-PBE method are in good agreement with the previous results (4.7001 Å) and other theoretical results [13, 15, 16]. For VSi_2, the calculated lattice parameters are found to be $a=b=4.5597$ Å, $c=6.3602$ Å, respectively, showing that they are in good agreement with the experimental values [17]. For V_5Si_3, the calculated lattice parameters are found to be $a=b=9.3997$ Å, $c=4.7252$ Å, respectively, are in good agreement with previous results [3, 7, 16]. For V_6Si_5, the calculated lattice parameters in this work are well consistent with the previous results [16, 18]. These agreements with the previous results provide a confirmation that this work is reliable.

The formation enthalpy E_f per atom of the V_xSi_y compounds can be expressed as

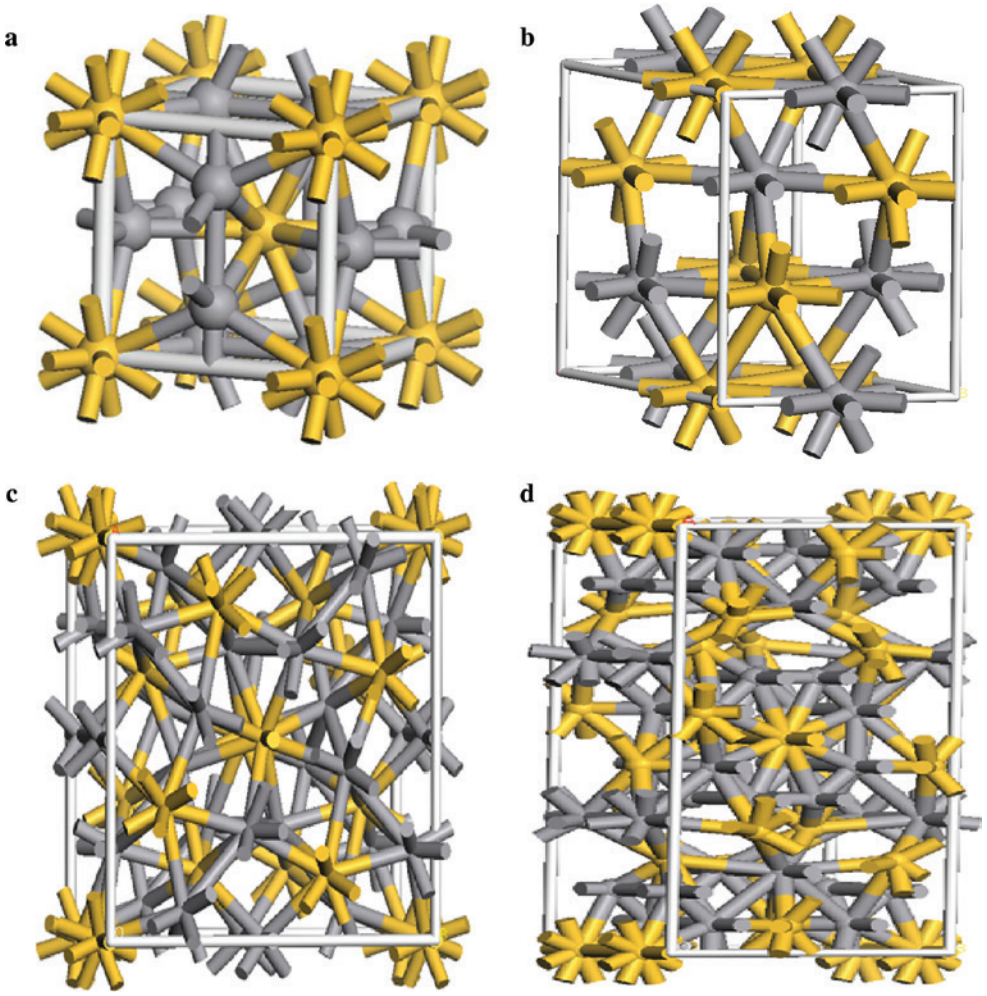

Figure 1: The crystal structure of V-Si compounds (a) V_3Si, (b) VSi_2, (c) V_5Si_3, and (d) V_6Si_5 (The V atoms are shown as gray spheres and the Si atoms as yellow spheres.).

Table 1: Calculated results with other theoretical and experimental lattice parameters (Å) and formation enthalpy (kJ/mol) of the V_3Si, VSi_2, V_5Si_3, and V_6Si_5.

System	Space group	*a*	*b*	*c*	E_f
V_3Si	*pm3n*	4.7021[a]			−44.78[a]
		4.735 [13]			−38.75 [14]
		4.727 [15]			−46.4 [13]
		4.7001 [16]			−44.6 [16]
VSi_2	$p6_422$	4.5597[a]	4.5597[a]	6.3602[a]	−54.26[a]
		4.57 [17]	4.57 [17]	6.37 [17]	−45.91 [5]
V_5Si_3	*I*4/*mcm*	9.3997[a]		4.7252[a]	−59.55[a]
		9.3930 [16]		4.7292 [16]	−56.5 [16]
		9.46 [7]		4.77 [7]	−53.73 [5]
		9.44 [7]		4.76 [7]	−59.00 ± 2 [13]
		9.3947 [3]		4.7265 [3]	−56.4 [3]
V_6Si_5	*Ibam*	15.9126[a]	7.4859[a]	4.8296[a]	−54.27[a]
		15.9419 [16]	7.4951 [16]	4.8100 [16]	−53 [16]
		15.966 [18]	7.501 [18]	4.858 [18]	−50.7 ± 2 [19–21]

[a]This work.

$$E_f = \frac{E_{tot}(V_xSi_y)}{x+y} - \frac{xE_{tot}(V) - yE_{tot}(Si)}{x+y} \quad (1)$$

where x and y are indices that give the amount of atoms of each atomic species within the unit cell of a structure V_xSi_y. E_{tot} is the total energy of atom of the elements or compound. The calculated formation enthalpies of V_3Si, VSi_2, V_5Si_3, and V_6Si_5 are also listed in Table 1, together with available experimental data and other theoretical results. For V_3Si, the formation enthalpy E_f is in good agreement with previous results [13, 14, 16]. The formation enthalpy of VSi_2 is also predicted in this work and in good agreement with theoretical results [5]. Compared to the experimental data [13], the present calculated formation enthalpy of the V_5Si_3 is also in good agreement and is coherent with other theoretical results [3, 5, 16]. For V_6Si_5, the calculated formation enthalpy E_f (–54.27 kJ/mol) in this work is in good agreement with the value –53 kJ/mol obtained by the GGA-PBE method [16] and other previous measurement results [19–21]. The deviation is only 6.57%.

3.2 Elastic Constants

The number of independent elastic constants is different for various crystal structures. For a cubic crystal, it has three independent elastic constants (C_{11}, C_{12}, and C_{44}). For a hexagonal crystal, it has five independent elastic constants (C_{11}, C_{12}, C_{13}, C_{33}, and C_{44}). For a tetragonal chalcopyrite crystal, it has six independent elastic constants (C_{11}, C_{12}, C_{13}, C_{33}, C_{44}, and C_{66}). For an orthorhombic crystal, it has nine elastic constants (C_{11}, C_{22}, C_{33}, C_{44}, C_{55}, C_{66}, C_{12}, C_{13}, and C_{23}). The mechanical stability criteria are given by [22–25].

As shown in Table 2, all of the elastic constants for V_3Si, VSi_2, V_5Si_3, and V_6Si_5 compounds satisfy the respective mechanical stability criteria. It indicates that all above structures are mechanically stable. The elastic constants for V_3Si are in agreement with the experimental data (at $T = 77$ K) [4]. It is worth pointing out that our theoretical calculations of the elastic constants for VSi_2 with space group $P6_422$ are in agreement with the experimental data [17]. The C_{ij} values

Table 2: Calculated results with other theoretical and experimental elastic constants C_{ij} (GPa) of the compounds in V_3Si, VSi_2, V_5Si_3, and V_6Si_5.

System		C_{11}	C_{12}	C_{13}	C_{22}	C_{23}	C_{33}	C_{44}	C_{55}	C_{66}
V_3Si	This work	241.78	169.56					78.60		
	[4]	233.6	151					77.1		
VSi_2	This work	375.46	62.70	76.39			426.99	144.94		
	[17]	357.8	50.6	68.1			422.3	135.7		
V_5Si_3	This work	397.23	104.46	99.91			341.07	104.09		129.06
	[3]	401.7	106.7	99.6			351.1	103.1		127.8
V_6Si_5	This work	392.70	123.69	80.59	331.60	91.74	343.01	136.12	98.89	114.54

Table 3: Calculated results with other theoretical and experimental bulk modulus B (GPa), shear modulus G (GPa), Young modulus E (GPa), Poisson's ratio σ, the ratio of the shear modulus G to the bulk modulus B, the compressional wave V_p (m/s), the shear velocities V_S (m/s), and average wave velocity V_m (m/s) of the compounds in V_3Si, VSi_2, V_5Si_3, and V_6Si_5.

System		B	G	E	σ	B/G	V_p	V_S	V_m
V_3Si	This work	193.64	57.52	157.01	0.364	3.37	6939.3	3154.8	3554.1
	[8]	213					7116	3819	
VSi_2	This work	178.29	153.15	357.18	0.166	1.16	9060.4	5733.2	6307
	Exp. [17]	167.2	147.9	342.6	0.158				
	[8]						8757	5535	
V_5Si_3	This work	193.26	121.69	301.74	0.239	1.59	8213.4	4805.3	5328.5
	[3]	195.8	122.1	303.1	0.24	1.60	8150	4755	5274
	[8]						7818	4380	
V_6Si_5	This work	183.71	120.16	295.95	0.232	1.53	9910.7	5858	6489.7

calculated by the GGA-PBE method of V_5Si_3 are also provided and compared. The calculated C_{ij} values in this work are well consistent with the previous results [3]. Unfortunately, there are no other theoretical and experimental results for comparison with our elastic results for V_6Si_5.

It is known that the mechanical properties are determined by the elastic modulus. The polycrystalline elastic properties, including bulk modulus B, shear modulus G, Young modulus E, and Poisson's ratio σ, can be obtained by Voigt–Reuss–Hill (VRH) approximation. The B, G, and E are listed in Table 3. As can be seen from Table 3, the bulk modulus B of for V-Si compounds follows the order $V_3Si > V_5Si_3 > V_6Si_5 > VSi_2$. V_3Si has the largest bulk modulus (193.64 GPa). The Young's modulus of for the V_3Si, VSi_2, V_5Si_3, and V_6Si_5 compounds follows the order $VSi_2 > V_5Si_3 > V_6Si_5 > V_3Si$.

According to Pugh's criterion [26], the ductility or brittleness of a solid material is judged by B/G ratio. The critical value which separates ductile and brittle material is $B/G = 1.75$. If $B/G > 1.75$, behaves in a ductile manner. Otherwise, behaves in a brittle. Moreover, the Poisson's ratio σ is consistent with B/G, which refers to a ductile compound has a large $\sigma > 0.26$ [27]. The values of B/G are larger than 1.75 and values of σ are larger than 0.26 for V_3Si in Table 3, which testify that they are ductile. The values of B/G and σ for VSi_2, V_5Si_3, and V_6Si_5 are less than 1.75 and 0.26, respectively. It shows that they are all brittle.

The values of the compressional velocity wave V_p and the shear wave velocity V_S can be obtained using the Navier's equation [28], where ρ is density of the compound.

$$V_p = \sqrt{(B + \frac{4}{3}G)\frac{1}{\rho}} \tag{2}$$

$$V_S = \sqrt{\frac{G}{\rho}} \tag{3}$$

The average wave velocity V_m can be calculated by

$$V_m = \left[\frac{1}{3}\left(\frac{2}{V_S^3} + \frac{1}{V_p^3}\right)\right]^{-1/3} \tag{4}$$

The calculated sound velocity of V_p, V_S, and V_m for the V_3Si, VSi_2, V_5Si_3, and V_6Si_5 compounds are listed in Table 3. In comparison, the calculated values of V_p and V_S for V_3Si at zero pressure are a little lower than reported by Fleischer et al. [8]. For VSi_2, the calculated values of V_p and V_S are in good agreement with those reported by Fleischer et al. [8]. For V_5Si_3, the calculated V_p and V_S in this work are in agreement with the values by the VASP-GGA method [3] and other previous results [8]. Without experimental data and theoretical results of the V_6Si_5, we cannot make any comparisons. We expect that our theoretical results provide the valuable reference for the further research.

As a method to study the elastic anisotropic behavior of a solid material, the 3D surface constructions of the directional dependences of reciprocals of Young's modulus E are very useful. The expressions of the reciprocals of Young's modulus for the V_3Si, VSi_2, V_5Si_3, and V_6Si_5 compounds are different for each other due to their various crystal structures [22].

In Figure 2, we show the mechanical stable structures of V_3Si, VSi_2, V_5Si_3, and V_6Si_5 compounds. The surface in each graph represents the magnitude of Young's modulus E along different orientations. From this figure, we can clearly see that the Young's modulus shows some anisotropy at different orientations. It also should be noted that the Young's modulus of V_3Si shows slight anisotropy and the Young's modulus of VSi_2, V_5Si_3, and V_6Si_5 shows some anisotropy for different orientations. As for the hexagonal VSi_2, the 3D directional dependences of the Young's modulus along z axis are more compressible than along x- and y-axes. The 3D figure of the Young's modulus for

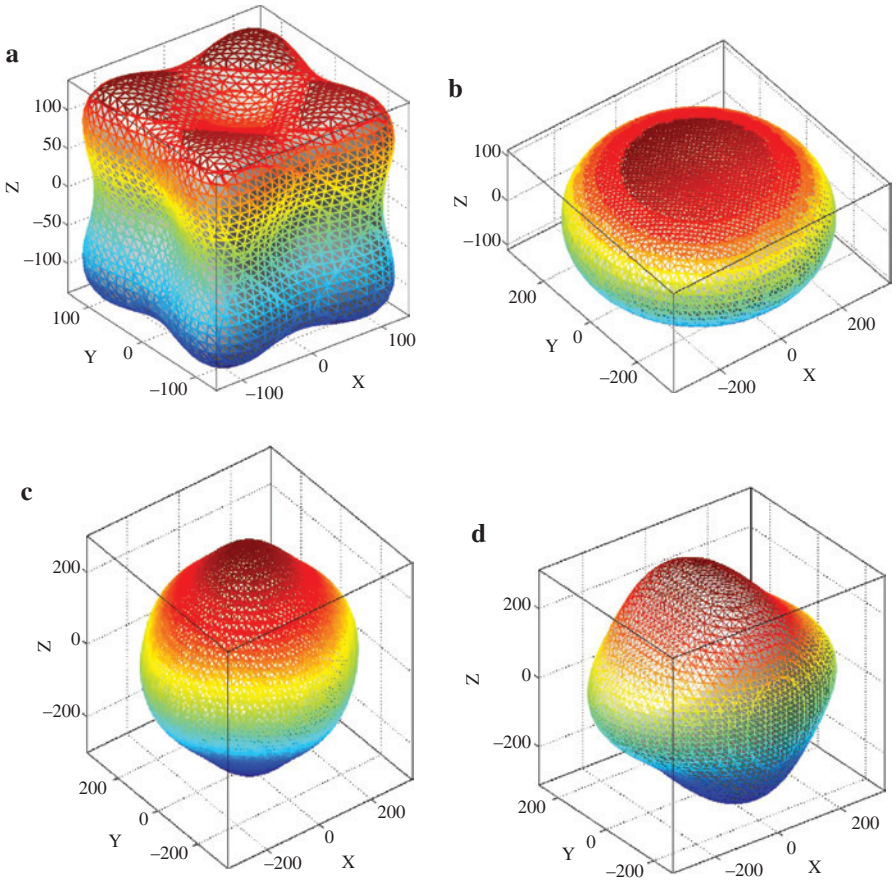

Figure 2: The directional dependence of the Young's modulus for the V_3Si, VSi_2, V_5Si_3, and V_6Si_5 compounds [(a) V_3Si, (b) VSi_2, (c) V_5Si_3, and (d) V_6Si_5]. The magnitude of Young's modulus at different directions is represented by the contour. The units are in GPa.

the tetragonal V_5Si_3 is characterised by more anisotropic along the *z*-axis than that along the *x*- and *y*-axes. As for the orthorhombic V_6Si_5, the 3D surface of Young's modulus along *x*-, *y*-, and *z*-axes is shown highly anisotropic.

3.3 Thermal Properties of V_3Si, VSi_2, V_5Si_3, and V_6Si_5 under High Temperature and High Pressure

In order to investigate the thermal properties of V_3Si, VSi_2, V_5Si_3, and V_6Si_5 compounds under high pressure (0–25 GPa) and melting points temperature [6], we have used the quasi-harmonic Debye model as implemented in the Gibbs code [29]. First, we obtain a set of total energy results versus unit-cell volumes around the equilibrium geometry. Then, the above-mentioned results are fitted to the equation of state in order to obtain different parameters as a function of pressure and temperature from standard thermal relations. By the above-mentioned method, we can get the internal energy *U*, the heat capacity of constant volume C_V, the heat capacity at constant pressure C_P, the entropy *S*, the thermal expansion coefficient α, Debye temperature Θ, and Grüneisen parameter γ.

The thermal properties of the V_3Si, VSi_2, V_5Si_3, and V_6Si_5 compounds are calculated at the different temperatures ranging from 0 to about melting points. The pressure effect is investigated in the range 0–25 GPa. Heat capacity belongs to one of the most important thermal properties of the materials. Figure 3 shows the calculated heat capacity at constant volume as functions of the temperature under zero GPa. It can be seen from Figure 3 that the heat capacity C_V increases exponentially with the temperature at $T<400$ K. At higher temperature, C_V follows the Debye model and approaches the Dulong–Petit limit indicating the thermal energy at high temperature excites all phonon modes.

As an important physical quantity, the Debye temperature could distinguish the physical properties between high- and low-temperature regions. The variation of the Debye temperature Θ (K) as a function of pressure and

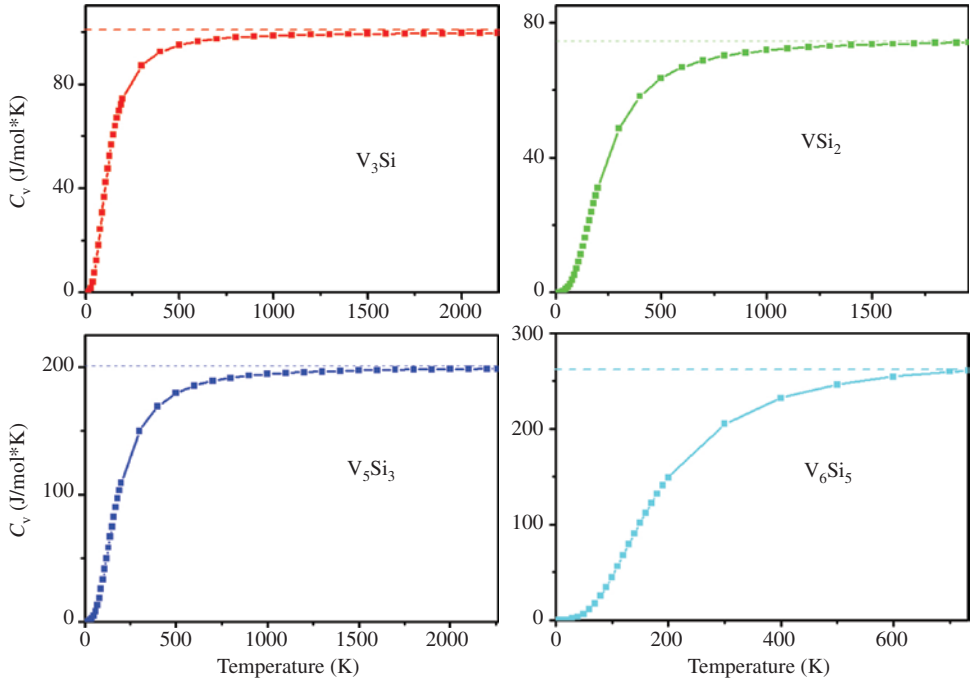

Figure 3: The heat capacity of constant volume C_V (J/mol K) for V_3Si, VSi_2, V_5Si_3, and V_6Si_5 in V-Si compounds at 0 GPa.

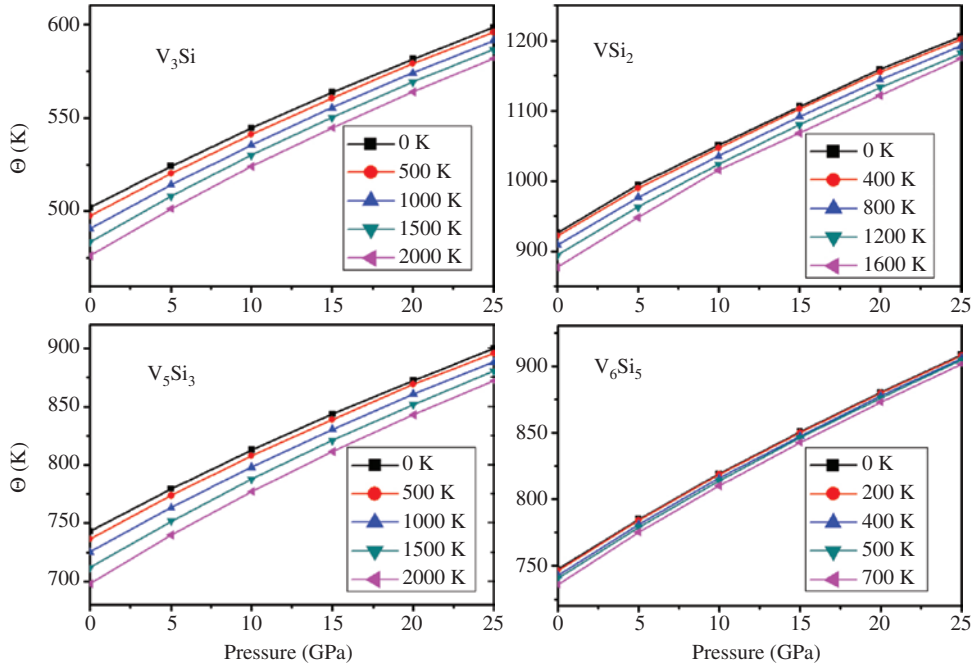

Figure 4: Debye temperature versus pressure at various temperatures for V_3Si, VSi_2, V_5Si_3, and V_6Si_5.

temperature is displayed in Figure 4. With the applied pressure increasing, the Debye temperatures are almost linearly increasing. The temperature and pressure dependence of Θ (K) reveals that the thermal vibration frequency of atoms in V-Si (V_3Si, VSi_2, V_5Si_3, and V_6Si_5) compounds changes with temperature and pressure.

Figure 5 shows the volume thermal expansion coefficient a of V_3Si, VSi_2, V_5Si_3, and V_6Si_5 across different pressures, from which it can be seen that the volume thermal expansion coefficient α increases quickly at a given temperature particularly at zero pressure below the temperature of 300 K. After a sharp increase, the volume thermal

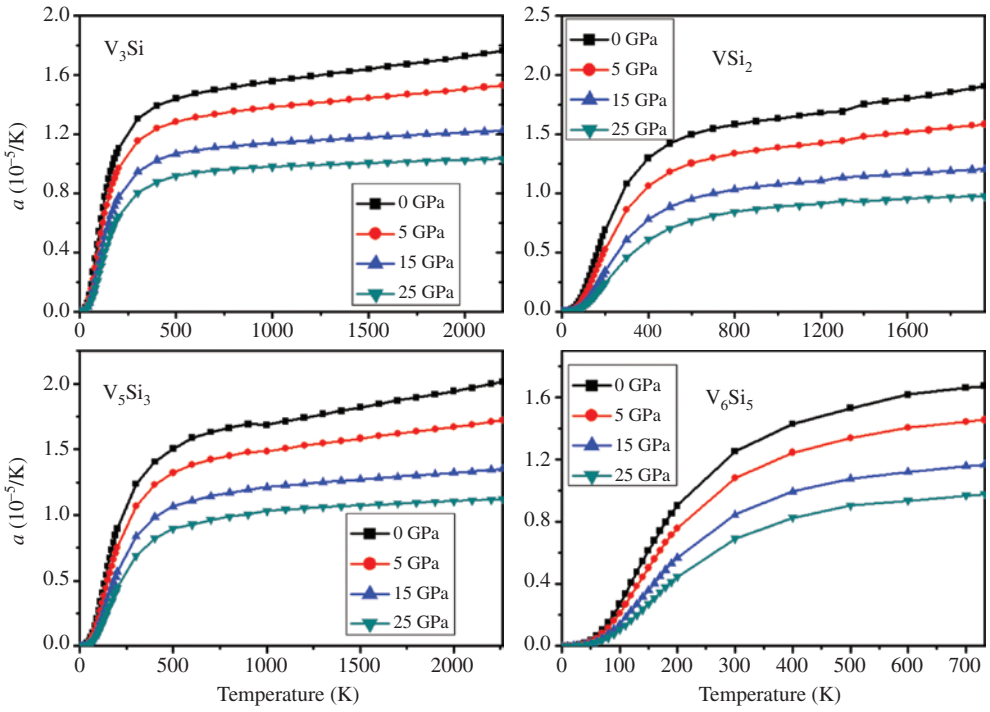

Figure 5: Thermal expansion coefficients versus temperature at various pressures for V_3Si, VSi_2, V_5Si_3, and V_6Si_5.

Table 4: The calculated internal energy U (kJ/mol), heat capacity of constant volume C_V (J/mol*K), heat capacity of constant pressure C_p (J/mol*K), Helmholtz free energy A (kJ/mol), entropy S (J/mol*K), Debye temperature Θ (K), Grüneisen parameter γ, and thermal expansion coefficient α (10^{-5}/K) for V_3Si, VSi_2, V_5Si_3, and V_6Si_5 at 300 K under different pressures.

P/GPa	*U*	C_V	C_p	*A*	*S*	Θ	γ	α
V_3Si								
0.00	33.96	87.19	87.79	7.35	88.69	499.87	1.768	1.31
5.00	34.31	86.15	86.66	8.85	84.87	522.37	1.705	1.16
10.00	34.65	85.17	85.61	10.19	81.56	543.00	1.653	1.04
15.00	34.98	84.24	84.62	11.40	78.62	562.16	1.609	0.95
20.00	35.30	83.35	83.69	12.40	75.98	580.12	1.571	0.87
25.00	35.60	82.50	82.80	13.52	73.59	597.14	1.537	0.80
VSi_2								
0.00	32.07	48.60	49.01	22.82	30.83	923.96	2.593	1.08
5.00	33.38	45.81	46.10	25.14	27.48	991.74	2.463	0.86
10.00	34.54	43.49	43.71	27.05	24.97	1049.19	2.369	0.72
15.00	35.69	41.31	41.48	28.84	22.80	1104.18	2.289	0.61
20.00	36.82	39.25	39.39	30.55	20.91	1157.32	2.221	0.52
25.00	37.84	37.51	37.62	32.02	19.40	1203.72	2.166	0.46
V_5Si_3								
0.00	76.91	149.88	150.97	42.94	113.23	740.44	1.973	1.24
5.00	78.52	145.85	145.85	46.70	106.07	777.18	1.899	1.07
10.00	80.06	142.12	142.12	50.08	99.93	811.02	1.837	0.94
15.00	81.51	138.69	139.25	53.11	94.67	841.96	1.786	0.84
20.00	82.90	135.46	136.00	55.90	90.01	871.07	1.742	0.76
25.00	84.25	132.42	132.98	58.49	85.86	899.48	1.704	0.69
V_6Si_5								
0.00	106.01	205.42	206.93	59.67	154.47	744.86	1.952	1.25
5.00	108.31	199.72	200.94	64.97	144.45	782.62	1.877	1.08
10.00	110.48	194.45	195.46	69.71	135.90	817.31	1.815	0.95
15.00	112.53	189.62	190.47	73.95	128.60	848.99	1.764	0.85
20.00	114.51	185.08	185.81	77.87	122.13	878.78	1.719	0.76
25.00	116.44	180.75	181.39	81.54	116.32	907.18	1.680	0.69

expansion coefficient of the V_3Si, VSi_2, V_5Si_3, and V_6Si_5 is nearly insensitive to the temperature above 300 K due to the electronic contributions. Thermal expansion coefficient α strongly decreases with pressure at a constant temperature.

Finally, we have also calculated the internal energy U, entropy S, thermal expansion coefficient α, heat capacity C_V and C_P, Helmholtz free energy A, Grüneisen parameter γ, and Debye temperature Θ for the V_3Si, VSi_2, V_5Si_3, and V_6Si_5 in V-Si at 300 K under different pressures. The theoretical results are presented in Table 4. However, there has been no experimental and theoretical data available for the thermal properties of V_3Si, VSi_2, V_5Si_3, and V_6Si_5 compounds so far. Therefore, our calculated results can provide support for future works on V_3Si, VSi_2, V_5Si_3, and V_6Si_5 compounds.

4 Conclusions

We have investigated the structural, elastic properties, elastic anisotropy, and thermodynamic properties of V_3Si, VSi_2, V_5Si_3, and V_6Si_5 compounds using first-principles calculations. The calculated elastic constants of compounds indicate that the V_3Si, VSi_2, V_5Si_3, and V_6Si_5 compounds are mechanically stable. Bulk modulus, shear modulus, Young's modulus, and Poisson's ratio have also been calculated and discussed. Moreover, we found that the pressure and temperature have important effects on the internal energy, heat capacity, Helmholtz free energy, entropy, Debye temperature, Grüneisen parameter, and thermal expansion coefficient.

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