

DFT Calculation for Elastic Constants of Tetragonal Structure of Crystalline Solids with WIEN2k Code: A New Package (*Tetra-elastic*)

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Tetra-elastic is a new package for calculating the elastic constants of tetragonal structure. It is compatible with the highly accurate all electron full potential linearized augmented plane wave plus local orbital [FP-(L)APW+lo] method as implemented in WIEN2k code. The package is released recently; the package and the user guide are available on (http://www.wien2k.at/reg_user/unsupported/). In this paper we provide detail description of the formalism of calculating the elastic constants of tetragonal structure. To testify the accuracy of the *Tetra-elastic* package several tetragonal structure compounds were used. The results show that the calculated elastic constants using *Tetra-elastic* exhibit better agreement with the available experimental data than the previous theoretical results used different methods. In this package the second-order derivative $E''(\varepsilon)$ of polynomial fit $E = E(\varepsilon)$ of energy vs strains at zero strain ($\varepsilon = 0$) is used to calculate the tetragonal elastic constants.

Keywords: Elastic constants; Tetra-elastic; tetragonal structure: FPLAPW; DFT

1. INTRODUCTION

The fast development in the computer's technology and theoretical techniques within density functional theory (DFT) make it possible to compute large and complex structures. The theoretical techniques are completely independent to solve the quantum mechanical Kohn Sham DFT equations.

One of the most accurate theoretical techniques is the *ab initio* DFT technique [1,2] which allows the structure to be efficiently optimized [3] and hence to obtain the elastic properties. It is well known that the elastic properties provide valuable information about the binding characteristic between adjacent atomic planes. Anisotropic characters of binding and structural stability are usually defined by the elastic constants C_{ij} . These constants have been often related to the shear modulus and Young's modulus, which are frequently measured for polycrystalline materials when investigating their hardness. The elastic moduli require knowledge of the derivative of the energy as a function of the lattice strain [4].

Recent developments in the theoretical calculation of the elastic properties within one of the highly accurate all electron full potential linearized augmented plane wave plus local orbital package [5] is a very attractive technique because many other mechanical properties such as bulk modulus, shear modulus, young's modulus, etc, can be derived from elastic constants. We should emphasize that the elastic constants determine the response of the materials to the external forces, as typified by bulk modulus, Young's modulus, shear modulus and Poisson's ratio which play a crucial role in determining the strength of the materials. The elastic properties define how a material that undergoes stress deforms and then recovers and returns to its original shape after stress ceases. The elastic constants of solids provide a link between the mechanical and dynamical behaviors of crystals and give important information concerning the nature of the forces operating in solids. These constants can be also predicting the structural stability of materials.

Based on our experiences in writing packages for calculating the elastic constants for different structures, namely cubic, hexagonal and orthorhombic [6-8]. In this work we have addressed ourselves to write a new package for calculating the elastic properties of the tetragonal structures by using second-order derivative within WIEN2k code. In order to testify our new *Tetra-elastic* package, several tetragonal structure compounds whose elastic constants are known experimentally and theoretically were used. We found that the *Tetra-elastic* give very accurate results which is in good agreement with the experimental data than the previous calculations.

2. THEORETICAL BACKGROUND

Theoretically the elastic constants are defined by means of a Taylor expansion of the total energy $E(V, \delta)$ for the system, with respect to a small strain (δ) of the lattice. If we consider the Bravais lattice vectors of tetragonal crystal structure as a matrix form (R) the distortion of the lattice (R') is expressed by multiplying R with a symmetric $\delta_{xy} = \delta_{yx}$ distortion matrix i.e. ($R' = R * D$), which is written as,

$$D = \begin{pmatrix} 1 + \delta_{xx} & \delta_{xy}/2 & \delta_{xz}/2 \\ \delta_{yx}/2 & 1 + \delta_{yy} & \delta_{yz}/2 \\ \delta_{zx}/2 & \delta_{zy}/2 & 1 + \delta_{zz}/2 \end{pmatrix}$$

And in Voigt notation (It is often convenient to change to the Voigt notation in order to reduce the number of indices. The Voigt notation replaces $xx \rightarrow 1$, $yy \rightarrow 2$, $zz \rightarrow 3$, zy (and yz) $\rightarrow 4$, xz (and zx) $\rightarrow 5$, xy (and yx) $\rightarrow 6$

$$D = \begin{pmatrix} 1 + \delta_1 & \delta_6/2 & \delta_5/2 \\ \delta_6/2 & 1 + \delta_2 & \delta_4/2 \\ \delta_5/2 & \delta_4/2 & 1 + \delta_3/2 \end{pmatrix}$$

we express the energy of the strained system by means of a Taylor expansion in the distortion parameters,

$$E(V, \delta) = E(V_0, 0) + V_0 \left(\sum_{i=1}^6 \tau_i \delta_i + \frac{1}{2} \sum_{i=1}^6 \sum_{j=1}^6 C_{ij} \delta_i \delta_j + O(\delta^3) \right)$$

The linear terms vanish if the strain causes no changes in the volume of the crystal. Otherwise, τ_i are related to the strain on the crystal and C_{ij} are elastic constants and V_0 is the volume of unstrained tetragonal system and we use it to evaluate the elastic constants.

To obtain elastic constants of tetragonal structure we have used the method obtained in Ref [9]. In this method elastic constants were calculated by applying small strains to the unstrained lattice.

There are six independent elastic constants for a tetragonal symmetry, called C_{11} , C_{12} , C_{13} , C_{33} , C_{44} , and C_{66} . Since we have six independent elastic constants, we need six different strains to determine these elastic constants. The six distortions used in the **Tetra-elastic** Package are described below. The first three distortions are written as

$$D_1 = \begin{pmatrix} 1 + \delta & 0 & 0 \\ 0 & 1 + \delta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$D_2 = \begin{pmatrix} 1 + \delta & 0 & 0 \\ 0 & 1 + \delta & 0 \\ 0 & 0 & \frac{1}{(1 + \delta)^2} \end{pmatrix}$$

and

$$D_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 + \delta \end{pmatrix}$$

These three distortions change the lattice parameter in the **a** and **c** directions. The symmetry of the strained lattice is therefore still tetragonal, however the volume of the distortion lattice changes by using D_1 and D_3 and the energy for these distortions can be obtained as

$$E(V, \delta) = E(V_0, 0) + V_0 \left((C_{11} + C_{12}) \delta^2 + O(\delta^3) \right)$$

$$E(V, \delta) = E(V_0, 0) + V_0 \left((C_{zz}) \delta^2 + O(\delta^3) \right)$$

$$C_{zz} = C_{11} + C_{12} + 2C_{33} - 4C_{13}$$

and

$$E(V, \delta) = E(V_0, 0) + V_0 \left(\frac{C_{33}}{2} \delta^2 + O(\delta^3) \right)$$

The second three type of distortions are volume conserved orthorhombic (D_4 and D_6) and monoclinic (D_5) distortions and written as

$$D_4 = \begin{pmatrix} \left(\frac{1+\delta}{1-\delta} \right)^{\frac{1}{2}} & 0 & 0 \\ 0 & \left(\frac{1-\delta}{1+\delta} \right)^{\frac{1}{2}} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$D_5 = \begin{pmatrix} 1 & 0 & \delta \\ 0 & 1 & \delta \\ \delta & \delta & 1 + \delta^2 \end{pmatrix}$$

and

$$D_6 = \begin{pmatrix} (1 + \delta^2)^{\frac{1}{2}} & \delta & 0 \\ \delta & (1 + \delta^2)^{\frac{1}{2}} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and the energy for these distortions can be obtained as

$$E(V, \delta) = E(V_0, 0) + V_0 \left((C_{11} - C_{12}) \delta^2 + O(\delta^4) \right)$$

$$E(V, \delta) = E(V_0, 0) + V_0 \left(4(C_{44}) \delta^2 + O(\delta^4) \right)$$

and

$$E(V, \delta) = E(V_0, 0) + V_0 \left(2(C_{66}) \delta^2 + O(\delta^4) \right)$$

respectively.

3. DETAILS OF CALCULATIONS AND STRUCTURAL ASPECTS

As the WIEN2k code officially doesn't include a package, which is completely compatible with it, to calculate the elastic properties of the tetragonal structure and since the elastic properties are very crucial because it is related to various fundamental properties. In order to fill this gap we have released a new package called *Tetra-elastic* for calculating the elastic properties of tetragonal structure compounds [10] within the framework of WIEN2k code. Based on the second-order derivative $E''(\varepsilon)$ of polynomial fit $E = E(\varepsilon)$ of energy vs. strains at zero strain ($\varepsilon = 0$), the *Tetra-elastic* package

calculates the tetragonal elastic constants. The *Tetra-elastic* package is compatible with the highly accurate all electron full-potential linearized augmented plane wave plus local orbital [FP-(L)APW+lo] method to solve the Kohn Sham DFT equations within the framework of the WIEN2K code [5]. The exchange and correlation potential was described by the generalized gradient approximation (GGA-PBE) formulated by Perdew et al [11]. In the [FP-(L)APW+lo] method, the unit cell volume is partitioned into the non-overlapping atomic spheres around each atom and the remaining interstitial area and two different sets of basis functions are used in these regions.

Table 1. The lattice constants obtained from different methods of calculations using different exchange correlation (XC) potentials in comparison with the available values.

Compound	Symmetry	XC	a (Å)	c (Å)
α -Pt ₂ Si ^a	139 (I4/mmn)	LDA	3.9196	5.9485
Exp ^b			3.9482	5.9628
AgGaSe ₂ ^c	122 (I42d)	LDA	6.0529	11.2100
AgGaSe ₂ ^d		GGA91	5.8380	11.0221
AgGaSe ₂ ^e		PBE	6.0579	11.2944
Exp ^f			5.9850	10.9047
MgF ₂ ^g	136 (P4 ₂ /mmm)	PBE	4.7086	3.0994
MgF ₂ ^g		PBE	4.6954	3.0983
Exp ^h			4.6150	3.0428
SnO ₂ ⁱ	136 (P4 ₂ /mmm) Rutile	LDA	4.7178	3.1798
SnO ₂ ⁱ		GGA	4.8179	3.3383
SnO ₂ ^j		PBE	4.8270	3.2486
Exp ^k			4.7370	3.1880
Exp ^l			4.7380	3.1887
TiO ₂ ^m	136 (P4 ₂ /mmm) Rutile	LDA	4.5669	2.93012
TiO ₂ ^m		GGA	4.6545	2.97608
Exp ^m			4.5936	2.95874
PtS ⁿ	131 (P4 ₂ /mmc)	LDA	3.4400	6.0900
PtS ⁿ		GGA91	3.5400	6.1700
Exp ^{o,p}			3.4700	6.1100
Ti ₂ B ^q	140 (I4/mcm)	PBE	5.6470	4.7410
Exp ^r			6.1000	4.5300
TiAl ^s	123(P4/mmm)	GGA	3.9890	4.0340
Exp ^s			3.9900	4.0700
TiO ₂ ^t	141 (I41/amd) Anatase	LDA	3.7604	9.7474
TiO ₂ ^t		GGA	3.8211	9.6712
Exp ^t			3.7845	9.5142

^a Ref. [18], ^b Ref. [22], ^c Ref. [23], ^d Ref. [24], ^e Ref. [9], ^f Ref. [25], ^g Ref. [13], ^h Ref. [26], ⁱ Ref. [12],
^j Ref. [27], ^k Ref. [28], ^l Ref. [29], ^m Ref. [12], ⁿ Ref. [19], ^o Ref. [30],
^p Ref. [31], ^q Ref. [20], ^r Ref. [32], ^s Ref. [21], ^t Ref. [12]

In the atomic spheres, wave functions are expanded into atomic orbitals while in the interstitial region a plane-wave basis set is used. Charge density and potential are expanded into lattice harmonics and Fourier series in the atomic spheres and interstitial regions, respectively. In order to get the total energy convergence the plane-wave expansion cutoff was $K_{\max}=7/R_{\text{mt}}$ ($K_{\max}=8/R_{\text{mt}}$) where R_{mt} is the smallest atomic muffin-tin sphere in the unit-cell and the maximum angular momentum of the atomic orbital basis functions was set to $l_{\max}=8$ (9), respectively. Since tetragonal compounds have internal coordinates, our calculations were optimized by minimization of the forces (1 mRy/au) acting on the atoms. To testify the accuracy of the newly released *Tetra-elastic* package several tetragonal structure compounds having different space group were used.

In Table 1, we have listed the cell parameters and the space groups of nine tetragonal structure compounds which were used in this work.

4. RESULTS AND DISCUSSION

Table 2. The calculated elastic constants in unit of (GPa) for AgGaSe₂ in comparison with experimental data and the previous theoretical results using different methods, lattice constants and exchange correlation (xc) potentials.

	AgGaSe ₂ ^a	AgGaSe ₂ ^b	AgGaSe ₂ ^c	AgGaSe ₂	AgGaSe ₂ ^d	AgGaSe ₂ ^e
Method	NPP	UPP	FPLAPW	FPLAPW	Exp	Exp
XC	LDA	GGA	PBE	PBE		
a (Å)	5.9340		6.0579	6.0579		
c (Å)	10.6693		11.2944	11.2944		
C11	92	86.4	74.95	70.95	89.8	80.1
C12	60	55.2	41.03	42.3	65.7	51.6
C13	56	52.9	43.03	41.2	45.1	52.6
C33	70	72.4	59.57	58.46	58.0	70.7
C44	26	20.3	30.10	23.66	21.7	21.2
C66	17	25.3	21.62	24.39	13.3	24.7

UPP : Ultrasoft pseudopotentials

NPP : Norm-conserving pseudopotentials

^a Ref. [16], ^b Ref. [17], ^c Ref. [9], ^d Ref. [14], ^e Ref. [15], **This work (Bold)**

The tetragonal symmetry possesses six independent elastic constants, namely; C_{11} , C_{12} , C_{13} , C_{33} , C_{44} , and C_{66} . In the Tables 2-9, we have listed the calculated elastic constants of nine tetragonal structure compounds using the newly released *Tetra-elastic* package.

Before attempting elastic constants calculations for tetragonal structure compounds whose elastic constants are unknown experimentally and theoretically. First we have calculated the elastic constants for several tetragonal structure compounds whose elastic constants are unknown

experimentally and theoretically to testified the accuracy of the *Tetra-elastic* package in comparison with the previously reported theoretical and experimental data. The calculated elastic constants of TiO₂(Rutile) [12], MgF₂ [13], and SnO₂(Rutile) [12] presented in Table 3, 4 , and 5 show that our calculated elastic constants show better agreement with the experimental data then the previous theoretical calculations.

Table 3. The calculated elastic constants in unit of (GPa) for α -Pt₂Si and TiO₂ (Rutile) in comparison with experimental data and the previous theoretical results using different methods, lattice constants and different exchange correlation (xc) potentials.

	α -Pt ₂ Si [†]	α -Pt ₂ Si	TiO ₂ ^g	TiO ₂ ^g	TiO ₂	TiO ₂ ^g
Method	FPLMTO	FPLAPW	UPP	UPP	FPLAPW	Exp
XC	LDA	PBE	LDA	GGA	PBE	
a (Å)	3.9196	3.9482	4.5669	4.6545	4.5937	4.5936
c (Å)	5.9485	5.9628	2.9301	2.9761	2.9581	2.9587
C11	332.4	324.8	293.8	270.1	268.3	269.0
C12	239.6	215.3	225.5	172.0	180.2	177.0
C13	169.4	182.5	171.0	147.0	146.4	146.0
C33	298.0	281.2	516.7	467.6	477.9	480.0
C44	62.7	71.0	122.7	115.9	122.3	124.0
C66	169.3	172.2	246.2	216.3	223.6	192.0

[†] Ref. [18], ^g Ref. [12], **This work (Bold)**

Table 4. The calculated elastic constants in unit of (GPa) for MgF₂ in comparison with the previous theoretical results using different methods, lattice constants and same exchange correlation (xc) potentials.

	MgF ₂ ^h	MgF ₂ ^h	MgF ₂	MgF ₂ ⁱ
Method	FPLAPW	PAW	FPLAPW	Exp
XC	PBE	PBE	PBE	
a (Å)	4.7086	4.6954	4.7086	
c (Å)	3.0994	3.0983	3.0994	
C11	130.0	127	128.3	123.7
C12	78.2	80.1	79.2	73.2
C13	54.7	57.3	61.9	53.6
C33	185.0	187.7	196.3	177.0
C44	50.5	50.8	51.2	55.2
C66	83.0	87.2	87.7	97.8

PAW : Projector augmented wave

^h Ref. [13], ⁱ Ref. [33], **This work (Bold)**

Table 2 presents the current results of the elastic constants of AgGaSe₂ compound in comparison with the experimental data [14,15] and the previous theoretical calculation using different

methods and different exchange correlation potentials [9,16,17]. Our calculated C_{12} and C_{66} are agreed with neutron measurements while C_{13} and C_{33} agree with ultrasonic measurements. Meanwhile one can see that our calculated C_{12} , C_{66} , C_{13} and C_{33} are in good agreement with previously reported FPLAPW results [9].

Table 3 presents the current results of the elastic constants of α -Pt₂Si [18] and TiO₂ (Rutile) [12] in comparison with experimental data and the previous theoretical results using different methods, different lattice constants and different exchange correlation potentials. One can see that our results for TiO₂ exhibit better agreements with the experimental data [12] than the previous calculations [12]. Meanwhile, Table 3 shows there is reasonable agreement between our calculated elastic constants of α -Pt₂Si-FPLAPW-PBE and the previously calculated elastic constants for α -Pt₂Si-FPLMTO-LDA.

Our calculated elastic constants of MgF₂ (FPLAPW-PBE) in comparison with the previous calculations using FPLAPW-PBE/PAW-PBE [13] are listed in Table 4. We noticed that there is fairly good agreement between our results and FPLAPW-PBE/PAW-PBE results. We should emphasize that our MgF₂-FPLAPW-PBE results agree with MgF₂-FPLAPW-PBE/PAW-PBE results in the matter of ordering the elastic constants, and the superposition of elastic constants obtained from our results agree well with FPLAPW-PBE/PAW-PBE results.

Table 5. The calculated elastic constants in unit of (GPa) for SnO₂ in comparison with the previous theoretical results using different method, lattice constants and different exchange correlation (xc) potentials.

	SnO ₂ ^f	SnO ₂ ^f	SnO ₂	SnO ₂ ^f
Method	UPP	UPP	FPLAPW	EXP
XC	LDA	GGA	PBE	
a (Å)	4.7178	4.8179	4.7370	
c (Å)	3.1798	3.3383	3.1880	
C11	246.2	218.2	228.2	261.7
C12	178.8	140.1	174.0	177.2
C13	149.3	126.9	148.0	155.5
C33	424.6	377.7	454.1	449.6
C44	97.5	87.2	89.7	103.1
C66	204.6	181.9	252.1	207.4

^f Ref. [12], **This work (Bold)**

Table 5 presents our calculated elastic constants of SnO₂ (SnO₂-FPLAPW-PBE) in comparison with the previous theoretical results using different method, different lattice constants and different exchange correlation potentials. One can see our results show better agreement with experimental values [12] and previous SnO₂-UPP-LDA calculations [12] than the previous SnO₂-UPP-GGA calculations [12].

In Table 6, the results of PtS [19] using UPP-GGA and UPP-LDA are compared with our FPLAPW-PBE. We should emphasize that our results show better agreement with the UPP-LDA data than the UPP-GGA calculations.

Table 6. The calculated elastic constants in unit of (GPa) for PtS in comparison with the previous theoretical results using different methods, lattice constants and exchange correlation (xc) potentials.

	PtS ^j	PtS ^j	PtS
Method	UPP	UPP	FPLAPW
XC	LDA	GGA91	PBE
a (Å)	3.4400	3.5400	3.4701
c (Å)	6.0900	6.1700	6.1092
C11	217.0	186.0	205.2
C12	73.0	53.0	63.1
C13	149.0	113.0	146.2
C33	343.0	283.0	328.2
C44	30.0	28.0	26.4
C66	12.0	13.0	16.4

^j Ref. [19], **This work (Bold)**

Table 7. The calculated elastic constants in unit of (GPa) for Ti₂B and TiAl in comparison with the previous theoretical results using different methods, and same lattice constants, and exchange correlation (xc) potentials

	Ti ₂ B ^k	Ti ₂ B	TiAl ^l	TiAl	TiAl ^l
Method	PAW	FPLAPW	UPP	FPLAPW	EXP
XC	PBE	PBE	GGA	PBE	
a (Å)	5.6470	5.6470	3.9890	3.9900	3.9900
c (Å)	4.7410	4.7410	4.0340	4.0700	4.0700
C11	321.0	291.1	170.0	177.7	183.0
C12	100.0	93.2	79.0	62.8	74.0
C13	94.0	126.5	78.0	65.1	74.0
C33	299.0	271.3	177.0	179.3	178.0
C44	105.0	114.0	113.0	79.81	105.0
C66	100.0	71.6	73.0	79.0	78.0

^k Ref. [20], ^l Ref. [21], **This work (Bold)**

Table 7 presents the current calculated elastic constants for Ti₂B [20] in comparison with the previous theoretical results using different methods, same lattice constants and same exchange correlation potentials. It is clear that there is a significant difference between the two methods. Since there are no experimental data available hence, we consider the present results as a prediction study. In addition the current calculated elastic constants for TiAl [21] along with the experimental data and previous theoretical results using different methods, different lattice constants and different

exchange correlation potentials are presented in Table 7. It is clear that our FPLAPW-PBE calculation using the experimental lattice constants show better agreement with the experimental data than that the UPP-GGA results.

In Table 8 the calculated elastic constants for TiO₂ (Anatase) [12] are presented in comparison with the previous theoretical results using different method, different lattice constants and different exchange correlation potentials. It is clear that the three different methods predict different values and since there are no experimental data are available to be compared with our and previous theoretical results, so based on our results which show good agreement with the experimental data (see Tables 3-5) hence, we consider the present results are more accurate, hoping that our present work will stimulate some more works on this material. Future experimental works will testify our calculated results.

Table 8. The calculated elastic constants in unit of (GPa) for TiO₂ (Anatase) in comparison with the previous theoretical results using different method, lattice constants and different exchange correlation (xc) potentials.

	TiO ₂ ^m	TiO ₂ ^m	TiO ₂
Method	UPP	UPP	FPLAPW
XC	LDA	GGA	PBE
a (Å)	3.7604	3.8211	3.7867
c (Å)	9.7474	9.6712	9.5149
C11	395.2	336.5	377.2
C12	153.9	138.6	111.7
C13	156.0	136.0	136.4
C33	195.9	192.1	192.4
C44	47.3	49.4	58.9
C66	59.5	58.3	82.9

^m Ref. [12], **This work (Bold)**

5. CONCLUSION

A new package called *Tetra-elastic* is released. This package is to calculate the elastic constants for tetragonal structure. The package is compatible with WIEN2k code. Several tetragonal structure compounds whose elastic constants are known experimentally and theoretically were used to testify the newly released *Tetra-elastic* package. We should emphasize that the calculated elastic constants using *Tetra-elastic* package exhibit better agreement with the available experimental data than the previous theoretical results obtained from different theoretical methods. The calculated elastic constants for several tetragonal structure compounds using the *Tetra-elastic* package are presented in comparison with the previous theoretical results using different method, different lattice constants and different exchange correlation potentials. It is clear that the different methods predict different values and since there are no experimental data are available for all compounds to be compared with our and previous theoretical results, so based on our results which show good agreement with the experimental

data (see Tables 3-5) hence, we consider the present results are more accurate, hoping that our present work will stimulate some more works on this material. Future experimental works will testify our calculated results.

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