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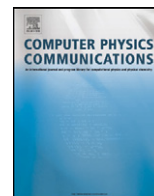


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# Calculations of single-crystal elastic constants made simple

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## ARTICLE INFO

### Article history:

Received 8 May 2009

Received in revised form 21 November 2009

Accepted 30 November 2009

Available online 4 December 2009

### Keywords:

Elasticity

## ABSTRACT

We present an efficient method to obtain single-crystal elastic constants. Using the method, the computation effort for the complete set of elastic constants (21 components for a triclinic crystal) of a crystal under a given strain state is similar to that for the bulk modulus, where the latter is normally calculated first together with the equilibrium volume by fitting the volume-dependent energy to an equation of state. The idea in the efficiency improvement is to apply linear-independent coupling strains to a crystal, and to extract the complete set of elastic constants simultaneously. For the new method, a single set of strains are universally applicable to all crystals, and less number of strains are needed for crystals of higher symmetry. Calculated single-crystal elastic constants of cubic diamond, hexagonal osmium, orthorhombic  $\text{TiSi}_2$  and monoclinic  $\text{Mg}_5\text{Si}_6$  are given as examples.

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## 1. Introduction

The elasticity is a fundamental property of crystalline materials and is of great importance in physical sciences, including materials science, solid state physics and chemistry, and geological sciences [1–3]. It describes the macroscopic response of crystals to external forces and directly relates to hardness and strength of materials, and the propagation of elastic waves in minerals. Many microscopic processes of materials, such as dislocation interactions and crack propagation, are analyzed based on the elasticity of materials [4]. More fundamentally, the elasticity of materials concerns the cohesion of solids and the thermodynamical properties, such as phonon spectra, the melting points, and Debye temperatures [2]. In this regard, the elastic constants are important parameters for the construction of interatomic potentials. Last, but far from least, the elasticity provides an important criterion for the mechanical stability of a crystal [1,5]. This information is quite helpful studying structural phase transitions and for searching new materials. A recent example is the story of platinum nitride, which had been unknown until synthesized in 2004 under high pressures and high temperatures, and filled the gap in the periodic table of nitrides [6]. The compound was initially proposed to be of the zinc-blende structure [6]. However, this structure was shown to be elastically unstable [7], which stimulated additional experimental and the-

oretical studies on this specific material, and provided important hints to understand and predict the crystal structures of other nitrides of noble transition metals [8–10].

The elasticity of a crystal is specified by a forth-rank tensor and can be described by a  $6 \times 6$  matrix [1,2]. The number of independent elastic constants depends on the symmetry of crystals. The lower the symmetry, the more the independent elastic constants: Cubic crystals have three but triclinic crystals have 21 independent elastic constants, for example. To measure the complete set of elastic constants experimentally, single crystals of macroscopic size are typically required. This makes the complete set of elastic constants available only for a very small portion of known materials, for which single crystals are available [11]. In some cases, such as metastable phases, grain boundary phases, and materials at extreme conditions, it is difficult and even impossible to grow a single crystal for elasticity measurements.

Alternatively, single-crystal elastic constants can be obtained from first-principles calculations (non-experimental method). Most of the previous calculations were based on fitting total energies [12–15] or stresses [16,17] of properly deformed crystals. The stress-based method is more efficient than the energy-based method, since for each deformation there are six stress components but only one energy available for the fitting. In these methods, different strain patterns are designed for crystals of different symmetry. For each strain pattern, energies or stress components are calculated step by step for a number of different strain magnitudes. Then the elastic constants are obtained by fitting the energy or stress as a function of the strain magnitude. Except for crystals of high symmetry, the procedure is computationally expensive and tedious. Very often, only the bulk modulus is calculated by

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**Table 1**

Components of six typical universal linear-independent coupling strains (in  $10^{-3}$ ). Note that the strains given here are not unique. Any strains of similar properties (see text for more details) can be used.

	$\varepsilon_1$	$\varepsilon_2$	$\varepsilon_3$	$\varepsilon_4$	$\varepsilon_5$	$\varepsilon_6$
$U_1$	1	2	3	4	5	6
$U_2$	−2	1	4	−3	6	−5
$U_3$	3	−5	−1	6	2	−4
$U_4$	−4	−6	5	1	−3	2
$U_5$	5	4	6	−2	−1	−3
$U_6$	−6	3	−2	5	−4	1

fitting the volume-dependent energy to an equation of state [18]. Approaches based on the linear response theory [19] or the interatomic force constants [5,20] were also used. These methods do not require explicit deformation on the reference crystal, but are generally more computationally demanding than the energy- or stress-based methods.

Here we present an efficient method that makes the computation effort required for the complete set of elastic constants of a crystal under a given strain state comparable to that required for the bulk modulus alone, even for crystals of the lowest symmetry. After the description of the method, examples are given for crystals of different symmetry.

## 2. Method

As in most previous calculations, the new method for single-crystal elastic constants is based on fitting the strain-stress relation of deformed crystals. Here the matrix notation, instead of tensor notation, is used to describe the single-crystal elastic constants, written as [1]

$$\begin{pmatrix} \sigma_1 \\ \sigma_2 \\ \sigma_3 \\ \sigma_4 \\ \sigma_5 \\ \sigma_6 \end{pmatrix} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ c_{12} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ c_{13} & c_{23} & c_{33} & c_{34} & c_{35} & c_{36} \\ c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} \\ c_{15} & c_{25} & c_{35} & c_{45} & c_{55} & c_{56} \\ c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} \end{pmatrix} \begin{pmatrix} \varepsilon_1 \\ \varepsilon_2 \\ \varepsilon_3 \\ \varepsilon_4 \\ \varepsilon_5 \\ \varepsilon_6 \end{pmatrix} \quad (1)$$

where  $\varepsilon_i$ ,  $\sigma_i$ , and  $c_{ij}$  are strain, stress, and single-crystal elastic (stiffness) constants, respectively. The stress tensor can be obtained from either first-principles or empirical potential methods. Once the stress is calculated for each strain, the single-crystal elastic constants are retrieved by linear least-squares fitting using singular value decomposition [21].

The improvement in the new method lies in the strains designed for universality and high efficiency. It is based on a simple idea: Each of the six stress components for a strain could be used as an independent ‘measurement’ of the elasticity of a crystal. The new strains are listed in Table 1. Abstractly, we say the six strain components  $\varepsilon_i$  span a 6-dimensional ‘strain space’, with the strain tensors as vectors in the space. Correspondingly, the calculated stress tensors represent vectors in a 6-dimensional ‘stress space’. The elastic constants matrix ( $c_{ij}$ ) is a mapping between the two spaces. The strains, named here ‘universal linear-independent coupling strains’ (ULICS), were designed to have the following three features. First, the strains are linear-independent to one another in the strain space. Second, all the stress components and elastic constants are coupled since there are no zero components in the strains. Third, the strains can be universally applied to crystals of any symmetry. For calculations of crystals of different symmetry, the only difference lies in the number of ULICS’s that are needed. More ULICS’s are needed for crystals of lower symmetry. The three features, as explained in more details in the following, are key points to the high efficiency of the new method.

**Table 2**

The angles ( $^\circ$ ) between the ULIC strains listed in Table 1, according to Eq. (2).

	$U_2$	$U_3$	$U_4$	$U_5$	$U_6$
$U_1$	90.0	90.0	90.0	90.0	90.0
$U_2$		90.6	95.7	68.7	114.0
$U_3$			86.9	98.2	98.2
$U_4$				102.1	80.5
$U_5$					115.4

**Table 3**

Number of ULICS required for the seven crystal systems.

Crystal system	Number of ULICS required
Cubic	1
Hexagonal	2
Rhombohedral	2
Tetragonal	2
Orthorhombic	3
Monoclinic	5
Triclinic	6

For the strain-stress fitting to be efficient, the sampling in both strain and stress spaces, and for the elastic constants, should be efficient. It requires strain and stress vectors to be linear independent; otherwise they would sample only certain subspaces. The angle between vectors, given by

$$\theta = \arccos\left(\frac{U_i \cdot U_j}{|U_i||U_j|}\right) \quad (2)$$

is a good measurement of linear-dependence. An angle of  $0^\circ$  means linear-dependent vectors. The larger the angle, the better the linear-independency. The angles between the ULICS in Table 1 are given in Table 2, which shows good linear-independency.

Note a trivial set of strains,  $[1 \ 0 \ 0 \ 0 \ 0 \ 0]$ ,  $[0 \ 1 \ 0 \ 0 \ 0 \ 0]$ ,  $[0 \ 0 \ 1 \ 0 \ 0 \ 0]$ ,  $[0 \ 0 \ 0 \ 1 \ 0 \ 0]$ ,  $[0 \ 0 \ 0 \ 0 \ 1 \ 0]$ , and  $[0 \ 0 \ 0 \ 0 \ 0 \ 1]$ , all in  $10^{-3}$ . Although linear-independent in the strain space, they sample only limited parts of strain and stress spaces. Taking  $[1 \ 0 \ 0 \ 0 \ 0 \ 0]$  as an example, its action on an orthorhombic crystal, according to Eq. (1), would give the stress of the form  $[\sigma_1 \ \sigma_2 \ \sigma_3 \ 0 \ 0 \ 0]$ . Thus only  $\sigma_1$ ,  $\sigma_2$ ,  $\sigma_3$  out of six stress components are sampled; and only  $c_{11}$ ,  $c_{21}$ ,  $c_{31}$  out of 9 independent elastic constants enters the above expression. Using the ULICS listed in Table 1, where the zero components are removed, all the stress components are sampled and all the elastic constants are coupled together.

Another feature of the ULIC strains listed in Table 1 is their universality: they are applicable to all the seven crystal systems. This is in contrast to current calculation methods, which require different strain patterns for different crystal systems. Thus the ULICS method makes the calculation of single-crystal elastic constants a simple, instead of a tedious process. The symmetry of the crystals can be utilized to reduce the computation further. The higher the symmetry, the less number of strains required. The numbers of required ULICS are listed in Table 3. Six ULICS are required for triclinic crystals, but only one ULICS is enough for cubic crystals. Taking the cubic case as a simple example, a ULICS (say  $U_1$ ,  $[1 \ 2 \ 3 \ 4 \ 5 \ 6] \times 10^{-3}$ ) gives a stress tensor of 6 components, with each one as a measurement of elasticity. The strain components  $\varepsilon_1$ ,  $\varepsilon_2$ ,  $\varepsilon_3$  couple  $c_{11}$  and  $c_{12}$  together to give  $\sigma_1$ ,  $\sigma_2$ ,  $\sigma_3$ . Thus  $c_{11}$  and  $c_{12}$  can be obtained from fitting the three measurements with one redundant,  $c_{44}$  from fitting  $\sigma_4$ ,  $\sigma_5$ ,  $\sigma_6$  with two redundant. For crystals of low symmetry, more ULICS’s in addition to those listed in Table 1, e.g.  $[6 \ 5 \ 4 \ 3 \ 2 \ 1] \times 10^{-3}$ , could be used to give larger redundancy. But our practice showed that the redundancy given by the ULICS of Table 3 is usually large enough. At high numerical accuracy normally adopted in calculations of elasticity, the differences in  $c_{ij}$  by using more ULICS are very small (about 1–2%). Examples are given in the next section.

**Table 4**The lattice parameters (in Å) of TiSi<sub>2</sub>.

	<i>a</i>	<i>b</i>	<i>c</i>
Cal. (present)	8.114	4.732	8.458
Exp. <sup>a</sup>	8.267	4.800	8.551
Cal. <sup>b</sup>	8.08	4.74	8.53

<sup>a</sup> Ref. [28].<sup>b</sup> Ref. [29].

Table 3 shows that six or less strains are required to retrieve the complete set of single-crystal elastic constants. As a comparison, about five volume strains are generally required to obtain only the bulk modulus of a crystal through the energy–volume fitting [18]. The high efficiency of the ULICS method is due to the linear-independence of the strains used, and the fact that the strains have no zero components. In this way, all the stress components are coupled together, making it possible to extract the complete set of elastic constants simultaneously, i.e., in a parallel mode. It should be mentioned that the ULICS's listed in Table 1 are by no means unique. Any strain combinations showing above three features would give similar efficiency and universality.

Many methods/codes could be employed to generate the stress tensor for each ULICS, including VASP, CASTEP, ABINIT, PWscf, and SIESTA, to name a few. In this paper we report the results using the projector augmented-wave method within density functional theory (DFT) [22,23], as implemented in the VASP code [24,25]. For the exchange and correlation functional the local density approximation (LDA) of the Perdew–Zunger parameterization [26] was used. Integrations over the Brillouin zone were performed using Monkhorst–Pack grids [27]. The *k*-point sampling in the Brillouin zone and the plane-wave cutoff energy were tested to ensure that the total energies converged to 1 meV per atom. The structural relaxations were performed until the residual forces and stresses (except the applied pressure) were less than 0.005 eV/Å and 0.05 GPa, respectively.

### 3. Applications and discussions

The ULICS method described above has been successfully applied to decades of crystals of different symmetry, from cubic to triclinic. Due to space limitation, the results for TiSi<sub>2</sub> (orthorhombic), diamond (cubic), Os (hexagonal), and Mg<sub>5</sub>Si<sub>6</sub> (monoclinic) are given in the following as examples. The data are given for materials at equilibrium volumes, which were evaluated from the Birch–Murnaghan fit to the total energies as a function of the unit cell volume. At each volume, the structure was fully relaxed.

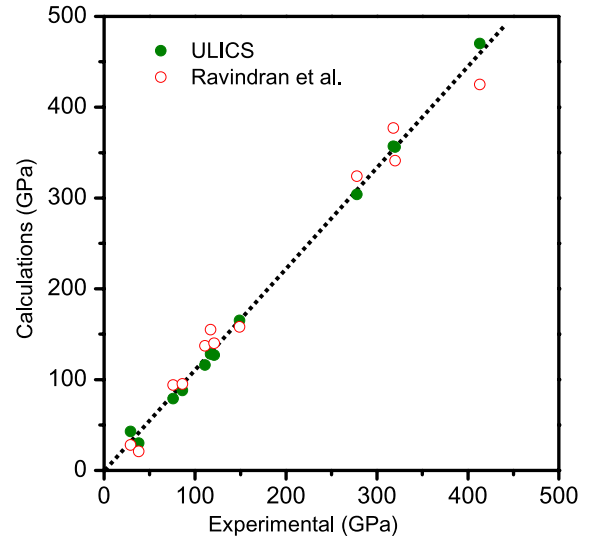
Titanium disilicide TiSi<sub>2</sub> has an orthorhombic lattice. It is widely used in the fabrication of integrated circuits as a contact material due to the high electrical and thermal conductivity, and the strong adhesion between TiSi<sub>2</sub> and silicon substrates. In addition, it exhibits high elastic stiffness, excellent oxidation resistance, high creep strength, and low density, very attractive for structural applications at temperatures up to 1300 °C and above. TiSi<sub>2</sub> has an orthorhombic structure, with the space group of Fddd (No. 70). The lattice parameters of TiSi<sub>2</sub> at equilibrium volume are given in Table 4. The experimental [28] and previously calculated [29] results are also listed for comparison. Table 5 lists the calculated single-crystal elastic constants of TiSi<sub>2</sub>, based on which the polycrystalline bulk modulus *B*, shear modulus *G*, Young's modulus *E*, and Poisson's ratio *ν* were obtained using the Voigt–Reuss–Hill averaging scheme [30]. All the elastic constants will be given in GPa except for the dimensionless Poisson's ratio. Three ULICS's, as listed in Table 3, were used in the calculations. Using more ULICS's resulted in less than 1% difference. The experimental [31] elastic constants and those calculated previously [29] are also given. For

**Table 5**The elastic constants of orthorhombic TiSi<sub>2</sub>. All the elastic constants will be given in GPa except for the dimensionless Poisson's ratio.

	<i>C</i> <sub>11</sub>	<i>C</i> <sub>22</sub>	<i>C</i> <sub>33</sub>	<i>C</i> <sub>44</sub>	<i>C</i> <sub>55</sub>	<i>C</i> <sub>66</sub>
Cal. (present)	357	356	470	116	79	128
Exp. <sup>a</sup>	318	320	413	111	76	117
Cal. <sup>b</sup>	377	341	425	137	94	155

	<i>C</i> <sub>12</sub>	<i>C</i> <sub>13</sub>	<i>C</i> <sub>23</sub>	<i>B</i>	<i>G</i>	<i>E</i>	<i>ν</i>
Cal. (present)	43	30	88	165	127	304	0.194
Exp. <sup>a</sup>	29	38	86	149	121	278	0.188
Cal. <sup>b</sup>	28	21	95	158	140	324	0.159

<sup>a</sup> Ref. [31].<sup>b</sup> Ref. [29].

**Fig. 1.** Comparison between calculated and experimental single-crystal elastic constants of TiSi<sub>2</sub>. The dotted line is an eye guide.

**Table 6**

The elastic constants of cubic diamond. All the elastic constants will be given in GPa except for the dimensionless Poisson's ratio.

	<i>C</i> <sub>11</sub>	<i>C</i> <sub>12</sub>	<i>C</i> <sub>44</sub>
Cal. (1 ULICS)	1077	143	586
Cal. (2 ULICS)	1097	145	585
Cal. (3 ULICS)	1095	144	589
Exp. <sup>a</sup>	1079	124	578
Cal. <sup>b</sup>	1099.6	142.8	587.0

<sup>a</sup> Ref. [36].<sup>b</sup> Ref. [37].

easy comparison, the data are plotted in Fig. 1. Generally, the error in elasticity calculations based on the DFT theory [22,23] is order of 10%, resulted mainly from the exchange–correlation approximation employed in the calculations [3], and the pseudopotentials if they are used. Considering the typical error, the agreement among the experimental, current and previous calculations is good. Note that 45 strains were used in the previous calculations [29]. In contrast, only 3 strains were used in the current calculations.

Diamond is one of the hardest materials in nature. It has a face-centered-cubic structure, with the space group of Fd $\bar{3}$ m (No. 227). The primitive unit cell contains two carbon atoms. The lattice parameter was calculated to be 3.536 Å, close to the experimental value 3.567 Å [32]. The single-crystal elastic constants of diamond are listed in Table 6. The data with one, two, and three ULICS are given. All the elastic constants are close to the experimental values. As can be seen, different numbers of ULICS resulted in only small changes in elastic constants.

**Table 7**

The elastic constants of Os. All the elastic constants will be given in GPa except for the dimensionless Poisson's ratio.

	$C_{11}$	$C_{12}$	$C_{13}$	$C_{33}$	$C_{55}$	$B$	$G$	$E$	$\nu$
Cal. (present)	839	246	257	925	279	458	293	725	0.236
Exp. <sup>a</sup>	763.3	227.9	218.0	843.2	269.3	410.3	274.3	673	0.227
Cal. <sup>b</sup>	894.5	249.2	245.6	1016.4	162.2	476.1			

<sup>a</sup> Ref. [38].

<sup>b</sup> Ref. [12].

**Table 8**

The lattice parameters  $a$  (in Å),  $b$  (in Å),  $c$  (in Å), and  $\beta$  (in degree) of  $\text{Mg}_5\text{Si}_6$ .

	$a$	$b$	$c$	$\beta$
Cal. (present)	14.95	3.89	7.00	110.18
Exp. <sup>a</sup>	15.16	4.05	6.74	105.3
Cal. <sup>b</sup>	14.88	3.97	6.83	110

<sup>a</sup> Ref. [33].

<sup>b</sup> Ref. [33,35].

**Table 9**

The elastic constants of monoclinic  $\text{Mg}_5\text{Si}_6$ . All the elastic constants will be given in GPa except for the dimensionless Poisson's ratio.

$C_{11}$	$C_{22}$	$C_{33}$	$C_{44}$	$C_{55}$	$C_{66}$
116	119	93	28	18	32
$C_{12}$	$C_{13}$	$C_{14}$	$C_{23}$	$C_{24}$	$C_{34}$
43	56	−6	45	12	10
$C_{46}$	$B$	$G$	$E$	$\nu$	
2	67	25	67	0.333	

Osmium has a hexagonal-close-packed structure, with the space group of  $P6_3/mmc$  (No. 194). The lattice parameters  $a$  and  $c$  were calculated to be 2.720 Å and 4.293 Å, respectively, quite close to the experimental values 2.735 Å and 4.319 Å. The single-crystal elastic constants are given in Table 7. Again, the agreement among the experimental, current and previous calculations is good.

$\text{Mg}_5\text{Si}_6$  is an important precipitation-hardening phase [33–35] in commercial aluminium alloys. In the Mg–Si binary system,  $\text{Mg}_2\text{Si}$  is the only equilibrium magnesium silicide.  $\text{Mg}_5\text{Si}_6$  is metastable and exists only in mechanically constrained conditions set up in the aluminium matrix. Since there is no free-standing  $\text{Mg}_5\text{Si}_6$  and their size is so small (typically  $4 \times 4 \times 50 \text{ nm}^3$  [33]), no experimental elastic properties of  $\text{Mg}_5\text{Si}_6$  are available.  $\text{Mg}_5\text{Si}_6$  has a monoclinic structure, with the space group of  $C2/m$  (No. 12). The lattice parameters of  $\text{Mg}_5\text{Si}_6$  at equilibrium volume are given in Table 8. Table 9 lists the calculated single-crystal elastic constants of  $\text{Mg}_5\text{Si}_6$  and the corresponding polycrystalline elastic constants. Five ULICS's were used in the calculations. The eigenvalues of the elastic-constant matrix were calculated, giving the lowest value of 13 GPa. It indicates that, although energetically metastable,  $\text{Mg}_5\text{Si}_6$  is elastically stable.

As the ULICS method provides high efficiency, it is now less computationally demanding to study the elastic constants of complex structures, and the trends in the elastic constants as a function of pressure, temperature or chemical composition. Soft deformation modes, which are of particular interest to study the mechanisms of phase transitions, can also be identified from the eigenvalues and eigenvectors of calculated elastic-constant matrix. It should be noted, however, since all the elastic constants are coupled, it is impossible to get the atomic configuration and the controlling electronic states of a particular elastic modulus. For this kind of purposes, additional calculations using individual (decoupled) strains will be needed.

We mentioned earlier that, using the ULICS method, the computation effort required for the complete set of elastic constants

of a crystal at a given strain state is comparable to that required for the bulk modulus alone. We note here, however, that the new method is not for the substitution of the calculations for the bulk modulus. In fact, for elastic constants at the equilibrium volume, one needs to calculate the latter first, normally by fitting the volume-dependent energy to an equation of state. The bulk modulus would be obtained at the same time during the fitting. Once the equation of state has been obtained, we have a one-to-one correspondence between the volume and the pressure. Thereafter, the single-crystal elastic constants at any given pressure can be easily calculated at the corresponding volume using the new method.

#### 4. Summary

In summary, we present here an efficient method to calculate single-crystal elastic constants. Besides the reduced computation costs, the simplicity that a single set of strains are applicable to all crystals would be more appealing. We expect the method will find a wide range of applications in solid state physics and chemistry, materials science, and geological sciences. The program implementing the method is available for free from the authors.

#### Acknowledgements

This work was supported by the National Natural Science Foundation of China (No. 50801040), the Foundation for the Author of National Excellent Doctoral Dissertation of PR China, the 985 Project of Tsinghua University, and the National 973 Project of China.

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