

Bachelorarbeit

Zur Erlangung des akademischen Grades Bachelor of Science (B.Sc.)

Implementing Third-Order Elastic Coefficients in ElaStic

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Abstract

I present my implementation of the third-order elastic constants into the **ElaStic** tool for those crystal systems not yet implemented. This includes the new “minimal-variation”-method, which automatizes the search for the ideal parameters for the fits to be performed, as well as changing the **ElaStic** tool to allow for an easier changing of strain types. Tests are performed for diamond and the titanium dioxide in the rutile phase for second and third-order elastic constants.

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Chapter 1

Introduction

The elastic constants of a material are properties of high concern as these constants determine the mechanical characteristics of the material. As such, a variety of methods are employed to obtain them, such as Raman spectroscopy [1] and shock wave measurements [2] from the experimental side, as well as theoretical approaches based on the Keating model [3] or modern *ab initio* calculations mainly using the density-functional theory [4].

This last method is the basis for the **ElaStic** tool [5]. **Elastic** calculates elastic constants of materials by computing their energies under deformation, performing fits onto the results and extracting the elastic constants from the fit parameters. However, until this work, the elastic constants of third order could be investigated with **ElaStic** only for a limited set of crystal systems .

Third-order elastic constants (TOECs) give the most important contribution to the anharmonic effects in a material. Knowledge of them allows one to predict, *e.g.*, how the second-order elastic constants (SOECs) change under pressure [6], the ductility of materials [7], and the Grüneisen parameters [8]. TOECs can also be used to construct models for interatomic potentials [9].

In this work, I present my implementation of the calculation of third-order elastic constants (TOECs) into the **ElaStic** tool, for those crystal groups not already implemented. To this end, I give some background on elastic theory as well as a short description of the **ElaStic** and **exciting** [10] software packages. Finally, I present what I implemented into **ElaStic** including the minimal-variation method and show applications performed using **exciting** of the new **ElaStic** code for the test cases of diamond and TiO_2 in the rutile phase.

Chapter 2

Theoretical Background

In this chapter, I give a background on the theory of elasticity describing strains and elastic constants as well as a short introduction of density-functional theory (DFT) which the **exciting** package is based on.

2.1 Elastic strains

Elastic strain describes a reversible deformation of an object. Macroscopic deformations can be complex, they can include bending or twisting of an object, but for many material properties, only microscopic deformations matter. On the microscopic scale any deformation can be approximated by a linear deformation: Deformations that compress the material in one dimension (uniaxial strain), deformations that shear the material (shearing strain), or any combination of uniaxial and shearing strains. An example in 2 dimensions of the different strain types is given in Fig. 2.1.

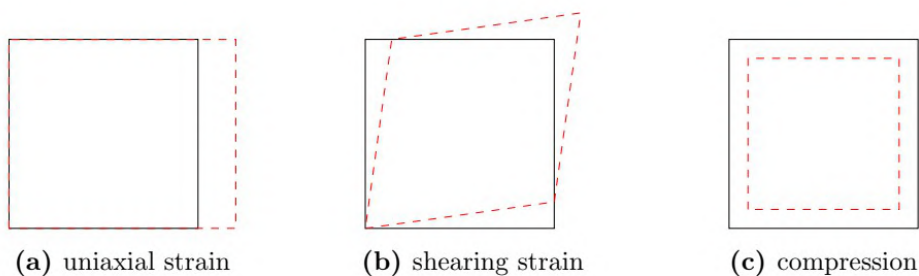


Figure 2.1: Visualization of different strain types in 2 dimensions.

Following Ref. [11], we describe these deformations by the physical strain tensor $\underline{\underline{\epsilon}}$, a symmetric second-order tensor:

$$\underline{\underline{\epsilon}} = \begin{pmatrix} \epsilon_{xx} & \epsilon_{xy} & \epsilon_{xz} \\ \epsilon_{xy} & \epsilon_{yy} & \epsilon_{yz} \\ \epsilon_{xz} & \epsilon_{yz} & \epsilon_{zz} \end{pmatrix} . \quad (2.1)$$

This tensor describes the deformation of a material that sends objects at position $\underline{x}$ to the position

$$(\mathbb{1} + \underline{\underline{\epsilon}}) \cdot \underline{x} . \quad (2.2)$$

For the purposes of deformations we only have to consider symmetric tensors, since any non-symmetric tensor gives a transformation of the object identical one from a symmetric tensor with a rotation.

However, this way of writing the strain depends on the point of origin and is, therefore, not “thermodynamically invariant”. For this reason, we use the Lagrangian strain $\underline{\underline{\eta}}$ in this thesis instead, which is defined by changes in the length of vectors:

$$|\underline{v}_{\text{new}}|^2 - |\underline{v}_{\text{old}}|^2 = 2 \underline{v}_{\text{old}} \cdot \underline{\underline{\eta}} \cdot \underline{v}_{\text{old}} . \quad (2.3)$$

The Lagrangian strain is related to the physical one by

$$\underline{\underline{\eta}} = \underline{\underline{\epsilon}} + \frac{1}{2} \underline{\underline{\epsilon}}^2 . \quad (2.4)$$

From now on, we describe the Lagrangian strain within the Voigt notation, in which the deformation is represented by a six dimensional vector:

$$\underline{\underline{\eta}} \equiv (\eta_1, \eta_2, \eta_3, \eta_4, \eta_5, \eta_6) \equiv (\eta_{xx}, \eta_{yy}, \eta_{zz}, 2\eta_{yz}, 2\eta_{xz}, 2\eta_{xy}) . \quad (2.5)$$

2.2 Elastic constants

We write the dependence of the elastic energy on the strain by performing a multi-dimensional Taylor expansion of the elastic energy around its equilibrium state:

$$E(\underline{\eta}) = E_0 + \frac{V_0}{2!} \sum_{ki} C_{ki}^{(2)} \eta_k \eta_i + \frac{V_0}{3!} \sum_{kij} C_{kij}^{(3)} \eta_k \eta_i \eta_j + \dots \quad (2.6)$$

Here $C_{ki}^{(2)}$ and $C_{kij}^{(3)}$ (with the Voigt indices $k, i, j = 1, \dots, 6$) are the second (SOECs) and third-order elastic constants (TOECs), respectively, that we are interested in. Furthermore, E_0 is the equilibrium energy and the linear term is omitted, as the energy is minimal at equilibrium, which necessitates the linear term to vanish. Finally, a pre-factor V_0 was chosen, since the energy is an extensive variable, and elastic constants are supposed to be material variables and therefore intensive.

The focus of this work is on the nonlinear elastic constants at the leading order, described by the third-order elastic tensor $\{C_{kij}^{(3)}\}$. This tensor is symmetric under permutation of indices:

$$C_{kij}^{(3)} = C_{kji}^{(3)} = C_{ikj}^{(3)} = C_{ijk}^{(3)} = C_{jki}^{(3)} = C_{jik}^{(3)}.$$

Furthermore, the symmetry of the crystal structure gives more restrictions on the elements of $\{C_{kij}^{(3)}\}$. For instance, for those crystals with a space group number from 177 to 194 (which we call “**Hexagonal 1**”) the third-order elastic tensor has the form shown in the next page.

$$\begin{aligned}
& C_{1ij}^{(3)} : \begin{pmatrix} C_{111} & C_{112} & C_{113} & 0 & 0 & 0 \\ C_{112} & \tilde{C}_{122} & C_{123} & 0 & 0 & 0 \\ C_{113} & C_{123} & C_{133} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{144} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{155} & 0 \\ 0 & 0 & 0 & 0 & 0 & \tilde{C}_{166} \end{pmatrix} & C_{2ij}^{(3)} : \begin{pmatrix} C_{112} & \tilde{C}_{122} & C_{123} & 0 & 0 & 0 \\ \tilde{C}_{122} & C_{222} & C_{113} & 0 & 0 & 0 \\ C_{123} & C_{113} & C_{133} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{155} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{144} & 0 \\ 0 & 0 & 0 & 0 & 0 & \tilde{C}_{266} \end{pmatrix}
\end{aligned}$$

$$\begin{aligned}
& C_{3ij}^{(3)} : \begin{pmatrix} C_{113} & C_{123} & C_{133} & 0 & 0 & 0 \\ C_{123} & C_{113} & C_{133} & 0 & 0 & 0 \\ C_{133} & C_{133} & C_{333} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{344} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{344} & 0 \\ 0 & 0 & 0 & 0 & 0 & \tilde{C}_{366} \end{pmatrix} & C_{4ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & C_{144} & 0 & 0 \\ 0 & 0 & 0 & C_{155} & 0 & 0 \\ 0 & 0 & 0 & C_{344} & 0 & 0 \\ C_{144} & C_{155} & C_{344} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \tilde{C}_{456} \\ 0 & 0 & 0 & 0 & \tilde{C}_{456} & 0 \end{pmatrix}
\end{aligned}$$

$$\begin{aligned}
& C_{5ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & 0 & C_{155} & 0 \\ 0 & 0 & 0 & 0 & C_{144} & 0 \\ 0 & 0 & 0 & 0 & C_{344} & 0 \\ 0 & 0 & 0 & 0 & 0 & \tilde{C}_{456} \\ C_{155} & C_{144} & C_{344} & 0 & 0 & 0 \\ 0 & 0 & 0 & \tilde{C}_{456} & 0 & 0 \end{pmatrix} & C_{6ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \tilde{C}_{166} \\ 0 & 0 & 0 & 0 & 0 & \tilde{C}_{266} \\ 0 & 0 & 0 & 0 & 0 & \tilde{C}_{366} \\ 0 & 0 & 0 & 0 & \tilde{C}_{456} & 0 \\ 0 & 0 & 0 & \tilde{C}_{456} & 0 & 0 \\ \tilde{C}_{166} & \tilde{C}_{266} & \tilde{C}_{366} & 0 & 0 & 0 \end{pmatrix}
\end{aligned}$$

Here, the $\{\tilde{C}_{kij}\}$ are expressed in terms of the other elastic constants as:

$$\begin{aligned}
\tilde{C}_{122} &= C_{111} + C_{112} - C_{222} & \tilde{C}_{166} &= \frac{1}{2}C_{112} - \frac{1}{2}C_{123} \\
\tilde{C}_{366} &= \frac{1}{2}C_{113} + \frac{1}{2}C_{123} & \tilde{C}_{456} &= -\frac{1}{2}C_{144} + \frac{1}{2}C_{155} \\
\tilde{C}_{266} &= \frac{1}{2}C_{111} - \frac{1}{4}C_{112} + \frac{1}{4}C_{222}
\end{aligned}$$

Table 2.1: Categorization of crystal systems by their space-group number with their respective number of independent SOECs and TOECs.

Name	Space group number	$\#C_{ki}^{(2)}$	$\#C_{kij}^{(3)}$
Cubic 1	207 to 230	3	6
Cubic 2	195 to 296	3	8
Hexagonal 1	177 to 194	5	10
Hexagonal 2	168 to 176	5	12
Trigonal 1	149 to 167	6	14
Trigonal 2	143 to 148	7	20
Tetragonal 1	89 to 142	6	12
Tetragonal 2	75 to 88	7	16
Orthorombic	16 to 74	9	20
Monoclinic	3 to 15	13	32
Triclinic	1 to 2	21	56

The form of the tensor for the other crystal systems, categorized in Table 2.1 is shown in Appendix A. These have been taken from Ref. [12].

2.3 Born-Oppenheimer approximation

In order to determine elastic constants, the **ElaStic** code has to compute the energy of the crystal system under strain. For the calculations in this thesis, this is done using the software package **exciting**, based on the solution of the quantum-mechanical problem of a crystal within the density-functional theory.

To calculate the energy of a state in quantum mechanics, one has to use the Schrödinger equation:

$$\hat{H} \Psi(r, R) = E \Psi(r, R) . \quad (2.7)$$

Here, the coordinate r is representing the set of positions of all the electrons, while R represents the set of positions of the nuclei. We can separate the full crystal Hamiltonian, $\hat{H}$, into kinetic and potential energies:

$$\hat{H} = \hat{T}_n + \hat{T}_e + \hat{V}_{ee} + \hat{V}_{en} + \hat{V}_{nn} , \quad (2.8)$$

where $\hat{T}_n$ is the kinetic energy of the nuclei and $\hat{T}_e$ the kinetic energy of the electrons, while V_{nn} , V_{en} and V_{ee} give us the potential energy between pairs of nuclei, between combinations of nucleus and electron, and pairs of electrons respectively.

To solve the Schrödinger equation, we use the adiabatic (Born-Oppenheimer) approximation [13], where the full wave function $\Psi(r, R)$ is written as a product of a function $\chi(R)$ that only depends on the coordinates of the nuclei and a function $\varphi(r; R)$ that depends on the coordinates of the electrons and, parametrically, on the nuclear coordinates:

$$\Psi(r, R) = \chi(R) \varphi(r; R) . \quad (2.9)$$

Using the Born-Oppenheimer approximation allows us to then write the Schrödinger equation as two connected equations:

$$[\hat{T}_e + \hat{V}_{en} + \hat{V}_{ee}] \varphi(r; R) = E(R) \varphi(r; R) \quad (2.10)$$

and

$$[\hat{T}_n + \hat{V}_{nn} + E(R)] \chi(R) = E_{\text{BO}} \chi(R) . \quad (2.11)$$

This means that we can get the total energy of a crystal for a fixed nuclear configuration (which is the elastic energy we are interested in) under the Born-Oppenheimer approximation by treating the nuclei like classical particles: We keep fixed their positions at coordinates R and solve Eq. (2.10) for the electronic ground-state energy $E(R)$. We add this to the classical coulomb potential $V_{nn}(R)$ and get the total energy of the crystal for the given nuclear configuration R :

$$E_{\text{total}} = V_{nn}(R) + E(R) . \quad (2.12)$$

In the following we always refer to the ground-state energy calculated for a fixed nuclear configuration by minimizing $E(R)$ over the electronic wave-function.

2.4 Density-functional theory

This section follows the description given in Chapter 3 of Ref. [14]. To calculate the electron energy, we use the Kohn-Sham scheme from density-functional theory (DFT). DFT is based on the Hohenberg-Kohn (HK) theorems described in the following.

The first HK theorem states that the outer potential of a system of electrons (and therefore any other information of the system) is uniquely defined by its ground-state (GS) electron density $n_{\text{GS}}(\underline{r})$. The second HK theorem states that for a given system, the ground-state energy functional is minimized at its ground-state electron density $n_{\text{GS}}(\underline{r})$. As such, its functional derivative under the constraint of normalization of the density vanishes at the ground-state electron density:

$$\left. \frac{\delta(E[n] - \mu N)}{\delta n} \right|_{n_{\text{GS}}} = 0, \quad (2.13)$$

where N is the number of electrons in the system and μ the electronic chemical potential. Then, following a schema first developed by Kohn and Sham (KS), we split the ground-state energy functional in a sum of different functionals, $T_0[n]$ for the kinetic energy of the KS system, $E_{\text{H}}[n]$ for the Hartree energy, the energy from interaction with the nuclei $E_{\text{ext}}[n]$, and the exchange-correlation functional $E_{\text{xc}}[n]$. The exchange-correlation functional represents the energy that is not contained in the other functionals, and has to be approximated. Using this separation, Equation (2.13) can be written as (the index GS is omitted in the following):

$$\frac{\delta T_0[n]}{\delta n} + \frac{\delta E_{\text{H}}[n]}{\delta n} + \frac{\delta E_{\text{ext}}[n]}{\delta n} + \frac{\delta E_{\text{xc}}[n]}{\delta n} - \mu = 0. \quad (2.14)$$

To solve this equation, one then introduces the Kohn-Sham system, a system of non-interacting electrons, that, nevertheless, possesses the same ground-state electron density as the actual system we want to examine. The minimization of the GS energy functional within the KS approach leads us to the KS equations ($\nu = 1, \dots, N$):

$$\hat{h}_{\text{KS}} \phi_{\nu}(\underline{r}) = \left[-\frac{1}{2} \nabla^2 + v_{\text{H}}(\underline{r}, [n]) + v_{\text{ext}}(\underline{r}) + v_{\text{xc}}(\underline{r}, [n]) \right] \phi_{\nu}(\underline{r}) = \varepsilon_{\nu} \phi_{\nu}(\underline{r}) \quad (2.15)$$

$$\text{with} \quad n(\underline{r}) = \sum_{\nu} |\phi_{\nu}(\underline{r})|^2 \quad \text{and} \quad v_{\text{xc}}(\underline{r}, [n]) = \frac{\delta E_{\text{xc}}[n]}{\delta n(\underline{r})}. \quad (2.16)$$

These equations have to be solved “self-consistently”. This means that a starting density $n(\underline{r})$ is chosen, then, Kohn-Sham states ϕ_{ν} are generated using this density and Eq. (2.15), and then a new density is calculated with Eq. (2.16). This process is repeated until the density converges, *i.e.*, the difference between the density from the previous step and the current one is smaller than a chosen margin of error.

2.5 Solving the KS equations numerically

For a numerical solution of the KS equations, the KS states need to be expanded into a finite set of basis functions $\{\varphi_j(\underline{r})\}$:

$$\phi_\nu(\underline{r}) = \sum_j^{j_{\max}} c_\nu^j \varphi_j(\underline{r}) . \quad (2.17)$$

Using this on the Eq. (2.15) transforms it into a matrix equation:

$$\left(\underline{\underline{H}} - \epsilon_\nu \underline{\underline{S}} \right) \cdot \underline{c}_\nu = 0 . \quad (2.18)$$

Here, $\underline{c}_\nu$ is the representation of eigenvector ϕ_ν in the basis $\{\varphi_j(\underline{r})\}$, $\underline{\underline{H}}$ is the KS Hamiltonian in that basis

$$H_{jk} = \langle \varphi_j | \hat{h}_{\text{KS}} | \varphi_k \rangle , \quad (2.19)$$

and $\underline{\underline{S}}$ is the overlap matrix

$$S_{jk} = \langle \varphi_j | \varphi_k \rangle . \quad (2.20)$$

Chapter 3

The **exciting** and **ElaStic** Packages

The main focus of this thesis is the implementation of the **ElaStic** package [5]. **ElaStic** is a tool that calculates elastic constants from first principles by calculating energies of deformed crystal systems, performing fits onto the results and then obtain the elastic constants from the fit parameters. To calculate the energy of a crystal system under deformation, **ElaStic** is interfaced with the **exciting** package [10].

3.1 The **exciting** code

exciting is a full-potential all-electron package based on density-functional theory (DFT). Basically, **exciting** implements the numerical solution of the Kohn-Sham (KS) equations by expanding the KS states in a finite set of basis functions.

3.1.1 **exciting** basis functions

In **exciting** the space in the unit cell is separated into two regions: For every nucleus, points that lie within a sphere centered on that atom are said to be in a “muffin tin” (MT). The radius R_{MT} of these spheres can be chosen by the user of **exciting**. The space that is not part of a “muffin-tin” is called the “interstitial” (I) region. This separation is done, because the wave functions vary very fast close to the nuclei, while varying slower in regions further away. **exciting** uses 3 types of basis functions. These are called: “augmented plane waves” (APW), “linearized augmented plane waves” (LAPW) and “local orbitals” (LO).

An APW basis function consists of two parts: Within the MT spheres, it is represented in terms of spherical harmonics, $\hat{Y}(\underline{r})$, and radial functions, $u(\underline{r})$, while in the interstitial region it is represented by a plane wave:

$$\varphi_{\underline{G}+\underline{k}}(\underline{r}) = \begin{cases} \sum_{lm} A_{lm\alpha}^{\underline{G}+\underline{k}} u_{l\alpha}(r_\alpha) Y_{lm}(\hat{r}_\alpha) & \text{if } r_\alpha \leq R_{\text{MT}}^\alpha, \\ \frac{1}{\sqrt{\Omega}} e^{i(\underline{k}+\underline{G})\cdot\underline{r}} & \text{else,} \end{cases} \quad (3.1)$$

here, Ω is the unit-cell volume and the factors $A_{lm\alpha}^{\underline{G}+\underline{k}}$ are chosen in a way that ensures continuity between the two regions.

LAPW basis functions function in a similar way, except that the first energy derivative of the radial functions, $\dot{u}(\underline{r})$, also appears, as well as a further type of coefficients, B , which ensure, that the function is not only continuous at the transition between the MT and I regions, but that its derivative is continuous too.

$$\varphi_{\underline{G}+\underline{k}}(\underline{r}) = \begin{cases} \sum_{lm} \left(A_{lm\alpha}^{\underline{G}+\underline{k}} u_{l\alpha}(r_\alpha; \epsilon_{l\alpha}) + B_{lm\alpha}^{\underline{G}+\underline{k}} \dot{u}_{l\alpha}(r_\alpha; \epsilon_{l\alpha}) \right) Y_{lm}(\hat{r}_\alpha) & \text{if } r_\alpha \leq R_{\text{MT}}^\alpha, \\ \frac{1}{\sqrt{\Omega}} e^{i(\underline{k}+\underline{G})\cdot\underline{r}} & \text{else.} \end{cases} \quad (3.2)$$

The LO basis functions only affect the MT sphere:

$$\varphi_\mu(\underline{r}) = \begin{cases} \delta_{\alpha\alpha_\mu} \delta_{ll_\mu} \delta_{mm_\mu} [a_\mu u_{l\alpha}(r_\alpha) + b_\mu \dot{u}_{l\alpha}(r_\alpha)] Y_{lm}(\hat{r}_\alpha) & \text{if } r_\alpha \leq R_{\text{MT}}^\alpha, \\ 0 & \text{else.} \end{cases} \quad (3.3)$$

Here, the coefficients a_μ and b_μ are chosen in such a way, that the function is continous at the MT boundary and that the function is normalized to 1.

The LO base functions are combined with either APW or LAPW functions to give the basis that the KS state is expressed as:

$$\phi_{n\underline{k}}(\underline{r}) = \sum_{\underline{G}} c_{n\underline{G}}^{\underline{k}} \varphi_{\underline{G}+\underline{k}}(\underline{r}) + \sum_{\mu} c_{n\mu} \varphi_\mu(\underline{r}). \quad (3.4)$$

where, the band index n and the wave-vector $\underline{k}$ have been introduced explicitly instead of the index ν , for taking into account the periodicity of the crystal.

3.1.2 Parameters in exciting

Many parameters can be chosen in the input file for a **exciting** calculation. Important for the calculations presented further below are the following:

- **rgkmax**

This parameter represents the product of $R_{\text{MT}} = \min_\alpha R_{\text{MT}}^\alpha$, the MT radius and $|\underline{G} + \underline{k}|_{\text{max}}$ the maximum length of $\underline{G} + \underline{k}$, which limits the size of our basis set of (L)APW functions.

- **ngridk**

To calculate the total energy, one needs to integrate over the first Brillouin zone. **exciting** approximates this by sampling over the Brillouin zone. The mesh for sampling is given by **ngridk**, a triplet of natural numbers which represents the density of the mesh along the 3 basis vectors of the reciprocal space.

- **gmaxvr**

This parameter gives the maximum length of reciprocal lattice vectors G considered in the Fourier expansion of the potential and the density for the interstitial region.

- **swidth**

To allow for partial occupation of states close to the Fermi energy in metals, **exciting** uses a smoothing function. The width of the smoothing function is controlled by this parameter.

3.2 The **ElaStic** workflow

The starting step of **ElaStic** is the determination of the space group of the material which is to be examined. Depending on this space group, **ElaStic** chooses a list of deformation types to be applied to the material. Then, for each strain in the list (from here on now called the “strain type”), **ElaStic** calculates the energy of the strained system under different strain amplitudes employing the **exciting** code. The amplitudes are chosen to be evenly distributed up to a maximum value, the number of deformations and maximum amplitude are chosen by the user.

After the calculations are completed, **ElaStic** performs for each strain type a polynomial fit of the strain amplitude onto the obtained energies. However, the appropriate choice of both the polynomial order and number of deformations actually used for each strain type is not trivial. Allowing large strain amplitudes to be fitted risks leaving the region for which the polynomial approximates the real curve well. On the other hand, a fit onto points with possible numerical errors is most precise when the distance between those points is at its largest. Additionally, in the spirit of Taylor’s expansion, choosing a polynomial of low order restricts the domain on which it is a good approximation (and therefore the number of points which can be fitted sensibly), but increasing the order of the polynomial increases the degrees of freedom, and therefore decreases the predictive power of the fitting procedure.

ElaStic’s approach to this problem is to perform the fit for the polynomials of order n equal to those of the elastic constants, as well as for the orders $n + 2$ and $n + 4$, for each possible maximum strain amplitude and to plot the resulting

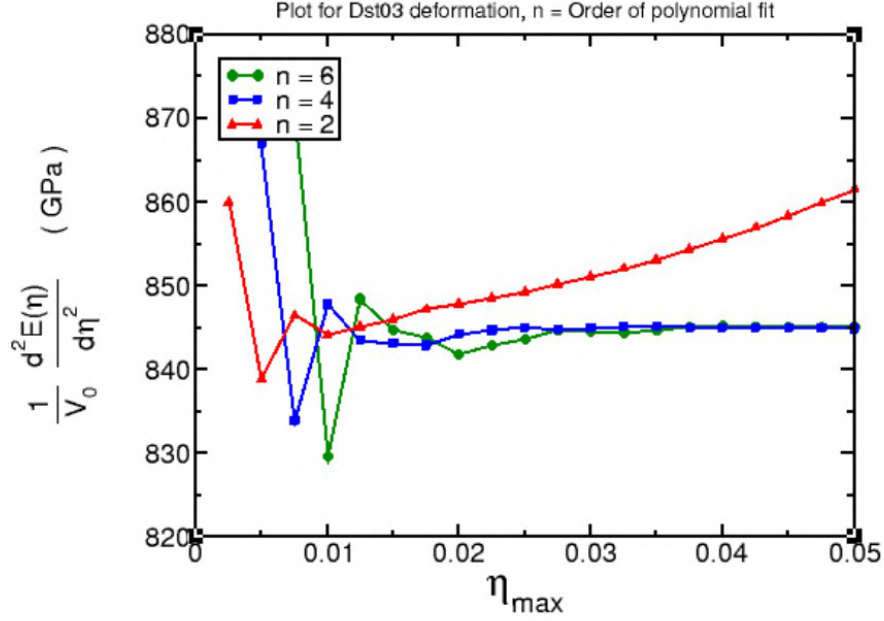


Figure 3.1: Fit parameter of order 2 (corresponding to the second derivative of the energy at equilibrium) in dependence of the maximum strain value and polynomial order of the fitting function for strain type 3 of TiO_2 in the rutile phase. Details of the calculation can be found in Section 5.2

fit parameters in dependence of the maximum strain amplitude to the user, as seen in the example shown in Fig. 3.1. The user can then choose the polynomial order and maximum strain with their own judgment of where they see a plateau for the fit parameter (since we expect “stability” from the correct maximum amplitude). Once this is done for each strain type, **ElaStic** then calculates the elastic constants from the fit parameters.

Chapter 4

A new implementation for **ElaStic**

The calculation of the third-order elastic constants (TOECs) of some crystal symmetries were already implemented in the **ElaStic** code. This concerns crystals with the following symmetries:

- **Cubic 1**,
- **Cubic 2**,
- **Hexagonal 1**,
- **Hexagonal 2**,
- **Trigonal 1**.

In this thesis, I implemented the remaining symmetries:

- ◇ **Trigonal 2**,
- ◇ **Tetragonal 1**,
- ◇ **Tetragonal 2**,
- ◇ **Orthorombic**,
- ◇ **Monoclinic**,
- ◇ **Triclinic**.

I also revised the symmetries already implemented, to allow for the changing of strain types without much effort, and implemented a procedure to automatize the choice of maximum fitted strain amplitude, which I call the “minimal-variation” method.

Finally, in order to do this implementation of the TOECs, I had to accomplish two tasks: (i) choosing the strain types for each symmetry type and (ii) figuring out the relationship between the elastic constants and the fitting parameters to implement the calculation of the elastic constants in the last step.

4.1 Calculating TOECs from the fit parameters

In order to get the relationship between the elastic constants of a given order and the fitting parameters, we use Eq. (2.6) as well as the polynomial fit, for a strain of $t \cdot \underline{\eta}^{(\nu)}$, where ν is the index indicating the strain type and t represents the strain amplitude:¹

$$\begin{aligned} E(t \cdot \underline{\eta}^{(\nu)}) &= A_0^{(\nu)} + A_2^{(\nu)} t^2 + A_3^{(\nu)} t^3 + \dots \\ &= E_0 + \left(\frac{V_0}{2!} \sum_{ki} C_{ki}^{(2)} \eta_k^{(\nu)} \eta_i^{(\nu)} \right) t^2 \\ &\quad + \left(\frac{V_0}{3!} \sum_{kij} C_{kij}^{(3)} \eta_k^{(\nu)} \eta_i^{(\nu)} \eta_j^{(\nu)} \right) t^3 + \dots \end{aligned} \quad (4.1)$$

Comparing the coefficients of t^3 (to get the third-order elastic constants) gives us

$$A_3^{(\nu)} = \frac{V_0}{3!} \sum_{kij} C_{kij}^{(3)} \eta_k^{(\nu)} \eta_i^{(\nu)} \eta_j^{(\nu)}. \quad (4.2)$$

However, the elastic constants, $C_{kij}^{(3)}$, are not all independent from each other. Therefore, we have to express the $C_{kij}^{(3)}$ in terms of independent parameters. These parameters happen to always be related linearly, thus, we can write:

$$C_{kij}^{(3)} = \sum_{\sigma} \lambda_{kij}^{\sigma} \Gamma_{\sigma}, \quad (4.3)$$

where the sum over σ is extended to number of independent TOECs, Γ_{σ} . Substituting this into Eq. (4.2), we obtain

$$A_3^{(\nu)} = \sum_{\sigma} \left(\frac{V_0}{3!} \sum_{kij} \lambda_{kij}^{\sigma} \eta_k^{(\nu)} \eta_i^{(\nu)} \eta_j^{(\nu)} \right) \Gamma_{\sigma}. \quad (4.4)$$

This equation defines a linear relationship between the fitting parameters $\{A_3^{(\nu)}\}$ and the independent TOECs, $\{\Gamma_{\sigma}\}$. Equation (4.4) can also be written in a matrix form as

$$\underline{A}_3 = \underline{B} \cdot \underline{\Gamma}, \quad (4.5)$$

where

$$B_{\nu\sigma} = \frac{V_0}{3!} \sum_{kij} \lambda_{kij}^{\sigma} \eta_k^{(\nu)} \eta_i^{(\nu)} \eta_j^{(\nu)}. \quad (4.6)$$

¹Notice that, here, t can assume positive or negative values. For the strain type $\nu = 1$, *e.g.*, positive (negative) values of t correspond to tensile (compression) strains.

If the number of strain types is equal to the number of independent TOECs and if the matrix $\underline{\underline{B}}$ is invertible, we can obtain the independent elastic constants $\{\Gamma_\sigma\}$ from the fitting parameters $\{A_3^{(\nu)}\}$, by simply multiplying Eq. (4.5) on the left by $\underline{\underline{B}}^{-1}$.

4.2 Choice of the strain types

When choosing the strain types for each crystal symmetry, one important issue to take into consideration is to choose them in such a way that the matrix $\underline{\underline{B}}$ is invertible. This means effectively that each strain type which is added needs to give us new information about the elastic constants.

The second consideration one has to make, is to choose strain types whose application onto the crystal leaves the crystal with as much symmetry as possible, as this speeds up the **exciting** calculations.

Thirdly, it is important to use as many strain types as possible which are already used for the calculation of the second-order elastic constants, as this allows for using one set of **exciting** calculations to be used for both the SOECs and TOECs.

Two test cases are given as example for the chosen strain types in Table 4.1, for **Cubic 1** as a representative for symmetry groups already implemented, and in Table 4.2, for **Tetragonal 1** as a representative for the newly implemented groups, respectively.

Table 4.1: TOECs strain types used for **Cubic 1** crystal structures in Voigt notation.

strain type	η_1	η_2	η_3	η_4	η_5	η_6
$\underline{\eta}^{(1)}$	η	η	η	0	0	0
$\underline{\eta}^{(2)}$	η	η	0	0	0	0
$\underline{\eta}^{(3)}$	0	0	0	0.5η	0.5η	0.5η
$\underline{\eta}^{(4)}$	η	η	$-\eta$	0	0	0
$\underline{\eta}^{(5)}$	η	0	0	0.5η	0	0
$\underline{\eta}^{(6)}$	η	0	0	0	0.5η	0

Table 4.2: Same as Table 4.1 for **Tetragonal 1** crystal structures.

strain type	η_1	η_2	η_3	η_4	η_5	η_6
$\underline{\eta}^{(1)}$	η	η	η	0	0	0
$\underline{\eta}^{(2)}$	0	0	η	0	0	0
$\underline{\eta}^{(3)}$	η	η	0	0	0	0
$\underline{\eta}^{(4)}$	0.5η	0.5η	$-\eta$	0	0	0
$\underline{\eta}^{(5)}$	η	0	η	0	0	0
$\underline{\eta}^{(6)}$	$-\eta$	0	η	0	0	0
$\underline{\eta}^{(7)}$	η	0	0	0.5η	0	0
$\underline{\eta}^{(8)}$	η	0	0	0	0.5η	0
$\underline{\eta}^{(9)}$	η	0	0	0	0	0.5η
$\underline{\eta}^{(10)}$	0	0	η	0.5η	0	0
$\underline{\eta}^{(11)}$	0	0	η	0	0	0.5η
$\underline{\eta}^{(12)}$	0	0	0	0.5η	0.5η	0.5η

4.3 Implementation of TOECs calculation

I implemented the procedure outlined in the Section 4.1 in two parts:

- (i) The steps until the expansion of fit parameters into independent elastic constants in Eq. (4.4) are done using **Wolfram Mathematica** [15].
- (ii) I have then used the results from the **Mathematica** notebook to write the **Python** code for **ElaStic**, which performs the remaining steps: The development of the matrix $\underline{\underline{B}}$ from Eq. (4.5), inverting $\underline{\underline{B}}$ and then applying $\underline{\underline{B}}^{-1}$ to the fitting parameters $\underline{A}_3$.

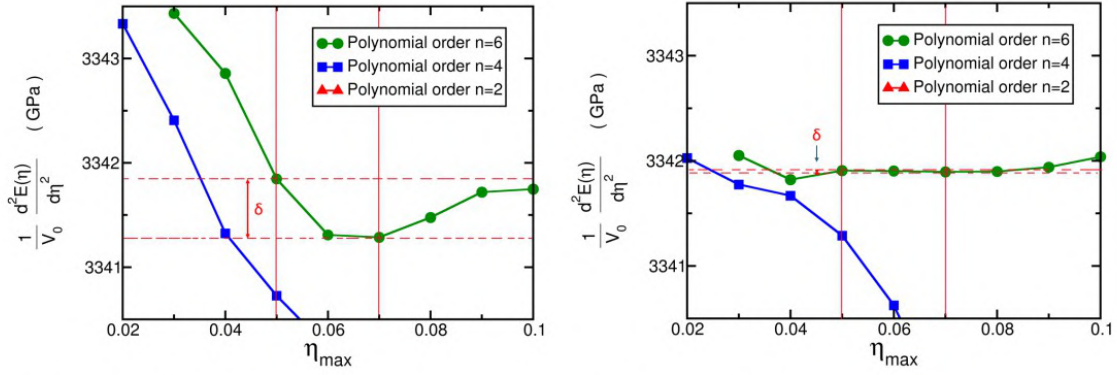
This approach has two benefits:

- It makes changing the types of strains in the future much easier, because the code can accommodate any list of strain types.
- This makes the expansion from Eq. (4.4) easier to verify as its results are written directly into the **Python** code.

4.4 The minimal-variation method

Further, I implemented a method that, during the “fitting stage” of **ElaStic**, avoid the human-eye inspection which characterize the current version of the code. Following Winter’s Bachelor’s thesis [16] (where it was called the ‘ δ -parameter” method), this method seeks to minimize the variation of the fit parameter in a certain interval. Using this method increases precision because it does not rely on the judgment and eyesight of the user to decide for which maximum strain amplitude the plot shows its most stable behaviour. The procedure established by the method is implemented in the following steps:

1. When obtaining the elastic constants from the calculated energies, the user can add two arguments: The first one assigns the order of the polynomial fit (default value is the order of elastic constants augmented by 4). The second one is the size of the “strain window” (interval) in terms of the number of stress points included in the interval (default value is 3).
2. The program then takes a set of fitting parameters calculated in the previous step, the number of which is equal to the chosen interval size, starting with the one for the smallest maximum strain value. The program calculates the



(a) Computational parameters:

`rgkmax=8`, `ngridk=12×12×12`, `gmaxvr=18`

(b) Computational parameters:

`rgkmax=8`, `ngridk=12×12×12`, `gmaxvr=25`

Figure 4.1: Visualization of the procedure used in the minimal-variation method proposed by Winter in his Bachelor’s thesis [16]. The solid red lines represent the selected interval, while the dashed red lines represent the greatest difference in that interval. This example is taken from Ref. [16], for a calculation of the second-order elastic constants of zincblende BN. Three strain points are considered to define the “strain window”.

difference between the smallest and the largest fit parameter value in this set as well as the average between them and stores these values.

3. The program then moves the interval by one strain point and repeats the process for this new set of strain values. New differences between smallest and largest strain value are generated, and if that difference is smaller than the one from the previous interval this new difference and the average of these strain values are stored replace the previous ones.
4. This process gets repeated, replacing stored values for “difference” and “average” whenever a new smallest difference is found until the fit parameter associated with the largest calculated strain value is reached. The stored value for “average” is then used for the further calculation of the elastic constants.

Chapter 5

Results

The new implementation of the **ElaStic** code has been tested for two materials: Diamond and TiO_2 in the rutile phase. For both materials, the calculations were done using for the exchange-correlation energy functional the generalized gradient approximation (GGA) in the form introduced by Perdew, Burke, and Enzerhof (PBE) [17]. The species files describing the constituent atoms and the type of basis functions in the muffin-tin region are taken from Ref. [18] and shown in Appendix C.

5.1 Diamond

The crystal structure of diamond has symmetry type **Cubic 1** and its primitive unit cell contains two carbon atoms. The conventional unit cell of diamond can be seen in Fig. 5.1. Diamond was chosen for its short calculation times and the large number of references for comparison. The equilibrium lattice constant $a_0 = 3.573 \text{ \AA}$ was taken from Ref. [19].

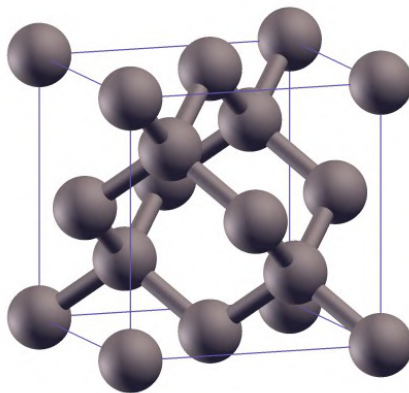


Figure 5.1: Conventional unit cell of diamond.

5.1.1 Second-order elastic constants of diamond

As it can be seen in Table 5.1, the strain types used for **Cubic 1** are the same as standard strain types from **ElaStic**, with the difference that for the strain type $\underline{\eta}^{(3)}$ the η_4 , η_5 , and η_6 entries are scaled by a factor 1/4. This was done to better match the strain amplitudes for the uniaxial deformations with those for the shearing deformations. The calculations presented in Table 5.2 were performed using **rgkmax**=9.0, **ngridk**=12×12×12, **gmaxvr**=25, and 21 strain amplitudes with a maximum Lagrangian strain of 0.05 for each strain type. The results show good agreement with the reference values, especially those from calculations performed with the same approximation for the exchange-correlation energy functional (PBE).

SOECs tensor for Cubic 1						Table 5.1: Strain types for SOECs (Cubic 1).						
$\begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}$						strain type	η_1	η_2	η_3	η_4	η_5	η_6
						$\underline{\eta}^{(1)}$	η	η	η	0	0	0
						$\underline{\eta}^{(2)}$	η	η	0	0	0	0
						$\underline{\eta}^{(3)}$	0	0	0	0.5η	0.5η	0.5η

Table 5.2: Calculated SOECs of diamond in units of [GPa] compared to other theoretical and experimental references.

Source	Type	E_{xc}	C_{11}	C_{12}	C_{44}
This work	DFT	PBE	1050.2	124.0	556.9
Ref. [20]	DFT	PBE	1054	124	559
Ref. [4]	DFT	PBE	1053	125	560
Ref. [4]	DFT	LDA	1106	149	592
Ref. [21]	Expt.		1079	124	578
Ref. [22]	Expt.		1079	127	578

5.1.2 Third-order elastic constants of diamond

The strain types used here for the determination of the TOECs of diamond can be found in Section 4.2. As seen in Table 5.3 for the TOECs different methods can give quite different results. However, when comparing our results to results obtained by PBE we see good agreement between them, in particular with those reported in Ref. [4].

Table 5.3: Calculated TOECs for diamond in units of [GPa] compared to other theoretical and experimental references.

Source	Type	E_{xc}	C_{111}	C_{112}	C_{123}	C_{144}	C_{155}	C_{456}
This work	DFT	PBE	-5893	-1624	612	-241	-2805	-1155
Ref. [4]	DFT	PBE	-5882	-1667	614	-212	-2814	-1157
Ref. [20]	DFT	PBE	-6026	-1643	606	-200	-2817	-1168
Ref. [20]	DFT	LDA	-6303	-1739	589	-196	-2911	-1074
Ref. [3]	Expt.		-7367	-2136	1040	186	-3292	76
Ref. [1]	Expt.		-6260	-2260	112	-674	-2860	-823

5.2 Titanium dioxide in the rutile phase

Rutile is a mineral of TiO_2 of symmetry type **Tetragonal 1**, its conventional unit cell can be seen in Fig. 5.2. Rutile was chosen because **Tetragonal 1** is among those crystal systems whose TOECs were newly implemented into **ElaStic**. More importantly, in his Bachelor’s thesis Weber [23] already calculated the TOECs of rutile TiO_2 using his own version of **ElaStic**. This makes it possible to skip the convergence process, by using Weber’s convergence parameters and allows for comparisons to a set of calculations made with a different version of **ElaStic** that still uses **exciting**.

The structural parameters, *i.e.*, the lattice constants, corresponding to equilibrium, $a = 4.646 \text{ \AA}$ and $b = 2.964 \text{ \AA}$, were taken from Ref. [23]. Our calculations were done using **rgkmax**=8.0, **ngridk**= $12 \times 12 \times 18$, and **gmaxvr**=20. For each strain type 41 calculations were done, up to a maximum strain amplitude of 0.05.

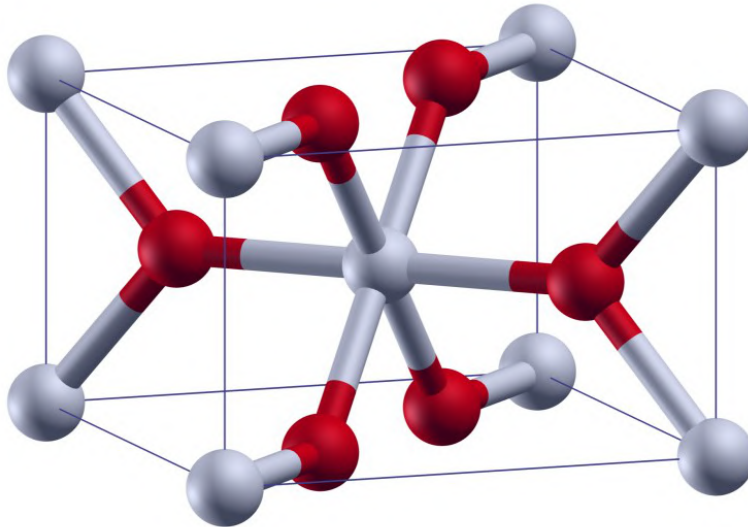


Figure 5.2: Unit cell of TiO_2 in rutile phase with titanium in white and oxygen in red.

5.2.1 Second-order elastic constants of rutile TiO_2

For the calculation of SEOEs of materials with the symmetry type **Tetragonal 1**, I have chosen a different set of strain types than the default set from **ElaStic**. This change was done to ensure that all calculations could be reused for the calculation of the TOECs. The explicit list of symmetry types used in the new implementation is shown in Table 5.4.

Our results for the SOECs are displayed in Table 5.5. We can see generally good agreement between our results and the reference values, in particular with those of Ref. [23], which were also obtained with **ElaStic**.

SOECs tensor for **Tetragonal 1**.

$$\begin{pmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{pmatrix}$$

Table 5.4: Same as Table 5.1 for **Tetragonal 1**.

strain type	η_1	η_2	η_3	η_4	η_5	η_6
$\underline{\eta}^{(1)}$	η	η	η	0	0	0
$\underline{\eta}^{(2)}$	0	0	η	0	0	0
$\underline{\eta}^{(3)}$	η	η	0	0	0	0
$\underline{\eta}^{(4)}$	η	0	η	0	0	0
$\underline{\eta}^{(5)}$	η	0	0	0.5η	0	0
$\underline{\eta}^{(6)}$	η	0	0	0	0	0.5η

Table 5.5: SOECs of rutile in [GPa] in comparison with other works.

Source	Type	E_{xc}	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}
This work	DFT	PBE	253.5	170.4	146.7	472.2	121.9	217.7
Ref. [23]	DFT	PBE	249.0	173.4	147.0	472.0	115.5	210.4
Ref. [24]	DFT	PBE	271	143	144	465	124	211
Ref. [25]	DFT	PBE	278	153	149	479	115	214
Ref. [26]	DFT	LDA	292	192	174	471	114	236
Ref. [27]	Expt.		267.3	174.1	146.4	483.9	123.9	190.4

Table 5.6: Calculated TOECs for rutile TiO_2 in [TPa] compared to those obtained by Weber in Ref. [23].

Source	C_{111}	C_{112}	C_{113}	C_{123}	C_{133}	C_{144}
This work	-1.654	-1.515	-0.522	-0.826	-0.357	-0.194
Weber [23]	-1.33	-1.58	0.38	-1.69	-0.41	-0.28
	C_{155}	C_{166}	C_{333}	C_{344}	C_{366}	C_{456}
This work	-0.432	-1.100	-4.342	-0.413	-0.604	-0.261
Weber [23]	-0.44	-1.25	-4.38	-0.40	-0.58	-0.26

5.2.2 Third-order elastic constants of rutile TiO_2

The strain types used for these calculations can be found in Section 4.2. Our results for the TOECs are displayed in comparison with those obtained (using both **ElaStic** and **exciting**) by Weber [23] in Table 5.6. We can see significant discrepancies in the results for C_{113} , C_{123} , and arguably C_{111} . The relative difference in C_{144} also seems large, but a low relative precision is expected for this value, as its calculation involves subtraction of strain parameters that results in a fairly small (compared to the other TOECs) value.

The reason of these discrepancies can be investigated by a direct inspection of Ref [23]. In Weber’s Bachelor’s thesis it is possible to identify a mistake in the expression for the calculation of C_{113} . Using the strain types from Ref [23] we obtain a slightly different expression for C_{113} :

$$C_{113} = A_3^{(2)} - 2 \left(A_3^{(1)} + A_3^{(3)} - A_3^{(8)} \right) - \frac{1}{2} \left(A_3^{(10)} + A_3^{(11)} \right),$$

the difference being the sign before $A_3^{(11)}$.

To check whether the further difference in the results comes from the use of different species files, I also calculated the strain type $\eta = (1, 0, 0, 0, 0, 0)$ that was used in the reference to calculate C_{111} directly, using the species files from the reference. As a result I obtained $C_{111} = -1.64$ TPa, which supports the results from this work over the results from the reference. As such, I tentatively trust the results from this work over the results from reference Ref. [23], though in the future further tests of the new implementation of **ElaStic** could lead to a final confirmation.

Chapter 6

Conclusions and Outlook

In this work, I have presented the implementation of the calculation of third order elastic constants into **ElaStic** for those crystal symmetries not already in **ElaStic**, namely

- **Trigonal 2**,
- **Tetragonal 1**,
- **Tetragonal 2**,
- **Orthorombic**,
- **Monoclinic**,
- **Triclinic**.

For all Laue groups, both those implemented already and those newly implemented, the choice of strain types has been revised in such a way that possible changes of the strain types require little implementation effort.

Additionally, the minimal-variation method has been implemented for the third-order elastic constants (TOECs). This reduces the error in the fitting procedure compared to estimating the point of least variation by human-eye inspection.

The new implementation was tested for two test cases: The materials diamond and TiO_2 in the rutile phase. All elastic constants for diamond and the second-order elastic constants (SOECs) for TiO_2 showed good agreement to the reference values. However, for the TOECs of rutile TiO_2 disagreements with the sole reference were found for some elastic constants, though there are tentative reasons to put more trust in the results from this work.

In the future further tests of this implementation should be done, especially for calculations of type **Tetragonal 1**, to gain explicit clarity on the discrepancies for TiO_2 found in this thesis.

For further future developments of the **ElaStic** package, aside from implementing methods to calculate elastic constants of order 4 and above, the code for the SOECs should be revised consistently to the case of the TOECs to also allow for a simple changing of strain types.

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Appendix A

Structure of TOECs Tensors

In this appendix, the structure of the third-order elastic tensors for each class of crystal symmetry is shown. The expressions are taken from Ref. [12].

A.1 Cubic 1

$$\begin{aligned}
& C_{1ij}^{(3)} : \begin{pmatrix} C_{111} & C_{112} & C_{112} & 0 & 0 & 0 \\ C_{112} & C_{112} & C_{123} & 0 & 0 & 0 \\ C_{112} & C_{123} & C_{112} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{144} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{155} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{155} \end{pmatrix} & C_{2ij}^{(3)} : \begin{pmatrix} C_{112} & C_{112} & C_{123} & 0 & 0 & 0 \\ C_{112} & C_{111} & C_{112} & 0 & 0 & 0 \\ C_{123} & C_{112} & C_{112} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{155} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{144} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{155} \end{pmatrix} \\
& C_{3ij}^{(3)} : \begin{pmatrix} C_{112} & C_{123} & C_{112} & 0 & 0 & 0 \\ C_{123} & C_{112} & C_{112} & 0 & 0 & 0 \\ C_{112} & C_{112} & C_{111} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{155} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{155} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{144} \end{pmatrix} & C_{4ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & C_{144} & 0 & 0 \\ 0 & 0 & 0 & C_{155} & 0 & 0 \\ 0 & 0 & 0 & C_{155} & 0 & 0 \\ C_{144} & C_{155} & C_{155} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{456} \\ 0 & 0 & 0 & 0 & C_{456} & 0 \end{pmatrix} \\
& C_{5ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & 0 & C_{155} & 0 \\ 0 & 0 & 0 & 0 & C_{144} & 0 \\ 0 & 0 & 0 & 0 & C_{155} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{456} \\ C_{155} & C_{144} & C_{155} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{456} & 0 & 0 \end{pmatrix} & C_{6ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & C_{155} \\ 0 & 0 & 0 & 0 & 0 & C_{155} \\ 0 & 0 & 0 & 0 & 0 & C_{144} \\ 0 & 0 & 0 & 0 & C_{456} & 0 \\ 0 & 0 & 0 & C_{456} & 0 & 0 \\ C_{155} & C_{155} & C_{144} & 0 & 0 & 0 \end{pmatrix}
\end{aligned}$$

A.2 Cubic 2

$$\begin{aligned}
 & C_{1ij}^{(3)} : \quad \begin{pmatrix} C_{111} & C_{112} & C_{113} & 0 & 0 & 0 \\ C_{112} & C_{113} & C_{123} & 0 & 0 & 0 \\ C_{113} & C_{123} & C_{112} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{144} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{155} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{166} \end{pmatrix} \quad C_{2ij}^{(3)} : \quad \begin{pmatrix} C_{112} & C_{113} & C_{123} & 0 & 0 & 0 \\ C_{113} & C_{111} & C_{112} & 0 & 0 & 0 \\ C_{123} & C_{112} & C_{113} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{166} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{144} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{155} \end{pmatrix}
 \end{aligned}$$

$$\begin{aligned}
 & C_{3ij}^{(3)} : \quad \begin{pmatrix} C_{113} & C_{123} & C_{112} & 0 & 0 & 0 \\ C_{123} & C_{112} & C_{113} & 0 & 0 & 0 \\ C_{112} & C_{113} & C_{111} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{155} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{166} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{144} \end{pmatrix} \quad C_{4ij}^{(3)} : \quad \begin{pmatrix} 0 & 0 & 0 & C_{144} & 0 & 0 \\ 0 & 0 & 0 & C_{166} & 0 & 0 \\ 0 & 0 & 0 & C_{155} & 0 & 0 \\ C_{144} & C_{166} & C_{155} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{456} \\ 0 & 0 & 0 & 0 & C_{456} & 0 \end{pmatrix}
 \end{aligned}$$

$$\begin{aligned}
 & C_{5ij}^{(3)} : \quad \begin{pmatrix} 0 & 0 & 0 & 0 & C_{155} & 0 \\ 0 & 0 & 0 & 0 & C_{144} & 0 \\ 0 & 0 & 0 & 0 & C_{166} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{456} \\ C_{155} & C_{144} & C_{166} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{456} & 0 & 0 \end{pmatrix} \quad C_{6ij}^{(3)} : \quad \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & C_{166} \\ 0 & 0 & 0 & 0 & 0 & C_{155} \\ 0 & 0 & 0 & 0 & 0 & C_{144} \\ 0 & 0 & 0 & 0 & C_{456} & 0 \\ 0 & 0 & 0 & C_{456} & 0 & 0 \\ C_{166} & C_{155} & C_{144} & 0 & 0 & 0 \end{pmatrix}
 \end{aligned}$$

A.3 Tetragonal 1

$$\begin{aligned}
& C_{1ij}^{(3)} : \begin{pmatrix} C_{111} & C_{112} & C_{113} & 0 & 0 & 0 \\ C_{112} & C_{112} & C_{123} & 0 & 0 & 0 \\ C_{113} & C_{123} & C_{133} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{144} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{155} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{166} \end{pmatrix} & C_{2ij}^{(3)} : \begin{pmatrix} C_{112} & C_{112} & C_{123} & 0 & 0 & 0 \\ C_{112} & C_{111} & C_{113} & 0 & 0 & 0 \\ C_{123} & C_{113} & C_{133} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{155} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{144} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{166} \end{pmatrix} \\
& C_{3ij}^{(3)} : \begin{pmatrix} C_{113} & C_{123} & C_{133} & 0 & 0 & 0 \\ C_{123} & C_{113} & C_{133} & 0 & 0 & 0 \\ C_{133} & C_{133} & C_{333} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{344} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{344} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{366} \end{pmatrix} & C_{4ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & C_{144} & 0 & 0 \\ 0 & 0 & 0 & C_{155} & 0 & 0 \\ 0 & 0 & 0 & C_{344} & 0 & 0 \\ C_{144} & C_{155} & C_{344} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{456} \\ 0 & 0 & 0 & 0 & C_{456} & 0 \end{pmatrix} \\
& C_{5ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & 0 & C_{155} & 0 \\ 0 & 0 & 0 & 0 & C_{144} & 0 \\ 0 & 0 & 0 & 0 & C_{344} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{456} \\ C_{155} & C_{144} & C_{344} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{456} & 0 & 0 \end{pmatrix} & C_{6ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & C_{166} \\ 0 & 0 & 0 & 0 & 0 & C_{166} \\ 0 & 0 & 0 & 0 & 0 & C_{366} \\ 0 & 0 & 0 & 0 & C_{456} & 0 \\ 0 & 0 & 0 & C_{456} & 0 & 0 \\ C_{166} & C_{166} & C_{366} & 0 & 0 & 0 \end{pmatrix}
\end{aligned}$$

A.4 Tetragonal 2

$$C_{1ij}^{(3)} : \begin{pmatrix} C_{111} & C_{112} & C_{113} & 0 & 0 & C_{116} \\ C_{112} & C_{112} & C_{123} & 0 & 0 & 0 \\ C_{113} & C_{123} & C_{133} & 0 & 0 & C_{136} \\ 0 & 0 & 0 & C_{144} & C_{145} & 0 \\ 0 & 0 & 0 & C_{145} & C_{155} & 0 \\ C_{116} & 0 & C_{136} & 0 & 0 & C_{166} \end{pmatrix} \quad C_{2ij}^{(3)} : \begin{pmatrix} C_{112} & C_{112} & C_{123} & 0 & 0 & 0 \\ C_{112} & C_{111} & C_{113} & 0 & 0 & \tilde{C}_{126} \\ C_{123} & C_{113} & C_{133} & 0 & 0 & \tilde{C}_{236} \\ 0 & 0 & 0 & C_{155} & \tilde{C}_{245} & 0 \\ 0 & 0 & 0 & \tilde{C}_{245} & C_{144} & 0 \\ 0 & \tilde{C}_{126} & \tilde{C}_{236} & 0 & 0 & C_{166} \end{pmatrix}$$

$$C_{3ij}^{(3)} : \begin{pmatrix} C_{113} & C_{123} & C_{133} & 0 & 0 & C_{136} \\ C_{123} & C_{113} & C_{133} & 0 & 0 & \tilde{C}_{236} \\ C_{133} & C_{133} & C_{333} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{344} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{344} & 0 \\ C_{136} & \tilde{C}_{236} & 0 & 0 & 0 & C_{366} \end{pmatrix} \quad C_{4ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & C_{144} & C_{145} & 0 \\ 0 & 0 & 0 & C_{155} & \tilde{C}_{245} & 0 \\ 0 & 0 & 0 & C_{344} & 0 & 0 \\ C_{144} & C_{155} & C_{344} & 0 & 0 & C_{446} \\ C_{145} & \tilde{C}_{245} & 0 & 0 & 0 & C_{456} \\ 0 & 0 & 0 & C_{446} & C_{456} & 0 \end{pmatrix}$$

$$C_{5ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & C_{145} & C_{155} & 0 \\ 0 & 0 & 0 & \tilde{C}_{245} & C_{144} & 0 \\ 0 & 0 & 0 & 0 & C_{344} & 0 \\ C_{145} & \tilde{C}_{245} & 0 & 0 & 0 & C_{456} \\ C_{155} & C_{144} & C_{344} & 0 & 0 & \tilde{C}_{556} \\ 0 & 0 & 0 & C_{456} & \tilde{C}_{556} & 0 \end{pmatrix} \quad C_{6ij}^{(3)} : \begin{pmatrix} C_{116} & 0 & C_{136} & 0 & 0 & C_{166} \\ 0 & \tilde{C}_{226} & \tilde{C}_{236} & 0 & 0 & C_{166} \\ C_{136} & \tilde{C}_{236} & 0 & 0 & 0 & C_{366} \\ 0 & 0 & 0 & C_{446} & C_{456} & 0 \\ 0 & 0 & 0 & C_{456} & \tilde{C}_{556} & 0 \\ C_{166} & C_{166} & C_{366} & 0 & 0 & 0 \end{pmatrix}$$

$$\tilde{C}_{226} = -C_{166}$$

$$\tilde{C}_{236} = -C_{136}$$

$$\tilde{C}_{245} = -C_{145}$$

$$\tilde{C}_{556} = -C_{446}$$

A.5 Orthorombic

$$\begin{aligned}
& C_{1ij}^{(3)} : \begin{pmatrix} C_{111} & C_{112} & C_{113} & 0 & 0 & 0 \\ C_{112} & C_{122} & C_{123} & 0 & 0 & 0 \\ C_{113} & C_{123} & C_{133} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{144} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{155} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{166} \end{pmatrix} & C_{2ij}^{(3)} : \begin{pmatrix} C_{112} & C_{122} & C_{123} & 0 & 0 & 0 \\ C_{122} & C_{222} & C_{223} & 0 & 0 & 0 \\ C_{123} & C_{223} & C_{233} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{244} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{255} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{266} \end{pmatrix} \\
& C_{3ij}^{(3)} : \begin{pmatrix} C_{113} & C_{123} & C_{133} & 0 & 0 & 0 \\ C_{123} & C_{223} & C_{233} & 0 & 0 & 0 \\ C_{133} & C_{233} & C_{333} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{344} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{355} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{366} \end{pmatrix} & C_{4ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & C_{144} & 0 & 0 \\ 0 & 0 & 0 & C_{244} & 0 & 0 \\ 0 & 0 & 0 & C_{344} & 0 & 0 \\ C_{144} & C_{244} & C_{344} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{456} \\ 0 & 0 & 0 & 0 & C_{456} & 0 \end{pmatrix} \\
& C_{5ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & 0 & C_{155} & 0 \\ 0 & 0 & 0 & 0 & C_{255} & 0 \\ 0 & 0 & 0 & 0 & C_{355} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{456} \\ C_{155} & C_{255} & C_{355} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{456} & 0 & 0 \end{pmatrix} & C_{6ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & C_{166} \\ 0 & 0 & 0 & 0 & 0 & C_{266} \\ 0 & 0 & 0 & 0 & 0 & C_{366} \\ 0 & 0 & 0 & 0 & C_{456} & 0 \\ 0 & 0 & 0 & C_{456} & 0 & 0 \\ C_{166} & C_{266} & C_{366} & 0 & 0 & 0 \end{pmatrix}
\end{aligned}$$

A.6 Hexagonal 1

$$\begin{aligned}
& C_{1ij}^{(3)} : \begin{pmatrix} C_{111} & C_{112} & C_{113} & 0 & 0 & 0 \\ C_{112} & \tilde{C}_{122} & C_{123} & 0 & 0 & 0 \\ C_{113} & C_{123} & C_{133} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{144} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{155} & 0 \\ 0 & 0 & 0 & 0 & 0 & \tilde{C}_{166} \end{pmatrix} & C_{2ij}^{(3)} : \begin{pmatrix} C_{112} & \tilde{C}_{122} & C_{123} & 0 & 0 & 0 \\ \tilde{C}_{122} & C_{222} & C_{113} & 0 & 0 & 0 \\ C_{123} & C_{113} & C_{133} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{155} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{144} & 0 \\ 0 & 0 & 0 & 0 & 0 & \tilde{C}_{266} \end{pmatrix} \\
& C_{3ij}^{(3)} : \begin{pmatrix} C_{113} & C_{123} & C_{133} & 0 & 0 & 0 \\ C_{123} & C_{113} & C_{133} & 0 & 0 & 0 \\ C_{133} & C_{133} & C_{333} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{344} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{344} & 0 \\ 0 & 0 & 0 & 0 & 0 & \tilde{C}_{366} \end{pmatrix} & C_{4ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & C_{144} & 0 & 0 \\ 0 & 0 & 0 & C_{155} & 0 & 0 \\ 0 & 0 & 0 & C_{344} & 0 & 0 \\ C_{144} & C_{155} & C_{344} & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & \tilde{C}_{456} \\ 0 & 0 & 0 & 0 & \tilde{C}_{456} & 0 \end{pmatrix} , \\
& C_{5ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & 0 & C_{155} & 0 \\ 0 & 0 & 0 & 0 & C_{144} & 0 \\ 0 & 0 & 0 & 0 & C_{344} & 0 \\ 0 & 0 & 0 & 0 & 0 & \tilde{C}_{456} \\ C_{155} & C_{144} & C_{344} & 0 & 0 & 0 \\ 0 & 0 & 0 & \tilde{C}_{456} & 0 & 0 \end{pmatrix} & C_{6ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & 0 & 0 & \tilde{C}_{166} \\ 0 & 0 & 0 & 0 & 0 & \tilde{C}_{266} \\ 0 & 0 & 0 & 0 & 0 & \tilde{C}_{366} \\ 0 & 0 & 0 & 0 & \tilde{C}_{456} & 0 \\ 0 & 0 & 0 & \tilde{C}_{456} & 0 & 0 \\ \tilde{C}_{166} & \tilde{C}_{266} & \tilde{C}_{366} & 0 & 0 & 0 \end{pmatrix}
\end{aligned}$$

$$\tilde{C}_{122} = C_{111} + C_{112} - C_{222}$$

$$\tilde{C}_{166} = \frac{1}{2}C_{112} - \frac{1}{2}C_{123}$$

$$\tilde{C}_{266} = \frac{1}{2}C_{111} - \frac{1}{4}C_{112} + \frac{1}{4}C_{222}$$

$$\tilde{C}_{366} = \frac{1}{2}C_{113} + \frac{1}{2}C_{123}$$

$$\tilde{C}_{456} = -\frac{1}{2}C_{144} + \frac{1}{2}C_{155}$$

A.7 Hexagonal 2

$$C_{1ij}^{(3)} : \begin{pmatrix} C_{111} & C_{112} & C_{113} & 0 & 0 & C_{116} \\ C_{112} & \tilde{C}_{122} & C_{123} & 0 & 0 & \tilde{C}_{126} \\ C_{113} & C_{123} & C_{133} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{144} & C_{145} & 0 \\ 0 & 0 & 0 & C_{145} & C_{155} & 0 \\ C_{116} & \tilde{C}_{126} & 0 & 0 & 0 & \tilde{C}_{166} \end{pmatrix} \quad C_{2ij}^{(3)} : \begin{pmatrix} C_{112} & \tilde{C}_{122} & C_{123} & 0 & 0 & \tilde{C}_{126} \\ \tilde{C}_{122} & C_{222} & C_{113} & 0 & 0 & C_{116} \\ C_{123} & C_{113} & C_{133} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{155} & \tilde{C}_{245} & 0 \\ 0 & 0 & 0 & \tilde{C}_{245} & C_{144} & 0 \\ \tilde{C}_{126} & C_{116} & 0 & 0 & 0 & \tilde{C}_{266} \end{pmatrix}$$

$$C_{3ij}^{(3)} : \begin{pmatrix} C_{113} & C_{123} & C_{133} & 0 & 0 & 0 \\ C_{123} & C_{113} & C_{133} & 0 & 0 & 0 \\ C_{133} & C_{133} & C_{333} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{344} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{344} & 0 \\ 0 & 0 & 0 & 0 & 0 & \tilde{C}_{366} \end{pmatrix} \quad C_{4ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & C_{144} & C_{145} & 0 \\ 0 & 0 & 0 & C_{155} & C_{245} & 0 \\ 0 & 0 & 0 & C_{344} & 0 & 0 \\ C_{144} & C_{155} & C_{344} & 0 & 0 & C_{145} \\ C_{145} & C_{245} & 0 & 0 & 0 & \tilde{C}_{456} \\ 0 & 0 & 0 & C_{145} & \tilde{C}_{456} & 0 \end{pmatrix}$$

$$C_{5ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & C_{145} & C_{155} & 0 \\ 0 & 0 & 0 & \tilde{C}_{245} & C_{144} & 0 \\ 0 & 0 & 0 & 0 & C_{344} & 0 \\ C_{145} & \tilde{C}_{245} & 0 & 0 & 0 & \tilde{C}_{456} \\ C_{155} & C_{144} & C_{344} & 0 & 0 & \tilde{C}_{556} \\ 0 & 0 & 0 & \tilde{C}_{456} & \tilde{C}_{556} & 0 \end{pmatrix} \quad C_{6ij}^{(3)} : \begin{pmatrix} C_{116} & \tilde{C}_{126} & 0 & 0 & 0 & \tilde{C}_{166} \\ \tilde{C}_{126} & C_{116} & 0 & 0 & 0 & \tilde{C}_{266} \\ 0 & 0 & 0 & 0 & 0 & \tilde{C}_{366} \\ 0 & 0 & 0 & C_{111} & \tilde{C}_{456} & 0 \\ 0 & 0 & 0 & \tilde{C}_{456} & \tilde{C}_{556} & 0 \\ \tilde{C}_{166} & \tilde{C}_{266} & \tilde{C}_{366} & 0 & 0 & \tilde{C}_{666} \end{pmatrix}$$

$$\tilde{C}_{122} = C_{111} + C_{112} - C_{222}$$

$$\tilde{C}_{126} = -C_{116}$$

$$\tilde{C}_{166} = \frac{1}{2}C_{112} - \frac{1}{2}C_{123}$$

$$\tilde{C}_{245} = -C_{145}$$

$$\tilde{C}_{266} = \frac{1}{2}C_{111} - \frac{1}{4}C_{112} + \frac{1}{4}C_{222}$$

$$\tilde{C}_{366} = \frac{1}{2}C_{113} + \frac{1}{2}C_{123}$$

$$\tilde{C}_{456} = -\frac{1}{2}C_{144} + \frac{1}{2}C_{155}$$

$$\tilde{C}_{556} = -C_{145}$$

$$\tilde{C}_{666} = -C_{116}$$

A.8 Trigonal 1

$$C_{1ij}^{(3)} : \begin{pmatrix} C_{111} & C_{112} & C_{113} & C_{114} & 0 & 0 \\ C_{112} & \tilde{C}_{122} & C_{123} & C_{124} & 0 & 0 \\ C_{113} & C_{123} & C_{133} & C_{134} & 0 & 0 \\ C_{114} & C_{124} & C_{134} & C_{144} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{155} & \tilde{C}_{156} \\ 0 & 0 & 0 & 0 & \tilde{C}_{156} & \tilde{C}_{166} \end{pmatrix} \quad C_{2ij}^{(3)} : \begin{pmatrix} C_{112} & \tilde{C}_{122} & C_{123} & C_{124} & 0 & 0 \\ \tilde{C}_{122} & C_{222} & C_{113} & \tilde{C}_{224} & 0 & 0 \\ C_{123} & C_{113} & C_{133} & \tilde{C}_{234} & 0 & 0 \\ C_{124} & \tilde{C}_{224} & \tilde{C}_{234} & C_{155} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{144} & \tilde{C}_{256} \\ 0 & 0 & 0 & 0 & \tilde{C}_{256} & \tilde{C}_{266} \end{pmatrix}$$

$$C_{3ij}^{(3)} : \begin{pmatrix} C_{113} & C_{123} & C_{133} & C_{134} & 0 & 0 \\ C_{123} & C_{113} & C_{133} & \tilde{C}_{234} & 0 & 0 \\ C_{133} & C_{133} & C_{333} & 0 & 0 & 0 \\ C_{134} & \tilde{C}_{234} & 0 & C_{344} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{344} & C_{134} \\ 0 & 0 & 0 & 0 & C_{134} & \tilde{C}_{366} \end{pmatrix} \quad C_{4ij}^{(3)} : \begin{pmatrix} C_{114} & C_{124} & C_{134} & C_{144} & 0 & 0 \\ C_{124} & \tilde{C}_{224} & \tilde{C}_{234} & C_{155} & 0 & 0 \\ C_{134} & \tilde{C}_{234} & 0 & C_{344} & 0 & 0 \\ C_{144} & C_{155} & C_{344} & C_{111} & 0 & 0 \\ 0 & 0 & 0 & 0 & \tilde{C}_{455} & \tilde{C}_{456} \\ 0 & 0 & 0 & 0 & \tilde{C}_{456} & C_{124} \end{pmatrix}$$

$$C_{5ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & 0 & C_{155} & \tilde{C}_{156} \\ 0 & 0 & 0 & 0 & C_{144} & \tilde{C}_{256} \\ 0 & 0 & 0 & 0 & C_{344} & C_{134} \\ 0 & 0 & 0 & 0 & \tilde{C}_{455} & \tilde{C}_{456} \\ C_{155} & C_{144} & C_{344} & \tilde{C}_{455} & 0 & 0 \\ \tilde{C}_{156} & \tilde{C}_{256} & C_{134} & \tilde{C}_{456} & 0 & 0 \end{pmatrix} \quad C_{6ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & 0 & \tilde{C}_{156} & \tilde{C}_{166} \\ 0 & 0 & 0 & 0 & \tilde{C}_{256} & \tilde{C}_{266} \\ 0 & 0 & 0 & 0 & C_{134} & \tilde{C}_{366} \\ 0 & 0 & 0 & 0 & \tilde{C}_{456} & C_{124} \\ \tilde{C}_{156} & \tilde{C}_{256} & C_{134} & \tilde{C}_{456} & 0 & 0 \\ \tilde{C}_{166} & \tilde{C}_{266} & \tilde{C}_{366} & C_{124} & 0 & 0 \end{pmatrix}$$

$$\tilde{C}_{122} = C_{111} + C_{112} - C_{222}$$

$$\tilde{C}_{156} = \frac{1}{2}C_{114} + \frac{3}{2}C_{124}$$

$$\tilde{C}_{166} = \frac{1}{2}C_{112} - \frac{1}{2}C_{123}$$

$$\tilde{C}_{224} = -C_{114} - 2C_{124}$$

$$\tilde{C}_{234} = -C_{134}$$

$$\tilde{C}_{256} = \frac{1}{2}C_{114} - \frac{1}{2}C_{124}$$

$$\tilde{C}_{266} = \frac{1}{2}C_{111} - \frac{1}{4}C_{112} + \frac{1}{4}C_{222}$$

$$\tilde{C}_{366} = \frac{1}{2}C_{113} + \frac{1}{2}C_{123}$$

$$\tilde{C}_{455} = -C_{444}$$

$$\tilde{C}_{456} = -\frac{1}{2}C_{144} + \frac{1}{2}C_{155}$$

A.9 Trigonal 2

$$C_{1ij}^{(3)} : \quad \begin{pmatrix} C_{111} & C_{112} & C_{113} & C_{114} & C_{115} & C_{116} \\ C_{112} & \tilde{C}_{122} & C_{123} & C_{124} & C_{125} & \tilde{C}_{126} \\ C_{113} & C_{123} & C_{133} & C_{134} & C_{135} & 0 \\ C_{114} & C_{124} & C_{134} & C_{144} & C_{145} & \tilde{C}_{146} \\ C_{115} & C_{125} & C_{135} & C_{145} & C_{155} & \tilde{C}_{156} \\ C_{116} & \tilde{C}_{126} & 0 & \tilde{C}_{146} & \tilde{C}_{156} & \tilde{C}_{166} \end{pmatrix} \quad C_{2ij}^{(3)} : \quad \begin{pmatrix} C_{112} & \tilde{C}_{122} & C_{123} & C_{124} & C_{125} & \tilde{C}_{126} \\ \tilde{C}_{122} & C_{222} & C_{113} & \tilde{C}_{224} & \tilde{C}_{225} & C_{116} \\ C_{123} & C_{113} & C_{133} & \tilde{C}_{234} & \tilde{C}_{235} & 0 \\ C_{124} & \tilde{C}_{224} & \tilde{C}_{234} & C_{155} & \tilde{C}_{245} & \tilde{C}_{246} \\ C_{125} & \tilde{C}_{225} & \tilde{C}_{235} & \tilde{C}_{245} & C_{144} & \tilde{C}_{256} \\ \tilde{C}_{126} & C_{116} & 0 & \tilde{C}_{246} & \tilde{C}_{256} & \tilde{C}_{266} \end{pmatrix}$$

$$C_{3ij}^{(3)} : \quad \begin{pmatrix} C_{113} & C_{123} & C_{133} & C_{134} & C_{135} & 0 \\ C_{123} & C_{113} & C_{133} & \tilde{C}_{234} & \tilde{C}_{235} & 0 \\ C_{133} & C_{133} & C_{333} & 0 & 0 & 0 \\ C_{134} & \tilde{C}_{234} & 0 & C_{344} & 0 & \tilde{C}_{346} \\ C_{135} & \tilde{C}_{235} & 0 & 0 & C_{344} & C_{134} \\ 0 & 0 & 0 & \tilde{C}_{346} & C_{134} & \tilde{C}_{366} \end{pmatrix} \quad C_{4ij}^{(3)} : \quad \begin{pmatrix} C_{114} & C_{124} & C_{134} & C_{144} & C_{145} & \tilde{C}_{146} \\ C_{124} & \tilde{C}_{224} & \tilde{C}_{234} & C_{155} & \tilde{C}_{245} & \tilde{C}_{246} \\ C_{134} & \tilde{C}_{234} & 0 & C_{344} & 0 & \tilde{C}_{346} \\ C_{144} & C_{155} & C_{344} & C_{444} & C_{445} & C_{145} \\ C_{145} & \tilde{C}_{245} & 0 & C_{445} & \tilde{C}_{455} & \tilde{C}_{456} \\ \tilde{C}_{146} & \tilde{C}_{246} & \tilde{C}_{346} & C_{145} & \tilde{C}_{456} & C_{124} \end{pmatrix}$$

$$C_{5ij}^{(3)} : \quad \begin{pmatrix} C_{115} & C_{125} & C_{135} & C_{145} & C_{155} & \tilde{C}_{156} \\ C_{125} & \tilde{C}_{225} & \tilde{C}_{235} & \tilde{C}_{245} & C_{144} & \tilde{C}_{256} \\ C_{135} & \tilde{C}_{235} & 0 & 0 & C_{344} & C_{134} \\ C_{145} & \tilde{C}_{245} & 0 & C_{445} & \tilde{C}_{455} & \tilde{C}_{456} \\ C_{155} & C_{144} & C_{344} & \tilde{C}_{455} & \tilde{C}_{555} & \tilde{C}_{556} \\ \tilde{C}_{156} & \tilde{C}_{256} & \tilde{C}_{134} & \tilde{C}_{456} & \tilde{C}_{556} & C_{125} \end{pmatrix} \quad C_{6ij}^{(3)} : \quad \begin{pmatrix} C_{116} & \tilde{C}_{126} & 0 & \tilde{C}_{146} & \tilde{C}_{156} & \tilde{C}_{166} \\ \tilde{C}_{126} & C_{116} & 0 & \tilde{C}_{246} & \tilde{C}_{256} & \tilde{C}_{266} \\ 0 & 0 & 0 & \tilde{C}_{346} & C_{134} & \tilde{C}_{366} \\ \tilde{C}_{146} & \tilde{C}_{246} & \tilde{C}_{346} & C_{145} & \tilde{C}_{456} & C_{124} \\ \tilde{C}_{156} & \tilde{C}_{256} & C_{134} & \tilde{C}_{456} & 0 & 0 \\ \tilde{C}_{166} & \tilde{C}_{266} & \tilde{C}_{366} & C_{124} & 0 & 0 \end{pmatrix}$$

$$\tilde{C}_{122} = C_{111} + C_{112} - C_{222}$$

$$\tilde{C}_{126} = -C_{116}$$

$$\tilde{C}_{146} = -\frac{1}{2}C_{115} - \frac{3}{2}C_{125}$$

$$\tilde{C}_{156} = \frac{1}{2}C_{114} + \frac{3}{2}C_{124}$$

$$\tilde{C}_{166} = \frac{1}{2}C_{112} - \frac{1}{2}C_{123}$$

$$\tilde{C}_{224} = -C_{114} - 2C_{124}$$

$$\tilde{C}_{225} = -C_{115} - 2C_{125}$$

$$\tilde{C}_{234} = -C_{134}$$

$$\tilde{C}_{235} = -C_{135}$$

$$\tilde{C}_{245} = -C_{145}$$

$$\tilde{C}_{246} = -\frac{1}{2}C_{115} + \frac{1}{2}C_{125}$$

$$\tilde{C}_{256} = \frac{1}{2}C_{114} - \frac{1}{2}C_{124}$$

$$\tilde{C}_{266} = \frac{1}{2}C_{111} - \frac{1}{4}C_{112} + \frac{1}{4}C_{222}$$

$$\tilde{C}_{366} = \frac{1}{2}C_{113} + \frac{1}{2}C_{123}$$

$$\tilde{C}_{455} = -C_{444}$$

$$\tilde{C}_{456} = -\frac{1}{2}C_{144} + \frac{1}{2}C_{155}$$

$$\tilde{C}_{555} = -C_{445}$$

A.10 Monoclinic

$$C_{1ij}^{(3)} : \begin{pmatrix} C_{111} & C_{112} & C_{113} & 0 & 0 & C_{116} \\ C_{112} & C_{122} & C_{123} & 0 & 0 & C_{126} \\ C_{113} & C_{123} & C_{133} & 0 & 0 & C_{136} \\ 0 & 0 & 0 & C_{144} & C_{145} & 0 \\ 0 & 0 & 0 & C_{145} & C_{155} & 0 \\ C_{116} & C_{126} & C_{136} & 0 & 0 & C_{166} \end{pmatrix} \quad C_{2ij}^{(3)} : \begin{pmatrix} C_{112} & C_{122} & C_{123} & 0 & 0 & C_{126} \\ C_{122} & C_{222} & C_{223} & 0 & 0 & C_{226} \\ C_{123} & C_{223} & C_{233} & 0 & 0 & C_{236} \\ 0 & 0 & 0 & C_{244} & C_{245} & 0 \\ 0 & 0 & 0 & C_{245} & C_{255} & 0 \\ C_{126} & C_{226} & C_{236} & 0 & 0 & C_{266} \end{pmatrix}$$

$$C_{3ij}^{(3)} : \begin{pmatrix} C_{113} & C_{123} & C_{133} & 0 & 0 & C_{136} \\ C_{123} & C_{223} & C_{233} & 0 & 0 & C_{236} \\ C_{133} & C_{233} & C_{333} & 0 & 0 & C_{336} \\ 0 & 0 & 0 & C_{344} & C_{345} & 0 \\ 0 & 0 & 0 & C_{345} & C_{355} & 0 \\ C_{136} & C_{236} & C_{336} & 0 & 0 & C_{366} \end{pmatrix} \quad C_{4ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & C_{144} & C_{145} & 0 \\ 0 & 0 & 0 & C_{245} & C_{245} & 0 \\ 0 & 0 & 0 & C_{344} & C_{345} & 0 \\ C_{144} & C_{244} & C_{344} & 0 & 0 & C_{446} \\ C_{145} & C_{245} & C_{345} & 0 & 0 & C_{456} \\ 0 & 0 & 0 & C_{446} & C_{456} & 0 \end{pmatrix}$$

$$C_{5ij}^{(3)} : \begin{pmatrix} 0 & 0 & 0 & C_{145} & C_{155} & 0 \\ 0 & 0 & 0 & C_{245} & C_{255} & 0 \\ 0 & 0 & 0 & C_{345} & C_{355} & 0 \\ C_{145} & C_{245} & C_{345} & 0 & 0 & C_{456} \\ C_{155} & C_{255} & C_{355} & 0 & 0 & C_{556} \\ 0 & 0 & 0 & C_{456} & C_{556} & 0 \end{pmatrix} \quad C_{6ij}^{(3)} : \begin{pmatrix} C_{116} & C_{126} & C_{136} & 0 & 0 & C_{166} \\ C_{126} & C_{226} & C_{236} & 0 & 0 & C_{266} \\ C_{136} & C_{236} & C_{336} & 0 & 0 & C_{366} \\ 0 & 0 & 0 & C_{446} & C_{456} & 0 \\ 0 & 0 & 0 & C_{456} & C_{556} & 0 \\ C_{166} & C_{266} & C_{366} & 0 & 0 & C_{666} \end{pmatrix}$$

A.11 Triclinic

$$C_{1ij}^{(3)} : \begin{pmatrix} C_{111} & C_{112} & C_{113} & C_{114} & C_{115} & C_{116} \\ C_{112} & C_{122} & C_{123} & C_{124} & C_{125} & C_{126} \\ C_{113} & C_{123} & C_{133} & C_{134} & C_{135} & C_{136} \\ C_{114} & C_{124} & C_{134} & C_{144} & C_{145} & C_{146} \\ C_{115} & C_{125} & C_{135} & C_{145} & C_{155} & C_{156} \\ C_{116} & C_{126} & C_{136} & C_{146} & C_{156} & C_{166} \end{pmatrix} \quad C_{2ij}^{(3)} : \begin{pmatrix} C_{112} & C_{122} & C_{123} & C_{124} & C_{125} & C_{126} \\ C_{122} & C_{222} & C_{223} & C_{224} & C_{225} & C_{226} \\ C_{123} & C_{223} & C_{233} & C_{234} & C_{235} & C_{236} \\ C_{124} & C_{224} & C_{234} & C_{244} & C_{245} & C_{246} \\ C_{125} & C_{225} & C_{235} & C_{245} & C_{255} & C_{256} \\ C_{126} & C_{226} & C_{236} & C_{246} & C_{256} & C_{266} \end{pmatrix}$$

$$C_{3ij}^{(3)} : \begin{pmatrix} C_{113} & C_{123} & C_{133} & C_{134} & C_{135} & C_{136} \\ C_{123} & C_{223} & C_{233} & C_{234} & C_{235} & C_{236} \\ C_{133} & C_{233} & C_{333} & C_{334} & C_{335} & C_{336} \\ C_{134} & C_{234} & C_{334} & C_{344} & C_{345} & C_{346} \\ C_{135} & C_{235} & C_{335} & C_{345} & C_{355} & C_{356} \\ C_{136} & C_{236} & C_{336} & C_{346} & C_{356} & C_{366} \end{pmatrix} \quad C_{4ij}^{(3)} : \begin{pmatrix} C_{114} & C_{124} & C_{134} & C_{144} & C_{145} & C_{146} \\ C_{124} & C_{224} & C_{234} & C_{244} & C_{245} & C_{246} \\ C_{134} & C_{234} & C_{334} & C_{344} & C_{345} & C_{346} \\ C_{144} & C_{244} & C_{344} & C_{444} & C_{445} & C_{446} \\ C_{145} & C_{245} & C_{345} & C_{445} & C_{455} & C_{456} \\ C_{146} & C_{246} & C_{346} & C_{446} & C_{456} & C_{466} \end{pmatrix}$$

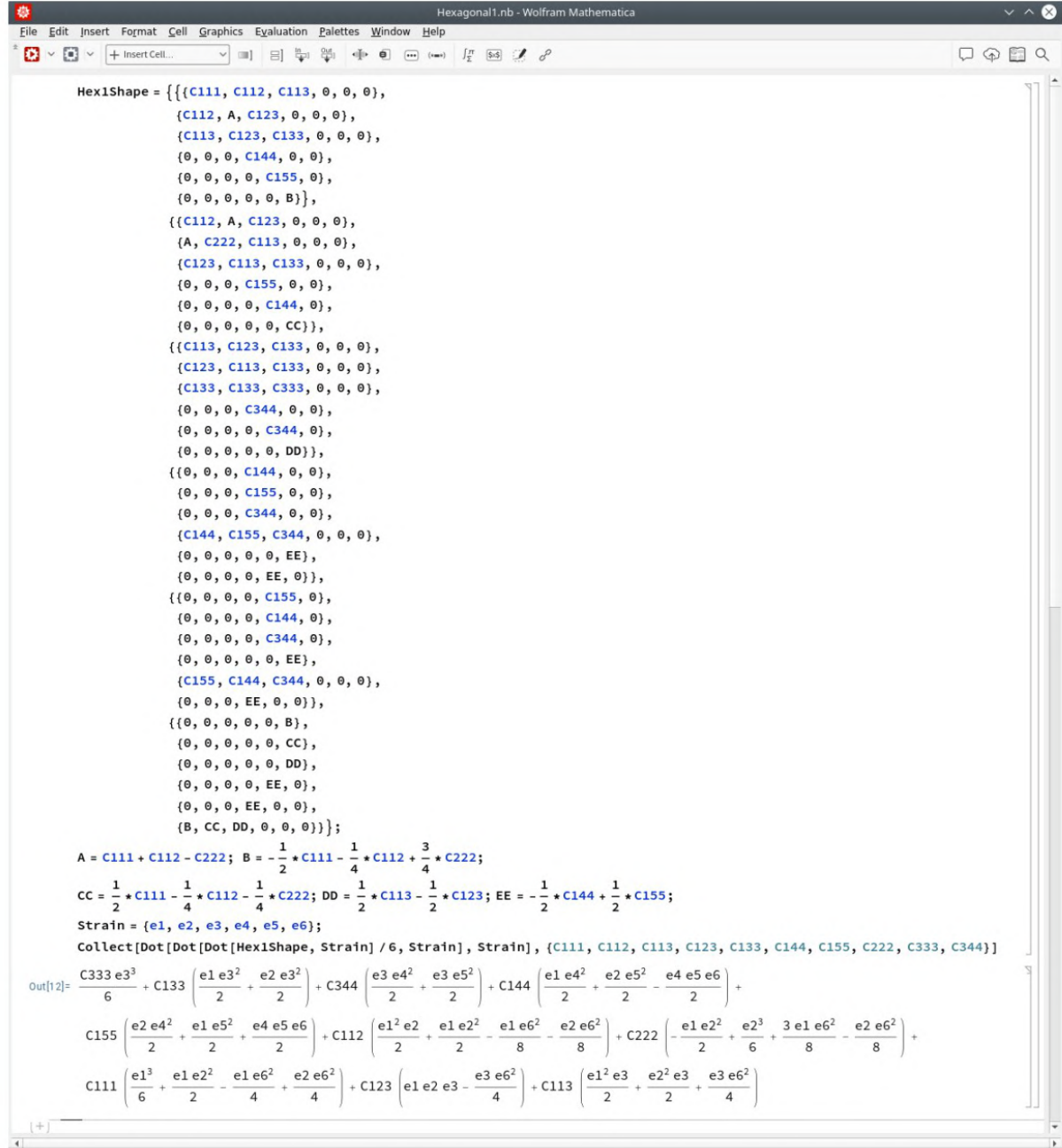
$$C_{5ij}^{(3)} : \begin{pmatrix} C_{115} & C_{125} & C_{135} & C_{145} & C_{155} & C_{156} \\ C_{125} & C_{225} & C_{235} & C_{245} & C_{255} & C_{256} \\ C_{135} & C_{235} & C_{335} & C_{345} & C_{355} & C_{356} \\ C_{145} & C_{245} & C_{345} & C_{445} & C_{455} & C_{456} \\ C_{155} & C_{255} & C_{355} & C_{455} & C_{555} & C_{556} \\ C_{156} & C_{256} & C_{356} & C_{456} & C_{556} & C_{566} \end{pmatrix} \quad C_{6ij}^{(3)} : \begin{pmatrix} C_{116} & C_{126} & C_{136} & C_{146} & C_{156} & C_{166} \\ C_{126} & C_{226} & C_{236} & C_{246} & C_{256} & C_{266} \\ C_{136} & C_{236} & C_{336} & C_{346} & C_{356} & C_{366} \\ C_{146} & C_{246} & C_{346} & C_{446} & C_{456} & C_{466} \\ C_{156} & C_{256} & C_{356} & C_{456} & C_{556} & C_{566} \\ C_{166} & C_{266} & C_{366} & C_{466} & C_{566} & C_{666} \end{pmatrix}$$

Appendix B

Example ElaStic Code

In order to give a better understanding of the practical realization of the contents of Section 4.3, an example for **Hexagonal 1** is presented in this appendix. Here, both the **Mathematica** notebook as well as the resulting actual **Python** implementation into **ElaStic** are shown.

B.1 Mathematica notebook for Hexagonal 1



```

Hex1Shape = {{(C111, C112, C113, 0, 0, 0),
  (C112, A, C123, 0, 0, 0),
  (C113, C123, C133, 0, 0, 0),
  {0, 0, 0, C144, 0, 0},
  {0, 0, 0, 0, C155, 0},
  {0, 0, 0, 0, 0, B}},
  {(C112, A, C123, 0, 0, 0),
  (A, C222, C113, 0, 0, 0),
  (C123, C113, C133, 0, 0, 0),
  {0, 0, 0, C155, 0, 0},
  {0, 0, 0, 0, C144, 0},
  {0, 0, 0, 0, 0, CC}},
  {(C113, C123, C133, 0, 0, 0),
  (C123, C113, C133, 0, 0, 0),
  (C133, C133, C333, 0, 0, 0),
  {0, 0, 0, C344, 0, 0},
  {0, 0, 0, 0, C344, 0},
  {0, 0, 0, 0, 0, DD}},
  {(0, 0, 0, C144, 0, 0),
  {0, 0, 0, C155, 0, 0},
  {0, 0, 0, C344, 0, 0},
  (C144, C155, C344, 0, 0, 0),
  {0, 0, 0, 0, 0, EE},
  {0, 0, 0, 0, EE, 0}},
  {(0, 0, 0, 0, C155, 0),
  {0, 0, 0, 0, C144, 0},
  {0, 0, 0, 0, C344, 0},
  {0, 0, 0, 0, 0, EE},
  (C155, C144, C344, 0, 0, 0),
  {0, 0, 0, EE, 0, 0}},
  {(0, 0, 0, 0, 0, B),
  {0, 0, 0, 0, 0, CC},
  {0, 0, 0, 0, 0, DD},
  {0, 0, 0, 0, EE, 0},
  {0, 0, 0, EE, 0, 0},
  (B, CC, DD, 0, 0, 0)});

A = C111 + C112 - C222; B = -1/2 * C111 - 1/4 * C112 + 3/4 * C222;
CC = 1/2 * C111 - 1/4 * C112 - 1/4 * C222; DD = 1/2 * C113 - 1/2 * C123; EE = -1/2 * C144 + 1/2 * C155;
Strain = {e1, e2, e3, e4, e5, e6};
Collect[Dot[Dot[Dot[Hex1Shape, Strain] / 6, Strain], Strain], {C111, C112, C113, C123, C133, C144, C155, C222, C333, C344}]

Out[12]= C333 e3^3 / 6 + C133 (e1 e3^2 / 2 + e2 e3^2 / 2) + C344 (e3 e4^2 / 2 + e3 e5^2 / 2) + C144 (e1 e4^2 / 2 + e2 e5^2 / 2 - e4 e5 e6 / 2) +
  C155 (e2 e4^2 / 2 + e1 e5^2 / 2 + e4 e5 e6 / 2) + C112 (e1^2 e2 / 2 + e1 e2^2 / 2 - e1 e6^2 / 8 - e2 e6^2 / 8) + C222 (-e1 e2^2 / 2 + e2^3 / 6 + 3 e1 e6^2 / 8 - e2 e6^2 / 8) +
  C111 (e1^3 / 6 + e1 e2^2 / 2 - e1 e6^2 / 4 + e2 e6^2 / 4) + C123 (e1 e2 e3 - e3 e6^2 / 4) + C113 (e1^2 e3 / 2 + e2^2 e3 / 2 + e3 e6^2 / 4)

```

Figure B.1: Screenshot of **Mathematica** Notebook used for the coefficients of Hexagonal 1

B.2 Implemented Python code for Hexagonal 1

```
M=np.zeros((ECs,ECs))
for j in range(ECs):

    %%!%!%--- Hexagonal I structures ---%!%!%!%!%!%!%!%!%!%!%!%!%!%!%!%
    if (LC == 'HI'):

        strainlist = ['01','26','04','03','17','30','08','02','10',
                      '14']

        e1=LS_Dic[strainlist[j]][0]
        e2=LS_Dic[strainlist[j]][1]
        e3=LS_Dic[strainlist[j]][2]
        e4=LS_Dic[strainlist[j]][3]
        e5=LS_Dic[strainlist[j]][4]
        e6=LS_Dic[strainlist[j]][5]

        #C111
        M[j][ 0] = (e1**3)/6 + (e1*e2**2)/2 - (e1*e6**2)/4 + (e2*e6
                    **2)/4
        #C112
        M[j][ 1] = (e1**2*e2)/2 + (e1*e2**2)/2 - (e1*e6**2)/8 - (e2
                    *e6**2)/8
        #C113
        M[j][ 2] = (e1**2*e3)/2 + (e2**2*e3)/2 + (e3*e6**2)/4
        #C123
        M[j][ 3] = e1*e2*e3 - (e3*e6**2)/4
        #C133
        M[j][ 4] = (e1*e3**2)/2 + (e2*e3**2)/2
        #C144
        M[j][ 5] = (e1*e4**2)/2 + (e2*e5**2)/2 - (e4*e5*e6)/2
        #C155
        M[j][ 6] = (e2*e4**2)/2 + (e1*e5**2)/2 + (e4*e5*e6)/2
        #C222
        M[j][ 7] = -(e1*e2**2)/2 + (e2**3)/6 + 3*(e1*e6**2)/8 - (e2
                    *e6**2)/8
        #C333
        M[j][ 8] = (e3**3)/6
        #C344
        M[j][ 9] = (e3*e4**2)/2 + (e3*e5**2)/2

Constants=np.matmul(np.linalg.inv(M),A3)
```

B.3 Python code for the minimal-variation method

```
def subroutine (steps, polyorder, order, ECnumber):
    tfact = np.math.factorial(order)

    A = []
    D = []
    L = []
    P = []

    for i in range(1, ECnumber+1):
        if (i<10):
            Dstn = 'Dst0'+str(i)
        else:
            Dstn = 'Dst' +str(i)

        derivative_file= open(Dstn+'_d'+str(order)+'E.dat', 'r')

        strain = []
        derivative = []

        if polyorder ==2:
            nth='2nd'
        elif polyorder ==3:
            nth='3rd'
        else:
            nth=str(polyorder)+'th'

        f=derivative_file.readlines()

        doappend=0
        for line in f:
            if doappend==1:
                if line.isspace():
                    break
                strain.append(float(line.split()[0].strip()))
                derivative.append(float(line.split()[1].strip())
                                /tfact)

            if nth in line:
                doappend=1

        strain = np.array(strain)
        derivative = np.array(derivative)
```

```

if len(strain)<steps:
    sys.exit('\n ERROR: For your choice of step size '+
            str(steps)+' and polynomial fitting order '+str(
            polyorder)+' , there are not enough data points ('
            +str(len(strain))+') to average once')

minRange = 1.e99
for j in range(len(derivative)-steps+1):
    tempList = []
    for l in range(dstps): tempList.append(derivative[j+
        l])

    Range = max(tempList)-min(tempList)

    if (Range < minRange):
        minRange = Range
        stableAverage = Average(tempList)
        stablePosition = strain[j+1]

A.append(stableAverage)
D.append(minRange)
L.append(stablePosition*100.)
P.append(abs(minRange/stableAverage*100.))

A = np.array(A)
D = np.array(D)
L = np.array(L)
P = np.array(P)
return A, D, L, P

```


Appendix C

Species Files

C.1 Carbon

```
<?xml version="1.0" encoding="UTF-8"?>
<spdb xsi:noNamespaceSchemaLocation="../../xml/species.xsd" xmlns:xsi="http://www.
w3.org/2001/XMLSchema-instance">
  <sp chemicalSymbol="C" name="carbon" z="-6.00000" mass="21894.16673">
    <muffinTin rmin="0.100000E-05" radius="1.2500" rinf="20.0" radialmeshPoints="
400"/>
    <atomicState n="1" l="0" kappa="1" occ="2.00000" core="false"/>
    <atomicState n="2" l="0" kappa="1" occ="2.00000" core="false"/>
    <atomicState n="2" l="1" kappa="1" occ="1.00000" core="false"/>
    <atomicState n="2" l="1" kappa="2" occ="1.00000" core="false"/>
    <basis>
      <default type="lapw" trialEnergy="0.1500" searchE="false"/>
      <custom l="0" type="lapw" trialEnergy="-0.5" searchE="false"/>
      <lo l="0">
        <wf matchingOrder="0" trialEnergy="-0.5" searchE="false"/>
        <wf matchingOrder="1" trialEnergy="-0.5" searchE="false"/></lo>
      <lo l="0">
        <wf matchingOrder="0" trialEnergy="-0.5" searchE="false"/>
        <wf matchingOrder="0" trialEnergy="-9.3" searchE="false"/></lo>
      <lo l="0">
        <wf matchingOrder="0" trialEnergy="-9.3" searchE="false"/>
        <wf matchingOrder="1" trialEnergy="-9.3" searchE="false"/></lo>
      <lo l="0">
        <wf matchingOrder="0" trialEnergy="-9.3" searchE="false"/>
        <wf matchingOrder="2" trialEnergy="-9.3" searchE="false"/></lo>
      <custom l="1" type="lapw" trialEnergy="0.15" searchE="false"/>
      <lo l="1">
        <wf matchingOrder="0" trialEnergy="0.15" searchE="false"/>
        <wf matchingOrder="1" trialEnergy="0.15" searchE="false"/></lo>
      <lo l="1">
        <wf matchingOrder="0" trialEnergy="0.15" searchE="false"/>
        <wf matchingOrder="2" trialEnergy="0.15" searchE="false"/></lo>
    </basis>
  </sp>
</spdb>
```

C.2 Titanium

```
<?xml version="1.0" encoding="UTF-8"?>
<spdb xsi:noNamespaceSchemaLocation="../../xml/species.xsd" xmlns:xsi="http://www.
w3.org/2001/XMLSchema-instance">
  <sp chemicalSymbol="Ti" name="titanium" z="-22.0000" mass="87256.20311">
    <muffinTin rmin="0.100000E-05" radius="2.0000" rinf="25.7965" radialmeshPoints=
      "1000"/>
    <atomicState n="1" l="0" kappa="1" occ="2.00000" core="true"/>
    <atomicState n="2" l="0" kappa="1" occ="2.00000" core="true"/>
    <atomicState n="2" l="1" kappa="1" occ="2.00000" core="true"/>
    <atomicState n="2" l="1" kappa="2" occ="4.00000" core="true"/>
    <atomicState n="3" l="0" kappa="1" occ="2.00000" core="false"/>
    <atomicState n="3" l="1" kappa="1" occ="2.00000" core="false"/>
    <atomicState n="3" l="1" kappa="2" occ="4.00000" core="false"/>
    <atomicState n="3" l="2" kappa="2" occ="2.00000" core="false"/>
    <atomicState n="4" l="0" kappa="1" occ="2.00000" core="false"/>
    <basis>
      <default type="lapw" trialEnergy="0.00" searchE="false"/>
      <custom l="0" type="lapw" trialEnergy="-2.30" searchE="false"/>
      <lo l="0"><wf matchingOrder="0" trialEnergy="-2.30" searchE="false"/>
        <wf matchingOrder="1" trialEnergy="-2.30" searchE="false"/></lo>
      <lo l="0"><wf matchingOrder="1" trialEnergy="-2.30" searchE="false"/>
        <wf matchingOrder="2" trialEnergy="-2.30" searchE="false"/></lo>
      <lo l="0"><wf matchingOrder="2" trialEnergy="-2.30" searchE="false"/>
        <wf matchingOrder="0" trialEnergy="0.00" searchE="false"/></lo>
      <lo l="0"><wf matchingOrder="0" trialEnergy="0.00" searchE="false"/>
        <wf matchingOrder="1" trialEnergy="0.00" searchE="false"/></lo>
      <custom l="1" type="lapw" trialEnergy="-1.42" searchE="false"/>
      <lo l="1"><wf matchingOrder="0" trialEnergy="-1.42" searchE="false"/>
        <wf matchingOrder="1" trialEnergy="-1.42" searchE="false"/></lo>
      <lo l="1"><wf matchingOrder="1" trialEnergy="-1.42" searchE="false"/>
        <wf matchingOrder="2" trialEnergy="-1.42" searchE="false"/></lo>
      <lo l="1"><wf matchingOrder="2" trialEnergy="-1.42" searchE="false"/>
        <wf matchingOrder="0" trialEnergy="1.0" searchE="false"/></lo>
      <lo l="1"><wf matchingOrder="0" trialEnergy="1.0" searchE="false"/>
        <wf matchingOrder="1" trialEnergy="1.0" searchE="false"/></lo>
      <lo l="1"><wf matchingOrder="1" trialEnergy="1.0" searchE="false"/>
        <wf matchingOrder="2" trialEnergy="1.0" searchE="false"/></lo>
      <custom l="2" type="lapw" trialEnergy="0.00" searchE="false"/>
      <lo l="2"><wf matchingOrder="0" trialEnergy="0.00" searchE="false"/>
        <wf matchingOrder="1" trialEnergy="0.00" searchE="false"/></lo>
      <lo l="2"><wf matchingOrder="1" trialEnergy="0.00" searchE="false"/>
        <wf matchingOrder="2" trialEnergy="0.00" searchE="false"/></lo>
      <lo l="2"><wf matchingOrder="2" trialEnergy="0.00" searchE="false"/>
        <wf matchingOrder="3" trialEnergy="0.00" searchE="false"/></lo>
      <lo l="3"><wf matchingOrder="0" trialEnergy="0.00" searchE="false"/>
        <wf matchingOrder="1" trialEnergy="0.00" searchE="false"/></lo>
      <lo l="3"><wf matchingOrder="1" trialEnergy="0.00" searchE="false"/>
        <wf matchingOrder="2" trialEnergy="0.00" searchE="false"/></lo>
      <lo l="4"><wf matchingOrder="0" trialEnergy="0.00" searchE="false"/>
        <wf matchingOrder="1" trialEnergy="0.00" searchE="false"/></lo>
      <lo l="4"><wf matchingOrder="1" trialEnergy="0.00" searchE="false"/>
        <wf matchingOrder="2" trialEnergy="0.00" searchE="false"/></lo>
    </basis>
  </sp>
</spdb>
```

C.3 Oxygen

```
<?xml version="1.0" encoding="UTF-8"?>
<spdb xsi:noNamespaceSchemaLocation="../../../xml/species.xsd" xmlns:xsi="http://www.
w3.org/2001/XMLSchema-instance">
  <sp chemicalSymbol="O" name="oxygen" z="-8.00000" mass="29165.12203">
    <muffinTin rmin="0.100000E-05" radius="1.4500" rinf="17.0873" radialmeshPoints=
      "600"/>
    <atomicState n="1" l="0" kappa="1" occ="2.00000" core="true"/>
    <atomicState n="2" l="0" kappa="1" occ="2.00000" core="false"/>
    <atomicState n="2" l="1" kappa="1" occ="2.00000" core="false"/>
    <atomicState n="2" l="1" kappa="2" occ="2.00000" core="false"/>
    <basis>
      <default type="lapw" trialEnergy="0.00" searchE="false"/>
      <custom l="0" type="lapw" trialEnergy="-0.87" searchE="false"/>
      <lo l="0">
        <wf matchingOrder="0" trialEnergy="-0.87" searchE="false"/>
        <wf matchingOrder="1" trialEnergy="-0.87" searchE="false"/></lo>
      <lo l="0">
        <wf matchingOrder="1" trialEnergy="-0.87" searchE="false"/>
        <wf matchingOrder="2" trialEnergy="-0.87" searchE="false"/></lo>
      <lo l="0">
        <wf matchingOrder="2" trialEnergy="-0.87" searchE="false"/>
        <wf matchingOrder="3" trialEnergy="-0.87" searchE="false"/></lo>
      <custom l="1" type="lapw" trialEnergy="-0.34" searchE="false"/>
      <lo l="1">
        <wf matchingOrder="0" trialEnergy="-0.34" searchE="false"/>
        <wf matchingOrder="1" trialEnergy="-0.34" searchE="false"/></lo>
      <lo l="1">
        <wf matchingOrder="1" trialEnergy="-0.34" searchE="false"/>
        <wf matchingOrder="2" trialEnergy="-0.34" searchE="false"/></lo>
      <lo l="1">
        <wf matchingOrder="2" trialEnergy="-0.34" searchE="false"/>
        <wf matchingOrder="3" trialEnergy="-0.34" searchE="false"/></lo>
      <lo l="2">
        <wf matchingOrder="0" trialEnergy="0.000" searchE="false"/>
        <wf matchingOrder="1" trialEnergy="0.000" searchE="false"/></lo>
      <lo l="2">
        <wf matchingOrder="1" trialEnergy="0.000" searchE="false"/>
        <wf matchingOrder="2" trialEnergy="0.000" searchE="false"/></lo>
      <lo l="3">
        <wf matchingOrder="0" trialEnergy="0.000" searchE="false"/>
        <wf matchingOrder="1" trialEnergy="0.000" searchE="false"/></lo>
      <lo l="3">
        <wf matchingOrder="1" trialEnergy="0.000" searchE="false"/>
        <wf matchingOrder="2" trialEnergy="0.000" searchE="false"/></lo>
    </basis>
  </sp>
</spdb>
```


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