DFT Calculations to Determine the Hardness of a Set of Quaternary Crystals

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Abstract: This article describes how DFT calculations were used to determine the hardest and softest stable crystal among a list of 23 quaternary crystals. First, input files were prepared for Quantum Espresso (QE) and convergence tests were performed to obtain the optimal trade-off between precision and calculation time. Subsequently, the elastic constants were calculated in order to calculate the hardness of the crystals. Finally, the obtained values were compared and the softest and hardest crystal was determined.

Keywords: DFT, elastic constants, generalized Hookes's law

I. INTRODUCTION

Quaternary alloys have the following structure: A_2BCD_4. The element A is Na, K, Rb or Cs. These elements are situated in group 1 of the periodic table. B and C can be picked from the 12 elements between Al, P, Tl and Bi. Element D is S, Se, Te or Po, those elements can be found in group 16 of the periodic table. In total, 2304 crystals can be built. However, only 23 were found to be stable according to DFT calculations [1]. Table I contains the 23 crystals that will be used for the DFT calculations. In Appendix A a visualization of the crystal can be seen.

Cs2BaGeSe4	Rb2BaSiSe4	K2BaSiSe4
Cs2BaSnSe4	Rb2CaSiSe4	K2CaSiSe4
Cs2CaGeSe4	Rb2CsPSe4	K2MgSiSe4
Cs2CaSnSe4	Rb2KPSe4	K2RbSiSe4
Cs2MgGeSe4	Rb2KSiSe4	K2SrSiSe4
Cs2MgSnSe4	Rb2MgSiSe4	
Cs2RbAsSe4	Rb2MgSiTe4	
Cs2SrGeSe4	Rb2NaPSe4	
Cs2SrSnSe4	Rb2SrSiSe4	

TABLE I. 23 stable quaternary crystals

II. PROCEDURE

First the cif files of the crystals were constructed. From this an input file could be made for QE. The next step was finding the k-mesh and basis set for the wave function (ecutwfc) and the density (ecutrho) for each crystal. It is of great importance to use correct cutoff parameters in order to be confident of the correctness of the calculated values, i.e. to make sure that the effective values are obtained and not random numerical noise. These parameters can be obtained by performing convergence tests. Important here is the trade-off between calculation precision and calculation time.
The following step was optimizing the geometry of each crystal in order to be able to start from a perfectly relaxed crystal.
Next, the elastic constants of the crystals were determined. These can be used to calculate other properties of the bulk crystals.
All these steps and the results are discussed in more detail in the next sections.

A. Convergence testing

The first step was determining the k-mesh. Like mentioned before, the k-mesh will be determined depending on the precision and calculation time. To know whether the values converge or not, the value of the hydrostatic pressure was observed for increasing values for the k-mesh. An example of convergence testing can be seen in Table II. It shows how the value of the hydrostatic pressure converges and how the calculation time increases for a more dense mesh. A 3x3x3 k-mesh was chosen for the calculations since convergence was already reached and the calculation time was still acceptable.
The same procedure was followed for ecutwfc and ecutrho. Generally ecutwfc=40 Ry was sufficient. Some crystals needed ecutwfc=80 Ry. Ecutrho was determined by varying the ratio between ecutwfc and ecutrho. A factor of 4 was sufficient but, since the calculation time for factor 5 didn't increase much compared to factor 4, factor 5 was preferred. This resulted in ecutrho=200 Ry

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or ecutrho=400 Ry. Finally the crystals were geometry optimized to obtain a perfectly relaxed crystal to start with.

k-mesh	Hydrostatic pressure (kbar)	Calculation time (s)
1x1x1	-26.92	165
3x3x3	-37.37	750
5x5x5	-37.36	2254
7x7x7	-37.36	4140
9x9x9	-37.36	6540

TABLE II. Convergence test: k-mesh

B. Elastic properties

Defining the elastic behaviour is the goal for this project. The elastic constants were obtained using the stress tensor procedure, by calculating the stiffness tensor. First, 6 independent deformations are applied to the unit cell (for all crystals studied in this project, the same deformations were used). This is done by multiplying the deformation matrix with the standard root tensor of the undeformed cell. These new calculated unit cell parameters are used to perform a relax-calculation, in order to obtain the stress tensors of the deformed unit cell with optimized positions for the atoms. Afterwards the stress-strain relations are written for each of these 6 deformations and this way Hooke's generealized law is obtained:

$$\begin{bmatrix} \sigma_{11} & \sigma_{12} & \sigma_{13} & \sigma_{14} & \sigma_{15} & \sigma_{16} \\ \sigma_{21} & \sigma_{22} & \sigma_{23} & \sigma_{24} & \sigma_{25} & \sigma_{26} \\ \sigma_{31} & \sigma_{32} & \sigma_{33} & \sigma_{34} & \sigma_{35} & \sigma_{36} \\ \sigma_{41} & \sigma_{42} & \sigma_{43} & \sigma_{44} & \sigma_{45} & \sigma_{46} \\ \sigma_{51} & \sigma_{52} & \sigma_{53} & \sigma_{54} & \sigma_{55} & \sigma_{56} \\ \sigma_{61} & \sigma_{62} & \sigma_{63} & \sigma_{64} & \sigma_{65} & \sigma_{66} \end{bmatrix} =$$

$$\begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix} \begin{bmatrix} \epsilon_{11} & \epsilon_{12} & \epsilon_{13} & \epsilon_{14} & \epsilon_{15} & \epsilon_{16} \\ \epsilon_{21} & \epsilon_{22} & \epsilon_{23} & \epsilon_{24} & \epsilon_{25} & \epsilon_{26} \\ \epsilon_{31} & \epsilon_{32} & \epsilon_{33} & \epsilon_{34} & \epsilon_{35} & \epsilon_{36} \\ 2\epsilon_{41} & 2\epsilon_{42} & 2\epsilon_{43} & 2\epsilon_{44} & 2\epsilon_{45} & 2\epsilon_{46} \\ 2\epsilon_{51} & 2\epsilon_{52} & 2\epsilon_{53} & 2\epsilon_{54} & 2\epsilon_{55} & 2\epsilon_{56} \\ 2\epsilon_{61} & 2\epsilon_{62} & 2\epsilon_{63} & 2\epsilon_{64} & 2\epsilon_{65} & 2\epsilon_{66} \end{bmatrix}$$

The strain tensor is obtained via the definition of the Green-Lagrange strain tensor, where F is the deformation matrix.

$$E = 1/2(F^T F - I)$$

By applying matrix manipulations, the stiffness tensor is obtained. The obtained stiffness tensor for $K_2MgSiSe_4$ is shown below in GPa:

$$\begin{bmatrix} 34.67 & 9.13 & 10.46 & 4.63 & 7.45 & 8.50 \\ 9.08 & 34.71 & 10.46 & 5.55 & 8.50 & 7.45 \\ 11.71 & 11.74 & 75.36 & 0.96 & 0.81 & 0.83 \\ 0 & 0 & 0 & 9.33 & 0 & 0 \\ 0 & 0 & 0 & 0 & 11.74 & 0 \\ 0 & 0 & 0 & 0 & 0 & 11.75 \end{bmatrix}$$

The stiffness tensor for all crystals can be found in Appendix B. Normally, the upper right and left block of the 6x6 matrix should be symmetric, but this isn't the case for any of our crystals. Some of them resemble almost symmetry, some of them don't. The correspondence to symmetry can give a good indication on how reliable further results will be.

III. RESULTS

The stiffness tensor is the gateway to obtain a set of elastic moduli. In the scope of this project, the bulk modulus (K) is first calculated directly from the stiffness tensor and, after calculating the shear modulus (G), the Young's modulus (E) and the Poisson constant (ν), also the micro-hardness could be calculated (H_v). The exact formulas can be found in Appendix C, based on [2]. Both parameters were calculated according to two formalisms, the Voigt (upper limit) and Reuss (lower limit) model.

A. Bulk modulus

In Appendix D the bulk moduli of all crystals are visualized. Both the Voigt and Reuss bulk moduli are shown. To be able to compare the crystals, the mean bulk modulus is also depicted. $Cs_2BaGeSe_4$ and $Rb_2SrSiSe_4$ show unreliable results. When observing the mean values, $Cs_2CaSnSe_4$ has the highest bulk modulus.

B. Micro-hardness

A visualization of the calculated micro-hardnesses can be found in Appendix D. For each crystal, the Voigt and Reuss micro-hardness are plotted. To compare the different crystals in a reliable way, the mean of the Voigt and Reuss micro-hardness is also plotted. Two crystals show unreliable data, $Cs_2CaSnSe_4$ and $Cs_2MgGeSe_4$. The Voigt and Reuss calculated micro-hardness for the two crystals differ respectively with 5 and 40 Hv. Based on the mean values, $Rb_2MgSiTe_4$ shows the highest micro-hardness. All crystals containing Mg show an increased hardness. The softest crystal, based on the mean value, is $Cs_2BaGeSe_4$. Physically interpreting this data is beyond the scope of this project.
Some research papers claim that the bulk modulus and the hardness are directly correlated: a material with a high bulk modulus generally has a high hardness [3]. In this project, however, this is certainly not the case. This correlation is indeed found to be not always correct [4]. The previous paper also states that the correlation between the shear modulus and the hardness is supposed to be better. Experimental values for the crystals are needed to confirm this statement.

IV. CONCLUSION

After dealing with start-up problems for the DFT calculations, due to incorrect pseudo-potentials, calculations went smoothly.

1. The calculated crystals(max. B= 60 GPa and Hv= 2) are generally soft for example in comparison with steel (B= 160 GPa, Hv= 10.61).[5]

2. For some crystals, unreliable data is obtained. The reason could be the choice of 3x3x3 k-mesh, where a 7x7x7 would be more precise in the case of these crystals. In the scope and time period of this project, achieving unreliable data for only a few crystals was acceptable.

3. Supposedly when the values of the cutoff parameters, in general, would be increased, more precise and accurate results for the hardness could be obtained. Only then a clear conclusion about the correlation between the bulk modulus and the microhardness can be made.

V. ACKNOWLEDGMENTS

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[1] M. Sluydts, M. Larmuseau, T. Crepain, K. Dumon, K. Lejaeghere, S. Cottenier, *How many materials are left to discover? An exploration of quaternary space*, ML4MS Conference (Finland) 2018 Center for Molecular Modeling, Ghent University

[2] Maarten De Jong, *Charting the complete elastic properties of inorganic crystalline compounds*, Scientific Data 2015 Department of Materials Science and Engineering, University of California

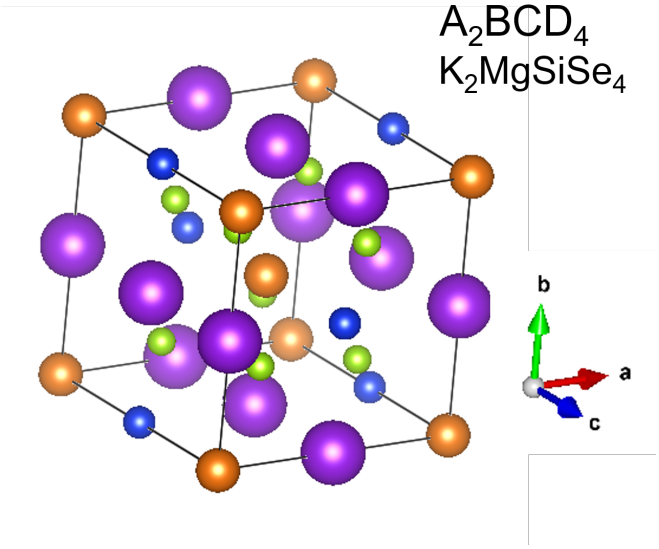
[3] Hongcun Zhai, Xiaofeng Li and Junyi Du *First-Principles Calculations on Elasticity and Anisotropy of Tetragonal Tungsten Dinitride under Pressure* Materials Transactions, Vol. 53, No. 7 (2012) pp. 1247 to 1251, The Japan Institute of Metals

[4] A.L. Ivanovskii *Mechanical and electronic properties of diborides of transition 3d5d metals from first principles: Toward search of novel ultra-incompressible and superhard materials* Progress in Materials Science 57 (2012) 184-228

[5] K. Persson *URL*, https://www.materialsproject.org/

Appendices

A. APPENDIX A: VISUALISATION OF THE UNIT CELL



B. APPENDIX B: STRESS TENSORS IN GPA

$$K2BaSiSe4 = \begin{bmatrix} 43.25 & 9.22 & 15.61 & 0.87 & 1.69 & 0.50 \\ 9.22 & 43.25 & 48.94 & 3.40 & 0.52 & 1.68 \\ 1.38 & 1.38 & 66.87 & 0.49 & 2.65 & 2.61 \\ 0 & 0 & 0 & 4.38 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3.75 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3.67 \end{bmatrix}$$

$$K2CaSiSe4 = \begin{bmatrix} 36.95 & 6.65 & 9.67 & 2.56 & 2.44 & 5.03 \\ 6.55 & 37.05 & 9.67 & 1.58 & 4.93 & 2.57 \\ 12.80 & 12.89 & 64.37 & 0.46 & 0.53 & 0.12 \\ 0 & 0 & 0 & 9.33 & 0 & 0 \\ 0 & 0 & 0 & 0 & 11.74 & 0 \\ 0 & 0 & 0 & 0 & 0 & 11.75 \end{bmatrix}$$

$$K2RbSiSe4 = \begin{bmatrix} 29.28 & 6.98 & 10.71 & 1.31 & 2.44 & 0.85 \\ 6.98 & 29.28 & 10.71 & 0.80 & 1.31 & 1.11 \\ 2.86 & 2.86 & 27.71 & 4.68 & 2.86 & 2.40 \\ 0 & 0 & 0 & 4.86 & 0 & 0 \\ 0 & 0 & 0 & 0 & 4.04 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3.94 \end{bmatrix}$$

$$Rb2SrSiSe4 = \begin{bmatrix} 32.19 & 78.16 & 57.68 & 23.88 & 23.24 & 23.67 \\ 63.95 & 76.65 & 57.68 & 23.67 & 22.67 & 22.81 \\ 51.17 & 62.85 & 0.91 & 20.14 & 18.09 & 20.78 \\ 0 & 0 & 0 & 17.13 & 0 & 0 \\ 0 & 0 & 0 & 0 & 3.79 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1.77 \end{bmatrix}$$

$$Rb2NaPSe4 = \begin{bmatrix} 33.18 & 2.58 & 9.07 & 0.67 & 0.67 & 1.04 \\ 11.87 & 3.89 & 8.81 & 1.11 & 0.56 & 1.46 \\ 8.23 & 4.14 & 38.20 & 1.16 & 1.11 & 0.94 \\ 0 & 0 & 0 & 0.48 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0.50 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3.66 \end{bmatrix}$$

$$Rb2MgSiTe4 = \begin{bmatrix} 23.18 & 4.43 & 4.40 & 1.47 & 1.16 & 1.67 \\ 7.72 & 4.44 & 4.40 & 1.74 & 1.59 & 1.61 \\ 6.61 & 1.39 & 45.59 & 0.82 & 1.20 & 0.87 \\ 0 & 0 & 0 & 7.71 & 0 & 0 \\ 0 & 0 & 0 & 0 & 24.07 & 0 \\ 0 & 0 & 0 & 0 & 0 & 6.91 \end{bmatrix}$$

$$Rb2MgSiSe4 = \begin{bmatrix} 31.18 & 8.20 & 12.02 & 2.27 & 1.22 & 1.09 \\ 8.20 & 31.21 & 12.02 & 2.86 & 0.91 & 0.80 \\ 4.42 & 4.42 & 71.84 & 1.11 & 0.94 & 0.86 \\ 0.00 & 0.00 & 0.00 & 9.70 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 2.18 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 7.11 \end{bmatrix}$$

$$Rb2KSiSe4 = \begin{bmatrix} 27.27 & 3.04 & 8.43 & 1.18 & 1.53 & 1.29 \\ 7.30 & 3.40 & 8.43 & 1.03 & 1.33 & 0.57 \\ 14.75 & 4.84 & 37.53 & 1.59 & 1.56 & 1.38 \\ 0.00 & 0.00 & 0.00 & 1.60 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 2.21 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 1.92 \end{bmatrix}$$

$$Rb2BaSiSe4 = \begin{bmatrix} 36.17 & 3.81 & 13.00 & 0.53 & 0.07 & 0.42 \\ 3.92 & 36.04 & 13.00 & 0.06 & 0.52 & 0.71 \\ 27.08 & 26.96 & 73.08 & 4.85 & 4.85 & 4.50 \\ 0.00 & 0.00 & 0.00 & 3.25 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 3.25 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 4.80 \end{bmatrix}$$

$$Rb2CaSiSe4 = \begin{bmatrix} 39.26 & 10.11 & 14.11 & 0.26 & 0.01 & 0.38 \\ 10.11 & 39.26 & 14.11 & 0.00 & 0.26 & 0.44 \\ 47.70 & 47.69 & 99.45 & 11.08 & 11.09 & 11.40 \\ 0.00 & 0.00 & 0.00 & 3.68 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 3.68 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 1.18 \end{bmatrix}$$

$$Rb2CsPSe4 = \begin{bmatrix} 32.93 & 20.30 & 11.94 & 0.12 & 0.59 & 0.54 \\ 9.10 & 44.44 & 11.94 & 0.44 & 0.27 & 0.29 \\ 2.44 & 13.69 & 27.97 & 1.78 & 1.63 & 1.83 \\ 0.00 & 0.00 & 0.00 & 3.11 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 3.13 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 4.31 \end{bmatrix}$$

$$Rb2KPSe4 = \begin{bmatrix} 32.76 & 8.26 & 8.88 & 0.58 & 0.10 & 0.63 \\ 8.26 & 32.76 & 8.88 & 0.10 & 0.58 & 0.78 \\ 20.98 & 20.98 & 47.75 & 4.02 & 4.02 & 3.53 \\ 0.00 & 0.00 & 0.00 & 3.37 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 3.37 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 2.38 \end{bmatrix}$$

$$K2SrSiSe4 = \begin{bmatrix} 47.02 & 11.58 & 16.67 & 0.36 & 0.81 & 0.01 \\ 11.59 & 47.00 & 16.67 & 1.10 & 0.02 & 0.14 \\ 52.36 & 52.34 & 100.28 & 11.53 & 11.15 & 10.70 \\ 0.00 & 0.00 & 0.00 & 1.70 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 2.64 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 2.23 \end{bmatrix}$$

$$Cs2BaGeSe4 = \begin{bmatrix} 34.33 & 9.65 & 14.13 & 0.06 & 0.39 & 0.72 \\ 9.65 & 34.33 & 14.13 & 0.39 & 0.06 & 0.56 \\ 13.73 & 13.63 & 5.17 & 0.10 & 0.11 & 0.16 \\ 0.00 & 0.00 & 0.00 & 1.23 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 1.23 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 2.83 \end{bmatrix}$$

$$Cs2MgGeSe4 = \begin{bmatrix} 8.42 & 12.57 & 16.60 & 6.22 & 6.96 & 7.83 \\ 12.57 & 8.40 & 16.60 & 6.96 & 6.22 & 7.49 \\ 1.24 & 1.24 & 61.17 & 0.43 & 0.43 & 2.62 \\ 0.00 & 0.00 & 0.00 & 6.99 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 6.99 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 5.06 \end{bmatrix}$$

$$Cs2MgSnSe4 = \begin{bmatrix} 3.50 & 25.63 & 28.38 & 12.69 & 13.21 & 12.98 \\ 25.63 & 3.50 & 28.38 & 13.22 & 12.69 & 12.60 \\ 0.29 & 0.29 & 57.68 & 3.05 & 3.05 & 3.77 \\ 0.00 & 0.00 & 0.00 & 7.92 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 7.91 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 5.14 \end{bmatrix}$$

$$Cs2BaSnSe4 = \begin{bmatrix} 17.91 & 7.56 & 3.48 & 5.49 & 5.17 & 5.04 \\ 7.56 & 17.91 & 3.48 & 5.17 & 5.49 & 5.12 \\ 7.96 & 7.96 & 46.87 & 1.89 & 1.89 & 1.62 \\ 0.00 & 0.00 & 0.00 & 0.13 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.13 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.77 \end{bmatrix}$$

$$Cs2RbAsSe4 = \begin{bmatrix} 20.80 & 1.89 & 1.42 & 1.82 & 1.92 & 1.85 \\ 1.89 & 20.80 & 1.42 & 1.92 & 1.82 & 1.15 \\ 8.14 & 8.14 & 28.57 & 1.01 & 1.01 & 0.52 \\ 0.00 & 0.00 & 0.00 & 2.87 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 2.87 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 2.21 \end{bmatrix}$$

$$Cs2CaGeSe4 = \begin{bmatrix} 31.54 & 0.90 & 9.45 & 0.85 & 0.97 & 0.41 \\ 0.90 & 31.54 & 9.45 & 0.97 & 0.85 & 0.15 \\ 10.75 & 10.75 & 58.31 & 0.29 & 0.29 & 0.06 \\ 0.00 & 0.00 & 0.00 & 3.90 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 3.90 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.23 \end{bmatrix}$$

$$Cs2SrGeSe4 = \begin{bmatrix} 18.49 & 6.00 & 3.10 & 5.18 & 5.22 & 4.98 \\ 6.00 & 18.49 & 3.10 & 5.22 & 5.18 & 4.20 \\ 9.72 & 9.70 & 52.43 & 0.44 & 0.44 & 0.71 \\ 0.00 & 0.00 & 0.00 & 1.85 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 1.85 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 0.58 \end{bmatrix}$$

$$Cs2CaSnSe4 = \begin{bmatrix} 104.88 & 7.46 & 12.04 & 9.55 & 9.11 & 5.94 \\ 7.46 & 104.88 & 12.04 & 9.11 & 9.55 & 6.85 \\ 19.70 & 19.70 & 238.81 & 5.16 & 5.16 & 4.33 \\ 0.00 & 0.00 & 0.00 & 0.17 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 16.67 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 8.07 \end{bmatrix}$$

$$Cs2SrSnSe4 = \begin{bmatrix} 4.03 & 21.24 & 18.38 & 10.20 & 10.30 & 10.26 \\ 21.24 & 4.03 & 18.38 & 10.31 & 10.18 & 9.57 \\ 4.08 & 4.07 & 46.85 & 2.58 & 2.56 & 2.85 \\ 0.00 & 0.00 & 0.00 & 3.12 & 0.00 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 3.12 & 0.00 \\ 0.00 & 0.00 & 0.00 & 0.00 & 0.00 & 1.21 \end{bmatrix}$$

C. APPENDIX C: EQUATIONS OF ELASTIC MODULI

$$9K_V = (C_{11}+C_{22}+C_{33}) + 2(C_{12}+C_{23}+C_{31})$$

$$1/K_R = (s_{11}+s_{22}+s_{33}) + 2(s_{12}+s_{23}+s_{31})$$

$$15G_V = (C_{11}+C_{22}+C_{33}) - (C_{12}+C_{23}+C_{31}) + 3(C_{44}+C_{55}+C_{66})$$

$$15/G_R = 4(s_{11}+s_{22}+s_{33}) - 4(s_{12}+s_{23}+s_{31}) + 3(s_{44}+s_{55}+s_{66})$$

$$2K_{VRH} = (K_V+K_R)$$

$$2G_{VRH} = (G_V+G_R)$$

$$E = \frac{9KG}{3B+G}$$

$$\nu = \frac{3K-2G}{2(3K+G)}$$

$$H_v = \frac{(1-2\nu)E}{6(1+\nu)}$$

D. APPENDIX D: RESULTS OF CALCULATIONS