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# Mechanical stability conditions for 3D and 2D crystals under arbitrary load

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The paper gathers and unifies mechanical stability conditions for all symmetry classes of 3D and 2D materials under arbitrary load. The methodology is based on the spectral decomposition of the fourth-order stiffness tensors mapped to second-order tensors using *orthonormal* (Mandel) notation, and the verification of the positivity of the so-called Kelvin moduli. An explicit set of stability conditions for 3D and 2D crystals of higher symmetry is also included, as well as a Mathematica notebook that allows mechanical stability analysis for crystals, stress-free and stressed, of arbitrary symmetry under arbitrary loads.

**Key words:** mechanical stability, Born's stability, 2D materials, Kelvin moduli, orthonormal notation.



## 1. Introduction

The examination of the mechanical stability of crystals is inextricably linked to the seminal paper of Max Born from 1940, in which he analyzed the stability of unstressed crystals with cubic symmetry [1]. This stability is often referred to as Born's stability. Stability conditions for unstressed 3D crystals of arbitrary symmetry can be found, for example, in [2]. Unfortunately, it uses non-tensorial Voigt notation and the principal minors of the stiffness tensor, making these conditions non-objective and thus dependent on the orientation of the crystal.

In general, checking the mechanical stability boils down to checking the positive definiteness of a certain fourth-order stiffness tensor, i.e., the non-negativity of a certain quadratic form for arbitrary values of incremental strains [3]. Historically, and especially in the field of continuum mechanics, there are at least four stability criteria for the loaded material, which differ in the choice of appropriate stiffness tensors [4, 5]. We denote these criteria by: $\mathbb{C}$, where the stiffness tensor is based on a symmetric Green strain; $\mathbb{A}$, where the stiffness tensor is based on an asymmetric deformation gradient; $\mathbb{Z}$, as $\mathbb{A}$ except that in the absence of rotation and the incremental stiffness tensor $\mathbb{L}$ giving the change in Cauchy stress with respect to strain. In the *ab initio* and molecular calculations, only the $\mathbb{L}$ and $\mathbb{C}$

criteria are relevant. Due to the polymorphism of the crystals, the stress-free configuration is not uniquely determined and only the current configuration is well defined. These criteria are also the most and least stringent [6]. If the crystal is in any stress-free configuration, then all of these criteria are equivalent.

The phonon (dynamical)- and mechanical (Born)-stability criteria are, in a sense, complementary and must be satisfied [7]. There are 3 acoustic branches of the phonon dispersion relation that start linearly at $\Gamma$ point. The slope of the dispersion curve near $\Gamma$ is the speed of sound. Knowing these slopes, the point symmetry of the crystal and its density, we can deduce the full stiffness tensor. The dynamical stability condition requires that all phonon modes have positive frequencies. Positive slopes of acoustic branches at $\Gamma$ point do not imply mechanical stability [8], these conditions are more complex.

When checking mechanical stability, the problem is not that its conditions are not known, but that they are defined by the fourth-order tensors and cannot be applied directly, they must be transformed into a useful matrix or lower-order tensor form. Even in this transformed form, for crystals of lower symmetry, this verification can be very cumbersome [2]. For the $\mathbb{L}$ criterion, only special, simplest cases are discussed in the literature, i.e., cubic crystals under hydrostatic pressure loading [9], uniaxial tensile deformation [10] and simple shear [3], respectively. The methodology proposed here does not require the checking of a list of conditions. Using the spectral decomposition of the fourth-order stiffness tensors mapped to a second-order tensors using *orthonormal* (Mandel) notation, for any material symmetry and any loading, amounts to computing Kelvin moduli, i.e., appropriate eigenvalues. The procedure requires only writing the calculated, either *ab initio* or atomistic, elastic constants and components of the stress tensor into the proper form of second-order tensors using *orthonormal* notation, and then solving the eigenproblem umerically.

The remainder of this paper is structured as follows: in Section 2 the differences between Voigt and *orthonormal* notations are discussed in detail, in Section 3 general mechanical stability conditions for stress-free systems of arbitrary symmetry written in *orthonormal* notation are discussed and in Section 4 the above stability conditions for stress-free systems were generalized to deformed and stressed systems. Additionally in Appendix A representations of the stiffness tensor for stress-free B2 NiAl written in *orthonormal* notation for three different orientations are shown, in Appendix B the application of general stability conditions to the cubic B2 NiAl crystal subjected to biaxial deformation, tension and compression, is presented. To complete the paper, an explicit set of stability conditions using both leading principal minors and Kelvin moduli is given in Appendix C for stress-free 3D systems with standard lattice vectors, and in Appendix D for 2D systems. Explicit formulas for homogenized isotropic bulk and shear modulus are given in Appendix E.

## 2. Voigt and *orthonormal* notation

In applied mathematics, physics [2, 11], continuum and computational mechanics [12, 13], *ab initio* and molecular codes [14], where symmetric tensors appear, it is common practice to use Voigt notation to reduce their order, so that second-order tensors (strain, stress) are written as vectors and fourth-order tensors (elasticity) as matrices [15, 16].

The most straightforward method for illustrating this notation is to consider the case of the generalized Hooke's law, which describes the linear relationship between strain and stress tensor:

$$\sigma_{ij} = C_{ijkl}\varepsilon_{kl} \rightarrow \boldsymbol{\sigma} = \mathbb{C}\boldsymbol{\varepsilon}, \tag{2.1}$$

where $\boldsymbol{\sigma}$ is the second-order Cauchy stress tensor, $\mathbb{C}$ is the fourth-order anisotropic stiffness tensor and $\boldsymbol{\varepsilon}$ is the second-order small strain tensor ($i, j, k = 1, 2, 3$ for 3D and $i, j, k = 1, 2$ for 2D problems), in accordance with the Einstein summation convention, repeated indices are to be understood as implicitly summed.

Since $\boldsymbol{\sigma}$ and $\boldsymbol{\varepsilon}$ are symmetric tensors, the following holds (minor symmetry)

$$C_{ijkl} = C_{jikl} = C_{ijlk}, \tag{2.2}$$

and from the thermodynamic requirement of the existence of a strain energy density function $W(\boldsymbol{\varepsilon})$ (hyperelastic material) [17] additionally holds (major symmetry)

$$C_{ijkl} = C_{klij}, \tag{2.3}$$

and hence the number of independent components of fourth-order $C_{ijkl}$ reduces to 21 in 3D [18] and to 6 in 2D [19, 20]. The non-tensorial Voigt notation aforementioned employs a 6×6 symmetric matrix in 3D:

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{33} \\ \sigma_{23} \\ \sigma_{13} \\ \sigma_{12} \end{bmatrix} = \left[\begin{array}{ccc|ccc} C_{1111} & C_{1122} & C_{1133} & C_{1123} & C_{1113} & C_{1112} \\ C_{1122} & C_{2222} & C_{2233} & C_{2223} & C_{2213} & C_{2212} \\ C_{1133} & C_{2233} & C_{3333} & C_{3323} & C_{3313} & C_{3312} \\ \hline C_{1112} & C_{2212} & C_{3323} & C_{2323} & C_{2313} & C_{2312} \\ C_{1113} & C_{2213} & C_{3313} & C_{2313} & C_{1313} & C_{1312} \\ C_{1112} & C_{2212} & C_{3312} & C_{2312} & C_{1312} & C_{1212} \end{array}\right] \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{33} \\ 2\varepsilon_{23} \\ 2\varepsilon_{13} \\ 2\varepsilon_{12} \end{bmatrix}, \tag{2.4}$$

or

$$\begin{bmatrix} \hat{\sigma}_1 \\ \hat{\sigma}_2 \\ \hat{\sigma}_3 \\ \hat{\sigma}_4 \\ \hat{\sigma}_5 \\ \hat{\sigma}_6 \end{bmatrix} = \begin{bmatrix} \hat{C}_{11} & \hat{C}_{12} & \hat{C}_{13} & \hat{C}_{14} & \hat{C}_{15} & \hat{C}_{16} \\ \hat{C}_{12} & \hat{C}_{22} & \hat{C}_{23} & \hat{C}_{24} & \hat{C}_{25} & \hat{C}_{26} \\ \hat{C}_{13} & \hat{C}_{23} & \hat{C}_{33} & \hat{C}_{34} & \hat{C}_{35} & \hat{C}_{36} \\ \hat{C}_{14} & \hat{C}_{24} & \hat{C}_{34} & \hat{C}_{44} & \hat{C}_{45} & \hat{C}_{46} \\ \hat{C}_{15} & \hat{C}_{25} & \hat{C}_{35} & \hat{C}_{45} & \hat{C}_{55} & \hat{C}_{56} \\ \hat{C}_{16} & \hat{C}_{26} & \hat{C}_{36} & \hat{C}_{46} & \hat{C}_{56} & \hat{C}_{66} \end{bmatrix} \begin{bmatrix} \hat{\varepsilon}_1 \\ \hat{\varepsilon}_2 \\ \hat{\varepsilon}_3 \\ \hat{\gamma}_4 \\ \hat{\gamma}_5 \\ \hat{\gamma}_6 \end{bmatrix} \rightarrow \hat{\boldsymbol{\sigma}} = \hat{\boldsymbol{C}}\hat{\boldsymbol{\varepsilon}}. \tag{2.5}$$

In 2D 3×3 symmetric matrix:

$$\begin{bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{12}\end{bmatrix} = \left[\begin{array}{cc|c} C_{1111} & C_{1122} & C_{1112}\\ C_{1122} & C_{2222} & C_{2212}\\ \hline C_{1112} & C_{2212} & C_{1212}\end{array}\right] \begin{bmatrix}\varepsilon_{11}\\ \varepsilon_{22}\\ 2\varepsilon_{12}\end{bmatrix}, \tag{2.6}$$

or

$$\begin{bmatrix}\hat{\sigma}_1\\ \hat{\sigma}_2\\ \hat{\sigma}_3\end{bmatrix} = \begin{bmatrix}\hat{C}_{11} & \hat{C}_{12} & \hat{C}_{13}\\ \hat{C}_{12} & \hat{C}_{22} & \hat{C}_{23}\\ \hat{C}_{13} & \hat{C}_{23} & \hat{C}_{33}\end{bmatrix} \begin{bmatrix}\hat{\varepsilon}_1\\ \hat{\varepsilon}_2\\ \hat{\gamma}_3\end{bmatrix} \rightarrow \hat{\boldsymbol{\sigma}} = \hat{\boldsymbol{C}}\hat{\boldsymbol{\varepsilon}}. \tag{2.7}$$

In this notation, the non-diagonal elements of the second-order strain tensor are doubled and denoted as $\hat{\gamma}_J$, and have the interpretation of engineering shear strains, for stresses there is no doubling.

The less popular is an *orthonormal*, also called Mandel, notation in 3D:

$$\begin{bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \sqrt{2}\sigma_{23}\\ \sqrt{2}\sigma_{13}\\ \sqrt{2}\sigma_{12}\end{bmatrix} = \left[\begin{array}{ccc|ccc} C_{1111} & C_{1122} & C_{1133} & \sqrt{2}C_{1123} & \sqrt{2}C_{1113} & \sqrt{2}C_{1112}\\ C_{1122} & C_{2222} & C_{2233} & \sqrt{2}C_{2223} & \sqrt{2}C_{2213} & \sqrt{2}C_{2212}\\ C_{1133} & C_{2233} & C_{3333} & \sqrt{2}C_{3323} & \sqrt{2}C_{3313} & \sqrt{2}C_{3312}\\ \hline \sqrt{2}C_{1112} & \sqrt{2}C_{2212} & \sqrt{2}C_{3323} & 2C_{2323} & 2C_{2313} & 2C_{2312}\\ \sqrt{2}C_{1113} & \sqrt{2}C_{2213} & \sqrt{2}C_{3313} & 2C_{2313} & 2C_{1313} & 2C_{1312}\\ \sqrt{2}C_{1112} & \sqrt{2}C_{2212} & \sqrt{2}C_{3312} & 2C_{2312} & 2C_{1312} & 2C_{1212}\end{array}\right] \begin{bmatrix}\varepsilon_{11}\\ \varepsilon_{22}\\ \varepsilon_{33}\\ \sqrt{2}\varepsilon_{23}\\ \sqrt{2}\varepsilon_{13}\\ \sqrt{2}\varepsilon_{12}\end{bmatrix}, \tag{2.8}$$

or

$$\begin{bmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\\ \sigma_4\\ \sigma_5\\ \sigma_6\end{bmatrix} = \begin{bmatrix}C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16}\\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26}\\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36}\\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46}\\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56}\\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66}\end{bmatrix} \begin{bmatrix}\varepsilon_1\\ \varepsilon_2\\ \varepsilon_3\\ \varepsilon_4\\ \varepsilon_5\\ \varepsilon_6\end{bmatrix} \rightarrow \tilde{\boldsymbol{\sigma}} = \tilde{\boldsymbol{C}}\tilde{\boldsymbol{\varepsilon}}. \tag{2.9}$$

In 2D:

$$\begin{bmatrix}\sigma_{11}\\ \sigma_{22}\\ \sqrt{2}\sigma_{12}\end{bmatrix} = \left[\begin{array}{cc|c} C_{1111} & C_{1122} & \sqrt{2}C_{1112}\\ C_{1122} & C_{2222} & \sqrt{2}C_{2212}\\ \hline \sqrt{2}C_{1112} & \sqrt{2}C_{2212} & 2C_{1212}\end{array}\right] \begin{bmatrix}\varepsilon_{11}\\ \varepsilon_{22}\\ \sqrt{2}\varepsilon_{12}\end{bmatrix}, \tag{2.10}$$

or

$$\begin{bmatrix}\sigma_1\\ \sigma_2\\ \sigma_3\end{bmatrix} = \begin{bmatrix}C_{11} & C_{12} & C_{13}\\ C_{12} & C_{22} & C_{23}\\ C_{13} & C_{23} & C_{33}\end{bmatrix} \begin{bmatrix}\varepsilon_1\\ \varepsilon_2\\ \varepsilon_3\end{bmatrix} \rightarrow \tilde{\boldsymbol{\sigma}} = \tilde{\boldsymbol{C}}\tilde{\boldsymbol{\varepsilon}}. \tag{2.11}$$

The difference between the Voigt notation and the *orthonormal* notation is not only the factor of 2 and its square root, but it is much more fundamental. In the Voigt notation, the elements of the matrix $\hat{\boldsymbol{C}}$ in Eqs. (2.5) and (2.7) are not the elements of a 2nd-order tensor, while in the *orthonormal* notation, the elements of $\tilde{\boldsymbol{C}}$ in Eqs. (2.9) and (2.11) are the elements of a 2nd-order tensor in six dimensions for 3D and three dimensions for 2D problems. The fourth-order tensor notation (2.1) and *orthonormal* notation (2.9, 2.11) are tensorially equivalent [19, 21]. It is also worth mentioning that in this notation the stiffness tensor $\tilde{\boldsymbol{C}}$ and the compliance tensor $\tilde{\boldsymbol{S}}$ have the same bases, are collinear (have the same eigenvectors and the eigenvalues of $\tilde{\boldsymbol{S}}$ are equal to the inverse of the eigenvalues of $\tilde{\boldsymbol{C}}$). There is also an equivalence of quadratic norms here [22]:

$$\|\boldsymbol{\sigma}\| = \sqrt{\sigma_{ij}\sigma_{ij}} = \|\tilde{\boldsymbol{\sigma}}\| = \sqrt{\sigma_I\sigma_I}, \tag{2.12}$$

$$\|\boldsymbol{\varepsilon}\| = \sqrt{\varepsilon_{ij}\varepsilon_{ij}} = \|\tilde{\boldsymbol{\varepsilon}}\| = \sqrt{\varepsilon_I\varepsilon_I}, \tag{2.13}$$

$$\|\mathbb{C}\| = \sqrt{C_{ijkl}C_{ijkl}} = \|\tilde{\boldsymbol{C}}\| = \sqrt{C_{IJ}C_{IJ}}. \tag{2.14}$$

For Voigt notation such equivalence of norms does not occur, see Section 6.

## 3. Internal stability criterion for stress-free lattice

The case of mechanical stability conditions for an unstressed system is considered first. These stability conditions are contained here in the requirement that the local quadratic approximation of the strain energy density function, $W(\boldsymbol{\varepsilon})$, is always positive, strictly convex:

$$W(\varepsilon_{ij}) = \frac{1}{2}\frac{\partial^2 W}{\partial\varepsilon_{ij}\partial\varepsilon_{kl}}\bigg|_{\boldsymbol{\varepsilon}=0}\varepsilon_{ij}\varepsilon_{kl} = \frac{1}{2}C_{ijkl}\varepsilon_{ij}\varepsilon_{kl} \to W(\boldsymbol{\varepsilon}) = \frac{1}{2}\boldsymbol{\varepsilon}\mathbb{C}\boldsymbol{\varepsilon} = \frac{1}{2}\boldsymbol{\varepsilon}\boldsymbol{\sigma}. \tag{3.1}$$

The meaning and properties of the quantities used here have already been explained in Section 2. However, this fourth-order tensor condition cannot be used directly. It is typically transformed into a matrix condition using Voigt notation. Then the positivity of the stiffness matrix, which is not a tensor in Voigt notation, is checked using the condition for positivity of the leading principal minors [2, 12, 23]. This condition is known as Sylvester's criterion and is equivalent to checking whether an upper triangular matrix has all positive diagonal elements after LU decomposition [24]. Still, there are several problems with this approach, it is not tensorially equivalent to the original problem, it depends on the choice of the base of the lattice vectors, and for low symmetries it is cumbersome. This will be clarified after discussing an alternative approach.

For an even-order tensor, the eigenvalue problem is well posed [25, 26], and the spectral decomposition of stiffness tensors can be equivalently expressed in both the fourth-order [27] and *orthonormal* notation:

$$\mathbb{C} = \sum_{I=1}^{6(3)} \lambda_I \boldsymbol{\varepsilon_I} \otimes \boldsymbol{\varepsilon_I} \leftrightarrow \tilde{\boldsymbol{C}} = \sum_{I=1}^{6(3)} \lambda_I \tilde{\boldsymbol{\varepsilon}}_{\boldsymbol{I}} \otimes \tilde{\boldsymbol{\varepsilon}}_{\boldsymbol{I}}, \tag{3.2}$$

where $\lambda_I$ are called the stiffness, Kelvin moduli [28] of $\mathbb{C}$ or $\tilde{\boldsymbol{C}}$, a $\boldsymbol{\varepsilon_I}$ here are the second-order symmetric eigenstate, eigenstrain tensors of $\mathbb{C}$, and $\tilde{\boldsymbol{\varepsilon}}_{\boldsymbol{I}}$ are eigenstate, eigenstrain vectors of $\tilde{\boldsymbol{C}}$ written in *orthonormal* notation ($I = 1, \ldots, 6$ for 3D (Eqs. (2.8) and (2.9)) and $I = 1, \ldots, 3$ for 2D (Eqs. (2.10) and (2.11))). The condition of the positivity of the Kelvin moduli is an alternative to the Sylvester criterion and guarantees the required positivity of the quadratic form in Eq. (3.1). And this approach, based on the spectral decomposition of the fourth-order stiffness tensors mapped to second-order tensors using *orthonormal* notation, and the verification of the positivity of the so-called Kelvin moduli, will be dominant in this study. It is worth making two further points before moving on to other considerations. First, the previously mentioned condition of positive slopes of acoustic branches of phonons at $\Gamma$ point corresponds to strong ellipticity in mathematical elasticity. This condition does not imply positivity of the strain energy density function, $W(\boldsymbol{\varepsilon})$ in Eq. (3.1), but the opposite implication appears [18]. The strong ellipticity condition allows the existence of a negative bulk modulus $B$ and Poisson's ratio $\nu$, which is only limited by the condition $\notin \left[\frac{1}{2}, 1\right]$, which seems to be unphysical [29]. Second, only the case of relaxed ions in the computational cell is considered here, i.e., when internal atomic coordinates are relaxed. In the case of clamped ions, without internal relaxation of the atoms, the mechanical and dynamical stability cannot be decoupled and the mechanical-phonon coupled system must be considered [30].

The symmetries of the stiffness tensor will now be discussed. Aspects of symmetry are known to be important in studying physical phenomena [11]. The crystal point group symmetry determines the symmetry of physical properties. The principle of symmetry (Neumann's Principle) directly states that: "The symmetry elements of any macroscopic physical property of a crystal must include the symmetry elements of the point group of the crystal" [31]. Since physical properties are represented by tensors, tensors for crystals must also have corresponding symmetries [32]. However, the symmetry classification of linear elastic materials is not related to crystallography. This is due to the properties of fourth-order Euclidean symmetric tensors (from the linearity of phenomenological Hooke's law and the properties of two, three-dimensional Euclidean space) [33]. For 3D linear hyperelastic materials, there are eight classes of symmetry [34] and four classes of symmetry for 2D [19, 35]. A classification of all symmetries of anisotropic elasticity, their relations to crystal systems, point and space groups, the corresponding number of distinct elastic constants and Kelvin moduli is gathered in Table 1 for 3D materials and Table 2 for 2D materials.

TABLE 1. The distinct symmetries of anisotropic elasticity and crystal systems for 3D materials.

| Material symmetry | Crystal system | Point group | Space group | No. of independent elastic constants | No. of distinct Kelvin moduli |
|---|---|---|---|---|---|
| Triclinic | Triclinic | $C_1$, $C_i$ | 1–2 | 21 | 6 |
| Monoclinic | Monoclinic | $C_2$, $C_s$, $C_{2h}$ | 3–15 | 13 | 6 |
| Orthotropic | Orthorhombic | $D_2$, $C_{2v}$, $D_{2h}$ | 16–74 | 9 | 6 |
| Tetragonal | Tetragonal | $C_4$, $S_4$, $C_{4h}$, $D_4$ $C_{4v}$, $D_{2d}$, $D_{4h}$ | 75–142 | 6 | 5 |
| Trigonal | Trigonal | $C_3$, $S_6$, $D_3$, $C_{3v}$, $D_{3d}$ | 143–167 | 6 | 4 |
| Transverse isotropy | Hexagonal | $C_6$, $C_{3h}$, $C_{6h}$, $D_6$ $C_{6v}$, $D_{3h}$, $D_{6h}$ | 168–194 | 5 | 4 |
| Cubic | Cubic | T, $T_h$, O, $T_d$, $O_h$ | 195–230 | 3 | 3 |
| Isotropy | | | | 2 | 2 |

TABLE 2. The distinct symmetries of anisotropic elasticity and crystal systems for 2D materials.

| Material symmetry | Crystal system | Point group | 2D Space system | No. of independent elastic constants | No. of distinct Kelvin moduli |
|---|---|---|---|---|---|
| Anisotropic | Oblique | $C_1$, $C_2$ | $p1, p2$ | 6 | 3 |
| Orthotropic | Rectangular | $D_1$, $D_2$ | $pm, pg, pmm, pmg$ | 4 | 3 |
| | Centered rectangular | $D_1$, $D_2$ | $cm, cmm, pgg$ | | |
| Tetragonal | Square | $C_4$, $D_4$ | $p4, p4m, p4g$ | 3 | 3 |
| Isotropy | Hexagonal | $C_3$, $D_3$, $C_6$, $D_6$ | $p3, p3m1, p31m, p6, p6m$ | 2 | 2 |

The number of distinct elastic constants requires some comment. Firstly, it is independent of the orientation of the crystallographic axis system only for isotropy. This is demonstrated in the representation of the stiffness tensor for NiAl, a crystal with cubic symmetry, in Appendix 6. Depending on the orientation of the crystal, we have 3 (A.1), 6 (A.2) and 9 (A.3) distinct elastic constants, respectively. As can be seen, the pattern of the stiffness tensor also changes, but the number of Kelvin moduli remains constant. In addition to rotating the structure in molecular or *ab initio* calculations, we do not always use conventional computational cells. Sometimes it is more convenient to convert non-orthogonal cells, such as hexagonal or trigonal cells, into orthogonal cells [36]. Secondly, some authors introduce two separate tetragonal and two

separate trigonal symmetries, differing in the number of distinct elastic constants [2, 11, 37]. Such a separation is unnecessary. They all have 6 distinct elastic constants when the proper substitution is made [38].

## 4. Internal stability criterion for deformed and stressed lattice

There are different internal stability criteria encountered in literature based on various tangent or incremental stiffness tensors [4]. In the present work, an internal stability criterion with respect to strain increments conjugated to Cauchy stress is applied [3, 39, 40]. The choice of this criterion is dictated by the fact that it reproduces well the observed physical instabilities and is among the two most stringent of the other proposed [6]. Incremental symmetrized tangent modulus $\mathbb{L}$ [3] is defined by

$$L_{ijkl} = C_{ijkl} + \frac{1}{2}\left(\sigma_{ik}\delta_{jl} + \sigma_{il}\delta_{jk} + \sigma_{jk}\delta_{il} + \sigma_{jl}\delta_{ik} - \sigma_{ij}\delta_{kl} - \sigma_{kl}\delta_{ij}\right) \to \mathbb{L} = \mathbb{C} + \mathbb{H}, \tag{4.1}$$

where $\mathbb{C}$ is the fourth-order anisotropic stiffness tensor calculated in the current (deformed, stressed) configuration chosen as reference configuration (stiffness tensor $\mathbb{C}$ in Eq. (2.1) is calculated in the stress-free configuration), $\boldsymbol{\sigma}$ is the second-order Cauchy stress tensor and $\boldsymbol{\delta}$ is the Kronecker delta tensor ($i, j, k = 1, 2, 3$ for 3D and $i, j, k = 1, 2$ for 2D problems). The tensors $\mathbb{C}$, $\mathbb{H}$ and $\mathbb{L}$ possess minor and major symmetry.

The necessary condition of internal stability requires positive definiteness of the quadratic form

$$L_{ijkl}\delta\varepsilon_{ij}\delta\varepsilon_{kl} \geq 0 \to \boldsymbol{\delta\varepsilon}\mathbb{L}\boldsymbol{\delta\varepsilon} \geq 0, \tag{4.2}$$

for all incremental strains $\forall \boldsymbol{\delta\varepsilon} \neq 0$.

Using the *orthonormal* notation described in more detail in Section 2, we can map the fourth-order tensors $\mathbb{C}$, $\mathbb{H}$ and $\mathbb{L}$ in Eq. (4.1) to tensorially equivalent symmetric tensors of the order two.

In 3D:

$$\mathbb{L} = \mathbb{C} + \mathbb{H} \to [\tilde{\boldsymbol{L}}_{\alpha\beta}] = [\tilde{\boldsymbol{C}}_{\alpha\beta}] + [\tilde{\boldsymbol{H}}_{\alpha\beta}], \tag{4.3}$$

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \to \begin{bmatrix} C_{1111} & C_{1122} & C_{1133} & \sqrt{2}C_{1123} & \sqrt{2}C_{1113} & \sqrt{2}C_{1112} \\ C_{1122} & C_{2222} & C_{2233} & \sqrt{2}C_{2223} & \sqrt{2}C_{2213} & \sqrt{2}C_{2212} \\ C_{1133} & C_{2233} & C_{3333} & \sqrt{2}C_{3323} & \sqrt{2}C_{3313} & \sqrt{2}C_{3312} \\ \sqrt{2}C_{1112} & \sqrt{2}C_{2212} & \sqrt{2}C_{3323} & 2C_{2323} & 2C_{2313} & 2C_{2312} \\ \sqrt{2}C_{1113} & \sqrt{2}C_{2213} & \sqrt{2}C_{3313} & 2C_{2313} & 2C_{1313} & 2C_{1312} \\ \sqrt{2}C_{1112} & \sqrt{2}C_{2212} & \sqrt{2}C_{3312} & 2C_{2312} & 2C_{1312} & 2C_{1212} \end{bmatrix}, \tag{4.4}$$

and

$$[\tilde{\boldsymbol{H}}_{\alpha\beta}] \to \begin{bmatrix} \sigma_{11} & \frac{-\sigma_{11}-\sigma_{22}}{2} & \frac{-\sigma_{11}-\sigma_{33}}{2} & -\frac{\sigma_{23}}{\sqrt{2}} & \frac{\sigma_{13}}{\sqrt{2}} & \frac{\sigma_{12}}{\sqrt{2}} \\ \frac{-\sigma_{11}-\sigma_{22}}{2} & \sigma_{22} & \frac{-\sigma_{22}-\sigma_{33}}{2} & \frac{\sigma_{23}}{\sqrt{2}} & -\frac{\sigma_{13}}{\sqrt{2}} & \frac{\sigma_{12}}{\sqrt{2}} \\ \frac{-\sigma_{11}-\sigma_{33}}{2} & \frac{-\sigma_{22}-\sigma_{33}}{2} & \sigma_{33} & \frac{\sigma_{23}}{\sqrt{2}} & \frac{\sigma_{13}}{\sqrt{2}} & -\frac{\sigma_{12}}{\sqrt{2}} \\ -\frac{\sigma_{23}}{\sqrt{2}} & \frac{\sigma_{23}}{\sqrt{2}} & \frac{\sigma_{23}}{\sqrt{2}} & \sigma_{22}+\sigma_{33} & \sigma_{12} & \sigma_{13} \\ \frac{\sigma_{13}}{\sqrt{2}} & -\frac{\sigma_{13}}{\sqrt{2}} & \frac{\sigma_{13}}{\sqrt{2}} & \sigma_{12} & \sigma_{11}+\sigma_{33} & \sigma_{23} \\ \frac{\sigma_{12}}{\sqrt{2}} & \frac{\sigma_{12}}{\sqrt{2}} & -\frac{\sigma_{12}}{\sqrt{2}} & \sigma_{13} & \sigma_{23} & \sigma_{11}+\sigma_{22} \end{bmatrix}, \tag{4.5}$$

or

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \to \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix}, \tag{4.6}$$

and

$$[\tilde{\boldsymbol{H}}_{\alpha\beta}] \to \begin{bmatrix} \sigma_1 & \frac{-\sigma_1-\sigma_2}{2} & \frac{-\sigma_1-\sigma_3}{2} & -\frac{\sigma_4}{2} & \frac{\sigma_5}{2} & \frac{\sigma_6}{2} \\ \frac{-\sigma_1-\sigma_2}{2} & \sigma_2 & \frac{-\sigma_2-\sigma_3}{2} & \frac{\sigma_4}{2} & -\frac{\sigma_5}{2} & \frac{\sigma_6}{2} \\ \frac{-\sigma_1-\sigma_3}{2} & \frac{-\sigma_2-\sigma_3}{2} & \sigma_3 & \frac{\sigma_4}{2} & \frac{\sigma_5}{2} & -\frac{\sigma_6}{2} \\ -\frac{\sigma_4}{2} & \frac{\sigma_4}{2} & \frac{\sigma_4}{2} & \sigma_2+\sigma_3 & \frac{\sigma_6}{\sqrt{2}} & \frac{\sigma_5}{\sqrt{2}} \\ \frac{\sigma_5}{2} & -\frac{\sigma_5}{2} & \frac{\sigma_5}{2} & \frac{\sigma_6}{\sqrt{2}} & \sigma_1+\sigma_3 & \frac{\sigma_4}{\sqrt{2}} \\ \frac{\sigma_6}{2} & \frac{\sigma_6}{2} & -\frac{\sigma_6}{2} & \frac{\sigma_5}{\sqrt{2}} & \frac{\sigma_4}{\sqrt{2}} & \sigma_1+\sigma_2 \end{bmatrix}. \tag{4.7}$$

In 2D:

$$[\tilde{\boldsymbol{L}}_{\alpha\beta}] = [\tilde{\boldsymbol{C}}_{\alpha\beta}] + [\tilde{\boldsymbol{H}}_{\alpha\beta}], \tag{4.8}$$

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \to \begin{bmatrix} C_{1111} & C_{1122} & \sqrt{2}C_{1112} \\ C_{1122} & C_{2222} & \sqrt{2}C_{2212} \\ \sqrt{2}C_{1112} & \sqrt{2}C_{2212} & 2C_{1212} \end{bmatrix}, \tag{4.9}$$

and

$$[\tilde{\boldsymbol{H}}_{\alpha\beta}] \to \begin{bmatrix} \sigma_{11} & \frac{-\sigma_{11}-\sigma_{22}}{2} & \frac{\sigma_{12}}{\sqrt{2}} \\ \frac{-\sigma_{11}-\sigma_{22}}{2} & \sigma_{22} & \frac{\sigma_{12}}{\sqrt{2}} \\ \frac{\sigma_{12}}{\sqrt{2}} & \frac{\sigma_{12}}{\sqrt{2}} & \sigma_{11}+\sigma_{22} \end{bmatrix}, \tag{4.10}$$

or

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \to \begin{bmatrix} C_{11} & C_{12} & C_{13} \\ C_{12} & C_{22} & C_{23} \\ C_{13} & C_{23} & C_{33} \end{bmatrix}, \tag{4.11}$$

and

$$[\tilde{\boldsymbol{H}}_{\alpha\beta}] \to \begin{bmatrix} \sigma_1 & \frac{-\sigma_1-\sigma_2}{2} & \frac{\sigma_3}{2} \\ \frac{-\sigma_1-\sigma_2}{2} & \sigma_2 & \frac{\sigma_3}{2} \\ \frac{\sigma_3}{2} & \frac{\sigma_3}{2} & \sigma_1+\sigma_2 \end{bmatrix}. \tag{4.12}$$

Having already mapped the $\tilde{\boldsymbol{L}}_{\alpha\beta}$ tensors, we need to determine the Kelvin moduli, i.e., their eigenvalues, for them. For a 2D problem, Eq. (4.8), this can be done analytically using the so-called Cardano formulas [41]. For 3D, except for special cases for the 6×6 tensors, Eq. (4.3), it is necessary to use numerical procedures using Mathematica [42], Python [43], Julia [44], or similar. The positivity of all Kelvin moduli guarantees the positive definiteness of the quadratic form in Eq. (4.2) and, consequently, mechanical stability (the tensors $\tilde{\boldsymbol{C}}_{\alpha\beta}$, $\tilde{\boldsymbol{H}}_{\alpha\beta}$ are symmetric and hence also $\tilde{\boldsymbol{L}}_{\alpha\beta}$, so Kelvin moduli are real).

## 5. Conclusions

As Ludwig Boltzmann is said to have said "Nothing is more practical than a good theory". The present work is somewhat in this spirit and boils down to a simple recipe for how to algorithmically check the mechanical stability of an arbitrarily loaded material with arbitrary symmetry. Whether it is a 3D or 2D material, the stiffness tensor in the current configuration can be calculated *ab initio* or atomistically, and if it is not a stress-free configuration, the Cauchy stress as well. It is important to use the *orthonormal* notation from Section 2 to represent the calculated quantities in terms of the corresponding second-order tensors $\tilde{\boldsymbol{C}}$, $\tilde{\boldsymbol{H}}$ and $\tilde{\boldsymbol{L}}$ from Eqs. (4.3)–(4.12). For the tensors of order two represented in this way, their eigenvalues, called Kelvin moduli, can be determined numerically. The positivity of these moduli indicates the mechanical stability of the material, structure, crystal analyzed.

## 6. Supplementary material

Mathematica notebook that allows mechanical stability analysis for crystals, stress-free and stressed, of arbitrary symmetry under arbitrary loads is available online at Supplementary material [45].

## Appendix A. NiAl-Stiffness tensors

Stiffness tensor for stress-free B2 NiAl written in *orthonormal* notation (2.8) for crystal orientation $X = [100]$, $Y = [010]$, $Z = [001]$ was taken from the paper [36], calculated using molecular statics (MS) approach in LAMMPS [14] and the Embedded Atom Model (EAM) [46].

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \rightarrow \begin{bmatrix} 190.868 & 142.908 & 142.908 & 0. & 0. & 0. \\ 142.908 & 190.868 & 142.908 & 0. & 0. & 0. \\ 142.908 & 142.908 & 190.868 & 0. & 0. & 0. \\ 0. & 0. & 0. & 242.971 & 0. & 0. \\ 0. & 0. & 0. & 0. & 242.971 & 0. \\ 0. & 0. & 0. & 0. & 0. & 242.971 \end{bmatrix}, \tag{A.1}$$

the same stiffness tensor for B2 NiAl but determined for crystal orientation $X = [110]$ $Y = [1\text{-}10]$ $Z = [001]$ (the *orthogonal* rotation tensor in 6-dimensional space can be found in [21])

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \rightarrow \begin{bmatrix} 288.374 & 45.402 & 142.908 & 0. & 0. & 0. \\ 45.402 & 288.374 & 142.908 & 0. & 0. & 0. \\ 142.908 & 142.908 & 190.868 & 0. & 0. & 0. \\ 0. & 0. & 0. & 242.971 & 0. & 0. \\ 0. & 0. & 0. & 0. & 242.971 & 0. \\ 0. & 0. & 0. & 0. & 0. & 47.960 \end{bmatrix}, \tag{A.2}$$

and the same stiffness tensor for B2 NiAl but determined for crystal orientation $X = [111]$ $Y = [1\text{-}10] Z = [11-2]$

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \rightarrow \begin{bmatrix} 320.876 & 77.904 & 77.904 & 0. & 0. & 0. \\ 77.904 & 288.374 & 110.406 & 0. & 0. & -65.004 \\ 77.904 & 110.406 & 288.374 & 0. & 0. & 65.004 \\ 0. & 0. & 0. & 177.968 & 91.929 & 0. \\ 0. & 0. & 0. & 91.929 & 112.964 & 0. \\ 0. & -65.004 & 65.004 & 0. & 0. & 112.964 \end{bmatrix}. \tag{A.3}$$

Depending on the orientation of the crystal, we have here 3 (A.1), 6 (A.2) and 9 (A.3) distinct elastic constants, respectively. As can be seen, the pattern of the stiffness tensor also changes, but the number of Kelvin moduli remains constant. For all 3 orientations, the Kelvin moduli are identical and are as follows $\lambda_i = (476.684, 242.971, 242.971, 242.971, 47.96, 47.96)$, $i = 1, \ldots, 6$.

## Appendix B. NiAl-Stability analysis

Let us consider the application of a homogeneous deformation to a monocrystal, in accordance with the Cauchy–Born rule (hypothesis) [13].

The order of indexes in the symmetric strain and stress tensor is here as follows: 1→11, 2→22, 3→33, 4→23, 5→13 and 6→12, whereas in LAMMPS [14] is assumed 1→11, 2→22, 3→33, 4→12, 5→13, 6→23, and in the Cartesian coordinate system, 1 is $X$, 2 is $Y$, and 3 is $Z$.

Consider a biaxial strain state, that is, one in which the deformation gradient $\mathbf{F}$ can be written in the following form

$$[\mathbf{F}_{ij}] \to \begin{bmatrix} \alpha & 0 & 0 \\ 0 & \alpha & 0 \\ 0 & 0 & 1 \end{bmatrix}, \tag{B.1}$$

where $\alpha$ is the stretch ratio, for $\alpha > 1$ we have tension and for $0 < \alpha < 1$ compression. The Lagrangian finite strain tensor, also called the Green strain tensor is defined as $\mathbf{E} = \frac{1}{2}(\mathbf{F^T F} - \mathbf{I})$. Linearization of the Green strain tensor yields the infinitesimal strain tensor $\boldsymbol{\varepsilon} = \frac{1}{2}(\mathbf{F^T} + \mathbf{F} - 2\mathbf{I})$, also called the linear strain tensor, or the small strain tensor [47].

For the B2 NiAl crystal oriented in the Cartesian coordinate system such that $X = [100]$ $Y = [010]$ $Z = [001]$ using molecular statics calculations we are looking for such an $\alpha$ that in the current, deformed configuration $\tilde{\boldsymbol{C}}_{\alpha\beta}$ in Eq. (4.4) becomes singular

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \to \begin{bmatrix} 12.351 & 12.375 & 5.225 & 0. & 0. & 0. \\ 12.375 & 12.351 & 5.225 & 0. & 0. & 0. \\ 5.225 & 5.225 & 54.415 & 0. & 0. & 0. \\ 0. & 0. & 0. & 61.726 & 0. & 0. \\ 0. & 0. & 0. & 0. & 61.726 & 0. \\ 0. & 0. & 0. & 0. & 0. & 84.722 \end{bmatrix}. \tag{B.2}$$

For biaxial tension and $\alpha$ equal to 1.15365, the Kelvin moduli are as follows $\lambda_i^{\tilde{\boldsymbol{C}}} = (84.722, 61.726, 61.726, 56.1524, 22.989, -0.024)$, $i = 1, \ldots, 6$ and $\tilde{\boldsymbol{C}}_{\alpha\beta}$ becomes singular.

We perform analogous calculations, but now require that $\tilde{\boldsymbol{L}}_{\alpha\beta}$ in Eq. (4.3) becomes singular

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \to \begin{bmatrix} 1.179 & 9.579 & 3.781 & 0. & 0. & 0. \\ 9.579 & 1.179 & 3.781 & 0. & 0. & 0. \\ 3.781 & 3.781 & 53.815 & 0. & 0. & 0. \\ 0. & 0. & 0. & 59.011 & 0. & 0. \\ 0. & 0. & 0. & 0. & 59.011 & 0. \\ 0. & 0. & 0. & 0. & 0. & 79.308 \end{bmatrix}. \tag{B.3}$$

For $\alpha$ equal to 1.15454, the Kelvin moduli are as follows $\lambda_i^{\tilde{\boldsymbol{C}}} = (79.308, 59.011, 59.011, 54.469, 10.105, -8.400)$, $i = 1, \ldots, 6$. As it can be seen, $\tilde{\boldsymbol{C}}_{\alpha\beta}$ alone is also singular here.

Since this is a deformed crystal, the stresses are not zero and are $\sigma_{11} = 27.060$, $\sigma_{22} = 27.060$, and $\sigma_{33} = 20.585$ GPa, respectively. For this stress state, the $\tilde{\boldsymbol{H}}_{\alpha\beta}$ tensor in Eq. (4.7) is

$$[\tilde{\boldsymbol{H}}_{\alpha\beta}] \to \begin{bmatrix} 27.060 & -27.060 & -23.823 & 0. & 0. & 0. \\ -27.060 & 27.060 & -23.823 & 0. & 0. & 0. \\ -23.823 & -23.823 & 20.585 & 0. & 0. & 0. \\ 0. & 0. & 0. & 47.645 & 0. & 0. \\ 0. & 0. & 0. & 0. & 47.645 & 0. \\ 0. & 0. & 0. & 0. & 0. & 54.120 \end{bmatrix}, \tag{B.4}$$

and the resulting $\tilde{\boldsymbol{L}}_{\alpha\beta}$ becomes

$$[\tilde{\boldsymbol{L}}_{\alpha\beta}] \to \begin{bmatrix} 28.239 & -17.481 & -20.042 & 0. & 0. & 0. \\ -17.481 & 28.239 & -20.042 & 0. & 0. & 0. \\ -20.042 & -20.042 & 74.400 & 0. & 0. & 0. \\ 0. & 0. & 0. & 106.656 & 0. & 0. \\ 0. & 0. & 0. & 0. & 106.656 & 0. \\ 0. & 0. & 0. & 0. & 0. & 133.427 \end{bmatrix}, \tag{B.5}$$

and the Kelvin moduli are as follows $\lambda_i^{\tilde{\boldsymbol{L}}} = (133.427, 106.656, 106.656, 85.193, 45.720, -0.034)$, $i = 1, \ldots, 6$ and $\tilde{\boldsymbol{L}}_{\alpha\beta}$ becomes singular. We see that for biaxial tension the singularity condition for $\tilde{\boldsymbol{C}}_{\alpha\beta}$ ($\alpha = 1.15365$) is somewhat more stringent than that for $\tilde{\boldsymbol{L}}_{\alpha\beta}$ ($\alpha = 1.15454$), while the crystal still remains mechanically stable.

Similar to the case of biaxial tension, biaxial compression is now analyzed. Again, we are looking for such an $\alpha$ that in the current, deformed configuration $\tilde{\boldsymbol{C}}_{\alpha\beta}$ in Eq. (4.4) becomes singular

$$[\tilde{\boldsymbol{C}}_{\alpha}] \to \begin{bmatrix} 1137.230 & 813.821 & 908.399 & 0. & 0. & 0. \\ 813.821 & 1137.230 & 908.399 & 0. & 0. & 0. \\ 908.399 & 908.399 & 845.906 & 0. & 0. & 0. \\ 0. & 0. & 0. & 399.541 & 0. & 0. \\ 0. & 0. & 0. & 0. & 399.541 & 0. \\ 0. & 0. & 0. & 0. & 0. & 1.875 \end{bmatrix}. \tag{B.6}$$

For biaxial compression and $\alpha$ equal to 0.7985, the Kelvin moduli are as follows $\lambda_i^{\tilde{\boldsymbol{C}}} = (2796.950, 399.541, 399.541, 323.411, 1.875, 0.011)$, $i = 1, \ldots, 6$ and $\tilde{\boldsymbol{C}}_{\alpha\beta}$ becomes singular.

We perform analogous calculations, but now require that $\tilde{\boldsymbol{L}}_{\alpha\beta}$ in Eq. (4.3) become singular

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \to \begin{bmatrix} 621.924 & 280.913 & 336.130 & 0. & 0. & 0. \\ 280.913 & 621.924 & 336.130 & 0. & 0. & 0. \\ 336.130 & 336.130 & 372.138 & 0. & 0. & 0. \\ 0. & 0. & 0. & 431.175 & 0. & 0. \\ 0. & 0. & 0. & 0. & 431.175 & 0. \\ 0. & 0. & 0. & 0. & 0. & 253.649 \end{bmatrix}. \tag{B.7}$$

For $\alpha$ equal to 0.9087, the Kelvin moduli are as follows $\lambda_i^{\tilde{\boldsymbol{C}}} = (1181.890, 431.175, 431.175, 341.011, 253.649, 93.083)$, $i=1,\ldots,6$. As can be seen, $\tilde{\boldsymbol{C}}_{\alpha\beta}$ alone is not singular here.

Since this is a deformed crystal, the stresses are not zero and are $\sigma_{11} = -59.567$, $\sigma_{22} = -59.567$, and $\sigma_{33} = -41.191$ GPa, respectively. For this stress state, the $\tilde{\boldsymbol{H}}_{\alpha\beta}$ tensor in Eq. (4.7) is

$$[\tilde{\boldsymbol{H}}_{\alpha\beta}] \to \begin{bmatrix} -59.567 & 59.567 & 50.379 & 0. & 0. & 0. \\ 59.567 & -59.567 & 50.379 & 0. & 0. & 0. \\ 50.379 & 50.379 & -41.191 & 0. & 0. & 0. \\ 0. & 0. & 0. & -100.758 & 0. & 0. \\ 0. & 0. & 0. & 0. & -100.758 & 0. \\ 0. & 0. & 0. & 0. & 0. & -119.134 \end{bmatrix}, \tag{B.8}$$

and the resulting $\tilde{\boldsymbol{L}}_{\alpha\beta}$ becomes

$$[\tilde{\boldsymbol{L}}_{\alpha\beta}] \to \begin{bmatrix} 562.357 & 340.480 & 386.508 & 0. & 0. & 0. \\ 340.480 & 562.357 & 386.508 & 0. & 0. & 0. \\ 386.508 & 386.508 & 330.947 & 0. & 0. & 0. \\ 0. & 0. & 0. & 330.417 & 0. & 0. \\ 0. & 0. & 0. & 0. & 330.417 & 0. \\ 0. & 0. & 0. & 0. & 0. & 134.515 \end{bmatrix}, \tag{B.9}$$

and the Kelvin moduli are as follows $\lambda_i^{\tilde{\boldsymbol{L}}} = (1233.770, 330.417, 330.417, 221.876, 134.515, 0.011)$, $i = 1,\ldots,6$ and $\tilde{\boldsymbol{L}}_{\alpha\beta}$ becomes singular. We see that for biaxial compression the singularity condition for $\tilde{\boldsymbol{L}}_{\alpha\beta}$ ($\alpha = 0.9087$) is much more stringent than that for $\tilde{\boldsymbol{C}}_{\alpha\beta}$ ($\alpha = 0.7985$), while the crystal still remains mechanically stable. Thus, it is recommended to check the condition on $\tilde{\boldsymbol{C}}_{\alpha\beta}$ as well as on $\tilde{\boldsymbol{L}}_{\alpha\beta}$. Similar observations were made in [6], where the behavior of a certain isotropic material subjected to different loads was analyzed.

The Mathematica notebook [42] that allows to analyze the mechanical stability of crystals, stress-free and stressed, of arbitrary symmetry subjected to arbitrary loads is available in the supplementary material in Section 6.

## Appendix C. 3D-Explicitly written out mechanical stability conditions

The following representations of stiffness tensor are given with respect to the symmetry axes, in a canonical base, with standard lattice vectors [37].

1. Cubic & isotropy → Cubic lattice (Table 1)
   (3 & 2 elastic constants; 3 &2 Kelvin moduli)

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \to \begin{bmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{bmatrix}, \tag{C.1}$$

   (For isotropy $C_{44} = C_{11} - C_{12}$)

   $C_{11} - C_{12} > 0$ & $C_{11} + 2C_{12} > 0$ & $C_{44} > 0$ or
   $\lambda_{I,II,III} = C_{44} > 0$ & $\lambda_{IV,V} = (C_{11} - C_{12}) > 0$ & $\lambda_{VI} = (C_{11} + 2C_{12}) > 0$.

2. Transverse isotropy → Hexagonal lattice (Table 1)
   (5 elastic constants; 4 Kelvin moduli)

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \to \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{11} - C_{12} \end{bmatrix}, \tag{C.2}$$

   $C_{11} > |C_{12}|$ & $2C_{13}^2 > C_{33}(C_{11} + C_{12})$ & $C_{44} > 0$ & $(C_{11} - C_{12}) > 0$ or
   $\lambda_{I,II} = C_{44} > 0$ & $\lambda_{III,IV} = (C_{11} - C_{12}) > 0$ &
   $\lambda_V = \frac{1}{2}(C_{11} + C_{22} + C_{33} - \bigstar) > 0$ & $\lambda_{VI} = \frac{1}{2}(C_{11} + C_{22} + C_{33} + \bigstar) > 0$,
   where $\bigstar = \sqrt{C_{11}^2 + 2C_{11}C_{12} + C_{12}^2 + 8C_{13}^2 - 2C_{11}C_{33} - 2C_{12}C_{33} + C_{33}^2}$.

3. Trigonal → Trigonal lattice (Table 1)
   (6 elastic constants; 4 Kelvin moduli)

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \to \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & 0 & 0 \\ C_{12} & C_{11} & C_{13} & -C_{14} & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ C_{14} & -C_{14} & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & \sqrt{2}C_{14} \\ 0 & 0 & 0 & 0 & \sqrt{2}C_{14} & C_{11} - C_{12} \end{bmatrix}. \tag{C.3}$$

   Some authors [2, 11, 37] distinguish a new Trigonal II class with seven, not six, distinct constants. However, this is not a new class and by a simple transformation can be reduced to the class above [38].

   $C_{11} > |C_{12}|$ & $C_{44} > 0$ & $2C_{13}^2 < C_{33}(C_{11} + C_{12})$ & $2C_{14}^2 < C_{44}(C_{11} - C_{12})$ or
   $\lambda_{I,II} = \frac{1}{2}(C_{11} - C_{12} + C_{44} - \diamond) > 0$ & $\lambda_{III,IV} = \frac{1}{2}(C_{11} - C_{12} + C_{44} + \diamond) > 0$,
   where $\diamond = \sqrt{C_{11}^2 + 2C_{11}C_{12} + C_{12}^2 + 8C_{14}^2 - 2C_{11}C_{44} + 2C_{12}C_{44} + C_{44}^2}$, &

$\lambda_V = \frac{1}{2}(C_{11} + C_{12} + C_{33} - \bigstar) > 0$ & $\lambda_{VI} = \frac{1}{2}(C_{11} + C_{12} + C_{33} + \bigstar) > 0$, where $\bigstar = \sqrt{C_{11}^2 + 2C_{11}C_{12} + C_{12}^2 + 8C_{13}^2 - 2C_{11}C_{33} - 2C_{12}C_{33} + C_{33}^2}$.

4. Tetragonal → Tetragonal lattice (Table 1)
(6 elastic constants; 5 Kelvin moduli)

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \to \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{13} & 0 & 0 & 0 \\ C_{13} & C_{13} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix}. \tag{C.4}$$

As above some authors [2, 11, 37] identify also a new Tetragonal II class with seven, not six, distinct constants and again, this is not a new class and can be simply transformed to the class above [38].

$C_{11} > |C_{12}|$ & $2C_{13}^2 < C_{33}(C_{11} + C_{12})$ & $C_{44} > 0$ & $C_{66} > 0$ or
$\lambda_{I,II} = C_{44} > 0$ & $\lambda_{III} = (C_{11} - C_{12}) > 0$ & $\lambda_{IV} = C_{66} > 0$ &
$\lambda_V = \frac{1}{2}(C_{11} + C_{22} + C_{33} - \bigstar) > 0$ & $\lambda_{VI} = \frac{1}{2}(C_{11} + C_{22} + C_{33} + \bigstar) > 0$, where $\bigstar = \sqrt{C_{11}^2 + 2C_{11}C_{12} + C_{12}^2 + 8C_{13}^2 - 2C_{11}C_{33} - 2C_{12}C_{33} + C_{33}^2}$.

5. Orthotropic → Orthorhombic lattice (Table 1)
(9 elastic constants; 6 Kelvin moduli)

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \to \begin{bmatrix} C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\ C_{12} & C_{22} & C_{23} & 0 & 0 & 0 \\ C_{13} & C_{23} & C_{33} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{66} \end{bmatrix}, \tag{C.5}$$

$C_{11} > 0$ & $C_{11}C_{22} > C_{12}^2$ & $C_{11}C_{22}C_{33} + 2C_{12}C_{13}C_{23} - C_{11}C_{23}^2 - C_{22}C_{13}^2 - C_{33}C_{12}^2 > 0$ & $C_{44} > 0$ & $C_{55} > 0$ & $C_{66} > 0$ or $\lambda_I = C_{44} > 0$ & $\lambda_{II} = C_{55} > 0$ & $\lambda_{III} = C_{66} > 0$ & $\lambda_{IV} = Root_I|\blacktriangle| > 0$ & $\lambda_V = Root_{II}|\blacktriangle| > 0$ & $\lambda_{VI} = Root_{III}|\blacktriangle| > 0$, where $\blacktriangle = C_{11}C_{22}C_{33} + 2C_{12}C_{13}C_{23} - C_{11}C_{23}^2 - C_{22}C_{13}^2 - C_{33}C_{12}^2$ (Roots calculated, e.g., from the Cardano formula [41]).

6. Monoclinic → Monoclinic lattice (Table 1)
(13 elastic constants; 6 Kelvin moduli)

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \to \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & 0 & 0 \\ C_{12} & C_{22} & C_{23} & C_{24} & 0 & 0 \\ C_{13} & C_{23} & C_{33} & C_{34} & 0 & 0 \\ C_{14} & C_{24} & C_{34} & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{55} & C_{56} \\ 0 & 0 & 0 & 0 & C_{56} & C_{66} \end{bmatrix}, \tag{C.6}$$

$\lambda_i > 0$ (all six eigenvalues of $\tilde{\boldsymbol{C}}_{\alpha\beta}$).

7. Triclinic → Triclinic lattice (Table 1)
   (21 elastic constants; 6 Kelvin moduli)

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \rightarrow \begin{bmatrix} C_{11} & C_{12} & C_{13} & C_{14} & C_{15} & C_{16} \\ C_{12} & C_{22} & C_{23} & C_{24} & C_{25} & C_{26} \\ C_{13} & C_{23} & C_{33} & C_{34} & C_{35} & C_{36} \\ C_{14} & C_{24} & C_{34} & C_{44} & C_{45} & C_{46} \\ C_{15} & C_{25} & C_{35} & C_{45} & C_{55} & C_{56} \\ C_{16} & C_{26} & C_{36} & C_{46} & C_{56} & C_{66} \end{bmatrix}, \tag{C.7}$$

   $\lambda_i > 0$ (all six eigenvalues of $\tilde{\boldsymbol{C}}_{\alpha\beta}$).

## Appendix D. 2D-Explicitly written out mechanical stability conditions

1. Full symmetry (isotropy) → Hexagonal lattice (Table 2)
   (2 elastic constants; 2 Kelvin moduli)

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \rightarrow \begin{bmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{11} & 0 \\ 0 & 0 & C_{11} - C_{12} \end{bmatrix}, \tag{D.1}$$

   $C_{11} > 0$ & $C_{11} > |C_{12}|$ or $\lambda_I = (C_{11} + C_{12}) > 0$ & $\lambda_{II} = (C_{11} - C_{12}) > 0$.

2. Symmetry of a square (tetragonal) → Square lattice (Table 2)
   (3 elastic constants; 3 Kelvin moduli)

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \rightarrow \begin{bmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{11} & 0 \\ 0 & 0 & C_{33} \end{bmatrix}, \tag{D.2}$$

   $C_{11} > 0$ & $C_{33} > 0$ & $C_{11} > |C_{12}|$ or $\lambda_I = (C_{11} + C_{12}) > 0$ & $\lambda_{II} = (C_{11} - C_{12}) > 0$ & $\lambda_{III} = C_{33} > 0$.

3. Symmetry of a rectangle (orthotropy)→ Rectangular & Centered rectangular lattice (Table 2)
   (4 elastic constants; 3 Kelvin moduli)

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \rightarrow \begin{bmatrix} C_{11} & C_{12} & 0 \\ C_{12} & C_{22} & 0 \\ 0 & 0 & C_{33} \end{bmatrix}, \tag{D.3}$$

   $C_{11} > 0$ & $C_{33} > 0$ & $C_{11}C_{22} > C_{12}^2$ or
   $\lambda_I = \frac{1}{2}(C_{11} + C_{22} + \sqrt{4C_{12}^2 - (C_{11} - C_{22})^2}) > 0$ & $\lambda_{II} = \frac{1}{2}(C_{11} + C_{22} - \sqrt{4C_{12}^2 - (C_{11} - C_{22})^2}) > 0$ & $\lambda_{III} = C_{33} > 0$.

4. No symmetry (anisotropy) → Oblique lattice (Table 2)
   (6 elastic constants; 3 Kelvin moduli)

$$[\tilde{\boldsymbol{C}}_{\alpha\beta}] \rightarrow \begin{bmatrix} C_{11} & C_{12} & C_{13} \\ C_{12} & C_{22} & C_{23} \\ C_{13} & C_{23} & C_{33} \end{bmatrix}, \tag{D.4}$$

   $C_{11} > 0$ & $C_{11}C_{22} > C_{12}^2$ & $\det(\tilde{\boldsymbol{C}}_{\alpha\beta}) > 0$ or $\lambda_I > 0$ & $\lambda_{II} > 0$ & $\lambda_{III} > 0$ (e.g., from the Cardano formula [41]).

If $C_{13}$ and/or $C_{23}$ are non-zero, it is difficult to determine if there is no symmetry or if the axes are incorrect [19]. To avoid this, the most general condition for anisotropy (D.4) should be checked.

## Appendix E. Homogenized isotropic bulk and shear modulus

In the *orthonormal* notation regardless of the choice of axes orientation we get:

*Voigt averaging:*
bulk modulus

$$B_V = \frac{1}{9}[(C_{11} + C_{22} + C_{33}) + 2(C_{12} + C_{13} + C_{23})]; \tag{E.1}$$

shear modulus

$$G_V = \frac{1}{15}\left[(C_{11} + C_{22} + C_{33}) - (C_{12} + C_{13} + C_{23}) + \frac{3}{2}(C_{44} + C_{55} + C_{66})\right]. \tag{E.2}$$

*Reuss averaging:*
bulk modulus

$$B_R = \frac{1}{[(S_{11} + S_{22} + S_{33}) + 2(S_{12} + S_{13} + S_{23})]}; \tag{E.3}$$

shear modulus

$$G_R = \frac{15}{[4(S_{11} + S_{22} + S_{33}) - 4(S_{12} + S_{13} + S_{23}) + 6(S_{44} + S_{55} + S_{66})]}, \tag{E.4}$$

where $S_{ij}$ are the elements of the compliance tensor $\tilde{\boldsymbol{S}} = \tilde{\boldsymbol{C}}^{-1}$.

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