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Original Research

Diagnosing Shear Conventions and Loading Constraints in a Crystal Elasticity Laboratory

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ABSTRACT

A computational laboratory is developed in which students diagnose errors in elastic-tensor notation, distinguish transverse boundary conditions, and decide whether an averaged modulus adequately describes a specified crystal direction. Complete stiffness matrices for inorganic structures are examined under infinitesimal uniaxial loading. An exact isotropic check shows that doubling the shear products in a directional-compliance calculation changes a prescribed 100 GPa response into apparent values between 28.571 and 100 GPa. Omitting those products instead produces values between 100 and 600 GPa. A separate comparison of constrained extension with free transverse contraction identifies discrepancies above twenty percent in investigated axial cases. For the correctly evaluated crystal responses, the Hill-derived modulus differs by more than twenty percent from at least one tested direction in 863 structures. The count is unchanged when angular sampling increases from 1,024 to 16,384 points. A CaO–BN exercise connects nearly identical averaged moduli to markedly different strain intervals, while a TiIr example separates a limiting direction from the fraction of orientations exceeding a tolerance. Eight independent visualizations display atomic positions, shear errors, loading constraints, directional strain, and angular resolution. The resulting three-hour exercise contains complete reference answers and individual transfer questions. Its numerical results are verified, but its effect on student understanding has not been measured.

KEYWORDS

computational laboratory; engineering shear; crystal elasticity; transverse contraction; directional strain; materials education

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1. INTRODUCTION

A material property becomes useful only after the loading conditions and the physical object to which it applies have been specified. Young's modulus provides a particularly clear example. A student can correctly remember a numerical value, substitute it into a stress–strain expression, and still obtain an inappropriate answer by applying an aggregate approximation to a particular crystal orientation. Another student can begin with the complete stiffness matrix and introduce a different error by confusing engineering shear with tensor shear. A third can select a diagonal matrix component while overlooking the transverse strain constraints implied by that choice. These mistakes are mathematically distinct, yet a conventional exercise that asks only for one final number can conceal all three. A laboratory that exposes their different signatures can connect elastic theory with a more careful interpretation of calculated material response.

Recent materials teaching has used mobile visualization and home-based activities to connect atomic arrangement with observable properties. An augmented-reality laboratory on metallic crystal structures demonstrated one route for presenting spatial information outside a conventional teaching room [1]. Instruction in materials characterization has likewise emphasized the relationship between a physical question, a suitable technique, and the interpretation of its output [2]. Computational undergraduate research activities can provide access to questions that would otherwise require substantial equipment or specialized facilities [3]. These developments support a computer laboratory on elasticity, but they also make its purpose more demanding than displaying an attractive crystal or running a prepared calculation. The student should identify which statement the calculation tests and which physical assumptions remain outside it.

Laboratory courses differ considerably in their goals, organization, and degree of student decision making. A broad examination of North American physics laboratories found substantial variation in the balance between reinforcing lecture content and developing investigative skills [4]. Comparisons across many courses associate skills-focused instruction with stronger critical-thinking performance and more productive views of experimentation than content reinforcement alone [5]. Such evidence does not transfer automatically to every computational activity. It instead provides a reason to formulate explicit actions that students must carry out. In the present exercise, those actions are to test a limiting case, diagnose a convention error, specify a boundary condition, compare two physically different quantities, and qualify a conclusion when angular resolution is finite.

A useful distinction follows between numerical agreement and justified interpretation. An output can agree with an expected answer because the same incorrect convention has been used twice. Conversely, two correct calculations can disagree because they describe different mechanical conditions. Critical-thinking assessment in laboratory settings addresses the use of evidence to choose what to trust and what to do [6]. The associated teaching literature emphasizes repeated comparisons between models and observations rather than an uninterrupted progression toward a known answer [7]. A crystal-elasticity exercise can adopt that discipline without pretending that numerical output is a new physical measurement. Its evidence consists of explicit constitutive relations, independent checks, and the consequences of changing clearly identified assumptions.

Students' reasoning about uncertainty provides another reason to separate the relevant questions. Comparisons between introductory and more advanced learners indicate that additional laboratory experience does not uniformly improve every aspect of uncertainty reasoning [8]. Instructor interviews also show differences in the emphasis assigned to uncertainty concepts and practices [9]. A finer angular grid can improve a directional search while leaving the accuracy of the underlying electronic-structure calculation unchanged. A wider interval of directional moduli can describe anisotropy without describing uncertainty in any one modulus. A tolerance used to accept an approximation can express an engineering requirement without becoming a confidence interval. These distinctions are central to the exercise because each can otherwise be obscured by the general statement that a calculation has become more accurate.

Crystal anisotropy already has a substantial instructional history. Three-dimensional tensor visualization has been used to connect equations with spatially varying crystal properties [10]. Directional elastic analysis is also available through established software, including ELATE and MechElastic [11, 12]. Large-scale investigations have examined elastic anisotropy across thousands of inorganic compounds [13], and equivariant learning methods now predict full elasticity tensors while respecting crystal symmetry [14]. Accordingly, neither directional Young's modulus nor its graphical representation is treated here as a new physical method. The contribution is a laboratory with inspectable error mechanisms, complete answers, and a sequence that distinguishes notation, boundary conditions, directional response, and numerical resolution.

The distinction between constrained and unconstrained deformation has particular educational value because it follows directly from a matrix already available to the learner. A diagonal stiffness coefficient gives the normal stress required when the corresponding normal strain is imposed and the remaining strain components are suppressed. Young's modulus describes uniaxial stress with the other stress components zero, allowing transverse and shear strains where coupling requires them. These conditions coincide only under special restrictions. Recent identification

methods for anisotropic structured materials explicitly account for multiple stiffness parameters and shear–normal coupling [15]. Deliberate mechanical coupling has also become a design variable in architectured materials [16]. The issue is therefore relevant beyond a notation exercise: a parameter acquires meaning through the conditions under which it is defined.

The selected crystal examples make the interpretation tangible without adding fabricated tensile observations. One example is a layered BN structure whose in-plane and out-of-plane responses differ strongly; another is a CaO structure with a narrow directional range. Measurements on atomically thin BN demonstrate the importance of interlayer interactions and also show why dimensionality and specimen form must be stated carefully [17]. A three-dimensional modulus in gigapascals cannot be substituted directly for a two-dimensional stiffness expressed per unit length. Similarly, a zero-temperature crystal calculation is not a certificate for the room-temperature performance of a porous, textured, or defective specimen. The structural image in this paper uses actual relaxed atomic positions, whereas the mechanical figures show calculations from the elastic coefficients.

A textbook treatment can prepare this distinction by presenting the same elastic relation in two forms. The scalar form answers a narrowly specified tensile question, while the matrix form retains coupling between the strain components. Students should be able to move between them without interpreting the shorter expression as universally more fundamental. An instructive question is whether suppressing transverse motion changes the measured slope even when the material remains isotropic. Another is whether agreement along a convenient axis establishes agreement after rotation. Both questions can be answered from the mathematical structure before any particular chemical composition is considered. This ordering helps separate a failure in the calculation from an unfamiliar material response. It also prevents chemical intuition from becoming the only way to recognize an implausible result, since a confident expectation about a familiar metal cannot replace a test of the constitutive expression. The exercise therefore uses an exact mechanical limit before introducing differences between crystal structures.

The laboratory is designed for students who can multiply matrices and have encountered linear elasticity, but who need not manipulate fourth-rank tensors fluently. A compact directional projection permits a derivation using a stress vector and a physical strain tensor. An isotropic solid then supplies an exact test with which to expose a smooth but incorrect angular response. The subsequent crystal calculations require the same algebra, so the transition does not depend on introducing a second computational language. NumPy supplies the matrix operations, and selected directional extrema are checked by numerical minimization using SciPy [18, 19]. The calculations remain short enough for students to explain rather than accept as an opaque software result.

The exercise supplies a complete mathematical and numerical task, not evidence that a particular class has learned more effectively. Research on students' expectations in nontraditional laboratories shows that learners may continue to seek confirmation of a predetermined result even when the activity permits more independent decisions [20]. The present design addresses that possibility by asking for a prediction before revealing a material pair, by making the first implementation intentionally incorrect, and by requiring a final statement for an unseen crystal. Whether these choices improve understanding remains open to direct evaluation. The following sections establish the physical calculations and reference answers needed for such an evaluation without inventing student responses or institutional implementation records.

2. ELASTIC COEFFICIENTS AND MECHANICAL DEFINITIONS

2.1. Material coverage and calculation conditions

The analysis uses the stiffness matrices accompanying the first-principles investigation of inorganic crystalline compounds and its linked numerical collection [21–23]. Those calculations were generated by the research team identified in these references; the directional calculations, diagnostic comparisons, and teaching exercises presented here are carried out independently. There are 1,181 distinct material identifiers and 1,087 distinct composition strings. Each entry supplies a complete six-by-six elastic matrix, its inverse, crystal information, aggregate moduli, and the reciprocal-space sampling setting. These variables are sufficient for calculating infinitesimal elastic response

in the stated coordinate frame. They do not provide repeated tensile specimens or independent observations for each loading direction.

The electronic calculations used projector-augmented-wave potentials and the Perdew–Burke–Ernzerhof approximation, with a Hubbard correction for selected oxides. They describe the zero-temperature and zero-pressure limit. The stated plane-wave cutoff is 700 eV, and the initial strain choices are minus and plus one-half and one percent, with further checks where required. The available reciprocal-space settings are 1,000, 7,000, 20,000, and 45,000, occurring in 37, 1,082, 60, and two entries, respectively. Complete final strain histories and electronic input decks are not available for every entry. Consequently, the present calculations evaluate the supplied elastic matrices rather than refitting stress–strain curves or assigning material-specific electronic-structure uncertainties.

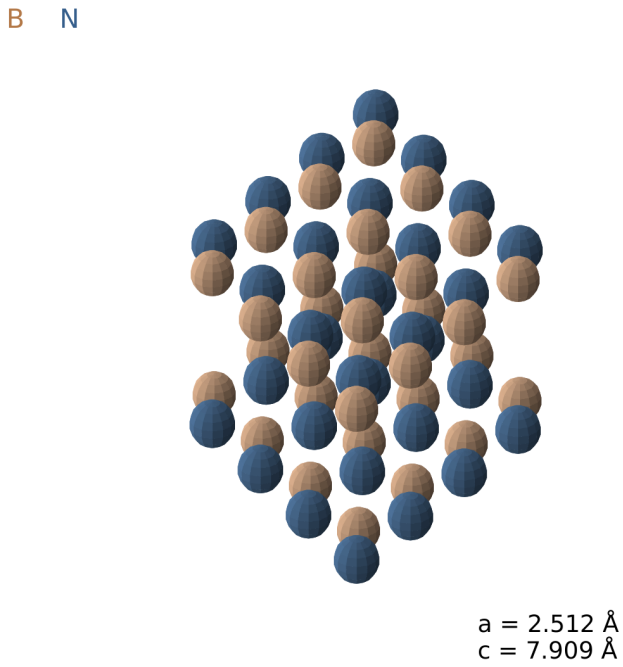


Figure 1: Layer geometry of the BN crystal mp-984. The rendering uses relaxed atomic coordinates, with boron in tan and nitrogen in blue.

Chemical similarity and alternative structures mean that the entries are not statistically independent experimental replicates. The principal counts therefore describe this finite collection directly. Directions within one crystal are evaluations of the same constitutive law, not additional specimens. No significance test treats them as independent observations. A separate composition check retains the entry with the lowest numerical material identifier for each composition string. This check examines whether repeated compositions strongly affect the main conclusion; it does not remove every chemical relationship between compounds. The distinction between a material calculation and a replicated experiment remains part of the student instructions.

Structural coordinates follow the representation distributed through the materials-analysis software collection [24]. For the layered BN example, the lattice parameters are $a = 2.512069$ and $c = 7.909136$ angstroms, with space group 194 and material identifier mp-984. Figure 1 displays a finite repetition of these relaxed coordinates. Sphere size and color identify atomic species and are visual choices; atomic positions and layer spacing follow the crystallographic values. The image is an atomistic rendering rather than microscopy. Its purpose is to establish which structure is being discussed before the directional calculations are interpreted.

2.2. Directional compliance and admissibility

Voigt order is $(11, 22, 33, 23, 13, 12)$. The stress vector contains physical shear stresses, whereas the strain vector contains engineering shear strains. Stiffness is expressed in gigapascals and compliance in inverse gigapascals. For a Cartesian unit loading direction $\mathbf{n}$, define

$$\boldsymbol{q}(\mathbf{n}) = \left(n_1^2, n_2^2, n_3^2, n_2n_3, n_1n_3, n_1n_2\right)^{\mathsf{T}}, \qquad \mathbf{S} = \mathbf{C}^{-1}. \tag{1}$$

A uniaxial stress $\sigma\mathbf{n}\otimes\mathbf{n}$ has vector representation $\sigma\boldsymbol{q}$. Applying compliance gives the engineering-strain vector. After converting its shear entries to physical tensor components, projection along the loading direction gives

$$E(\mathbf{n}) = \left[\boldsymbol{q}^{\mathsf{T}}\mathbf{S}\boldsymbol{q}\right]^{-1}, \qquad \varepsilon_{\parallel}(\mathbf{n}) = \frac{\sigma}{E(\mathbf{n})}. \tag{2}$$

The products in the final three positions of $\boldsymbol{q}$ are not doubled. Their interaction with engineering shear already enters through the strain representation. Coordinate directions refer to the standardized Cartesian frame of the tensor. Assigning crystallographic indices to an arbitrary direction requires the corresponding lattice transformation and cannot be inferred from a formula alone.

Every matrix must be finite and symmetric to an absolute tolerance of 10^{-8} GPa. Stability is checked in Kelvin notation using $\mathbf{C}_K = \mathbf{DCD}$, where $\mathbf{D} = \mathrm{diag}(1, 1, 1, \sqrt{2}, \sqrt{2}, \sqrt{2})$. The smallest eigenvalue must exceed 10^{-8} times the largest. Positive definiteness is the relevant elastic admissibility condition at zero stress [25], while Kelvin mapping preserves the tensor inner product in matrix form [26]. Passing this check does not establish thermodynamic phase stability or experimental synthesizability. No negative eigenvalue is clipped, and no stiffness matrix is replaced by an isotropic approximation.

2.3. An exact check for engineering-shear errors

An isotropic solid with $E_0 = 100$ GPa and Poisson's ratio $\nu_0 = 0.25$ is used only to test the algebra. Let k multiply the final three components of $\boldsymbol{q}$, with $k = 1$ denoting the correct expression. Define $T = n_1^2n_2^2 + n_1^2n_3^2 + n_2^2n_3^2$. Direct substitution into the isotropic compliance matrix gives

$$E_k(\mathbf{n}) = \frac{E_0}{1 + 2(1+\nu_0)(k^2-1)T}, \qquad 0 \le T \le \frac{1}{3}. \tag{3}$$

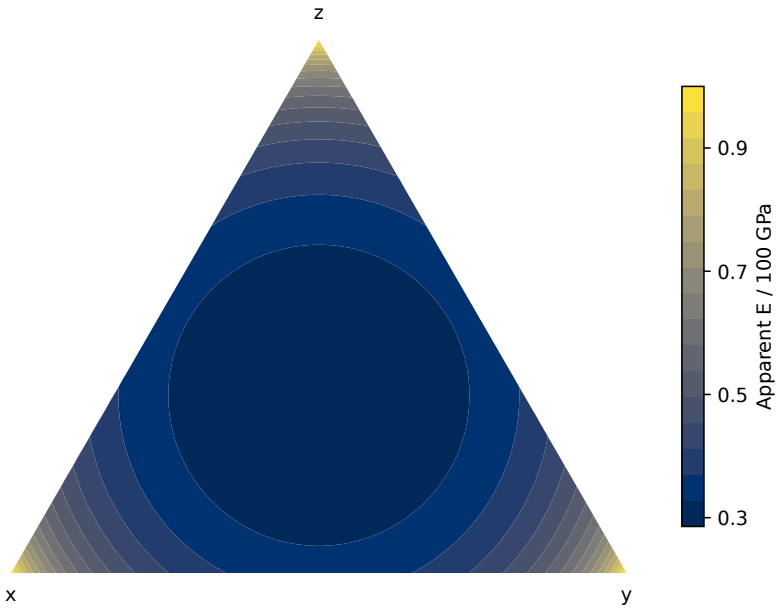


Figure 2: False directional variation produced by doubling shear products in a 100 GPa isotropic solid. The triangle coordinates are squared direction cosines; its corners correspond to the Cartesian axes.

The expression establishes a closed-form reference for the entire sphere. Doubling shear products corresponds to $k = 2$; omitting them corresponds to $k = 0$. Both errors leave coordinate-axis responses unchanged because T

vanishes there. A test confined to the coordinate axes therefore cannot detect either mistake. Figure 2 displays the apparent response for doubled products across the positive direction-cosine triangle. Each interior point represents squared direction cosines summing to unity, so the figure is a precise angular calculation rather than a diagram of material texture.

2.4. Transverse constraints and an averaged reference

Under uniaxial stress along Cartesian axis i, free transverse deformation gives $E_i = 1/S_{ii}$. Under imposed axial strain with all remaining strain components zero, the associated stress coefficient is C_{ii}. Their relative difference is

$$P_i = C_{ii}S_{ii} - 1. \tag{4}$$

For a positive-definite elastic matrix, the Schur complement makes this quantity nonnegative. It measures the penalty associated with suppressing coupled deformation, not angular anisotropy by itself. An isotropic solid with nonzero Poisson contraction can therefore have a nonzero penalty. This observation supplies a second exact diagnostic that remains independent of the engineering-shear check. A small numerical difference does not establish that the two mechanical definitions have become identical.

The order of checks is consequential. A failed isotropic test should stop the material comparison because every subsequent directional value would inherit the same convention error. Passing that test permits the student to examine loading constraints, but it does not make every matrix component a tensile modulus. Only after both definitions are settled should the angular search begin. This ordering makes the exercise efficient without hiding the reasoning behind it. It also provides a diagnostic record when two groups obtain different answers: they can identify the first check at which their results diverged. An instructor can then distinguish a coding problem from a difference in the physical question before discussing material chemistry. The resulting record is concise enough to retain within an ordinary laboratory notebook and precise enough to support an individual explanation after the group activity. In particular, the first failed check should be named explicitly rather than replaced by a general statement that the program was corrected until its output appeared reasonable to the student.

The nonnegative constraint penalty follows by partitioning the stiffness matrix into the selected axial component and all remaining components. If the remaining stresses are set to zero, the remaining strains relax in response to the off-diagonal coupling. Eliminating them reduces the effective axial stiffness by a quadratic coupling term containing the inverse of the remaining stiffness block. Positive definiteness makes that reduction nonnegative. This argument explains why the comparison does not require a change in crystal orientation or a change in the material itself. It also provides a useful answer when a student asks which of two disagreeing numbers is correct: both can be correct when their boundary conditions differ. The numerical task becomes one of identifying the requested experiment rather than choosing the number that is closer to a familiar handbook value.

The averaged reference follows the arithmetic mean of the Voigt and Reuss bulk and shear bounds [27]. Let a, b, and c denote the sums of normal diagonal stiffnesses, distinct normal off-diagonal stiffnesses, and shear diagonal stiffnesses, respectively. Let x, y, and z denote the corresponding compliance sums. Then

$$K_V = \frac{a+2b}{9}, \quad G_V = \frac{a-b+3c}{15}, \quad K_R = \frac{1}{x+2y}, \quad G_R = \frac{15}{4(x-y)+3z}. \tag{5}$$

With $K_H = (K_V + K_R)/2$ and $G_H = (G_V + G_R)/2$, the scalar reference is

$$E_H = \frac{9K_HG_H}{3K_H + G_H}. \tag{6}$$

All quantities are recalculated from the same stiffness matrix and its inverse. The exercise compares this aggregate reference with single-crystal response; it does not interpret their difference as a failure of aggregate elasticity. Actual textured polycrystals require additional information about orientation distributions and intergranular interaction, as illustrated by resonant-ultrasound investigations [28]. The constrained coefficient, the directional modulus, and the aggregate reference therefore answer three different mechanical questions.

2.5. Angular search and numerical checks

A Fibonacci sphere supplies approximately equal-area loading directions [29]. For $i = 0, \ldots, N-1$, the coordinates follow $z_i = 1 - 2(i + 1/2)/N$ and $\phi_i = i\pi(3 - \sqrt{5})$, with the remaining components obtained from the unit-circle radius at z_i. The main calculation uses 4,096 directions. Three Cartesian axes, six face diagonals, and four body diagonals are added for limiting-value searches. Antipodal equivalents provide the same elastic response. Separate calculations use 1,024 and 16,384 sphere points, while retaining the same additional directions.

Signed discrepancy is $d(\mathbf{n}) = E_H/E(\mathbf{n}) - 1$, with the directional modulus in the denominator. The largest tested absolute discrepancy and the orientation fraction beyond a tolerance are

$$B_N = \max_{\mathbf{n} \in \Omega_N \cup R} |d(\mathbf{n})|, \qquad F_{20,N} = \frac{1}{N} \sum_{\mathbf{n} \in \Omega_N} \mathbb{I}\left(|d(\mathbf{n})| > 0.20\right). \tag{7}$$

Only equal-area sphere points enter the fraction. Adding selected reference directions to its denominator would give those orientations disproportionate weight. The twenty-percent tolerance is an explicit teaching choice, not a recognized uncertainty limit. Values above unity are possible for the largest discrepancy because a scalar can greatly overestimate a compliant direction. Neither quantity is a probability of specimen failure.

Uniform angular weighting also requires an explicit geometrical choice. Sampling polar angle at equal increments places too much weight near the poles if each point is counted equally. The sphere construction used here instead distributes points approximately uniformly in height and azimuth, making the direction fraction an estimate under uniform solid angle. That estimate describes neither a preferred manufacturing orientation nor a measured grain distribution. A student examining a rolled sheet or a single-crystal component would need a different orientation weighting or a specified direction. The present uniform weighting is useful because it defines an inspectable question without assuming such additional information. Students should therefore state it alongside the angular fraction, just as they state the denominator alongside a relative discrepancy. Omitting either choice leaves the numerical answer insufficiently specified.

Two independent operations check the projection. One calculates the quadratic form directly; the other constructs the physical strain tensor after multiplying stress by compliance and then evaluates the longitudinal contraction. The isotropic expression is checked against Eq. (3) over the sphere. For six teaching crystals, local minimization from fifteen distinct starting directions also checks the directional extrema. Those searches confirm the selected examples but are not presented as a proof that every extremum of every crystal has been obtained. A finite angular search can miss a narrow region even when a collection-wide count remains unchanged.

3. RESULTS AND MECHANICAL INTERPRETATION

3.1. Notation errors produce convincing but incorrect responses

The correct isotropic calculation returns 100 GPa for every tested direction, with a maximum absolute deviation of 8.53×10^{-14} GPa on the refined sphere. Doubling the shear products produces a minimum of 200/7 GPa, while suppressing them produces a maximum of 600 GPa. The doubled expression gives 34.783 GPa along the equal-x–y direction, and the omitted expression gives 266.667 GPa there. These values follow analytically from Eq. (3); their agreement with numerical evaluation is not an agreement between two independent physical experiments.

The false variation is especially instructive because its appearance is orderly. It respects the coordinate axes, changes continuously, and has symmetry-related extrema. A learner inspecting only smoothness or familiar-looking symmetry could therefore mistake it for a legitimate crystal property. At the refined angular resolution, the doubled expression exceeds a twenty-percent discrepancy over 95.85 percent of directions, while the omitted expression does so over 86.71 percent. These percentages describe deliberately incorrect mathematics applied to one artificial isotropic solid. They are kept separate from every count involving actual crystal coefficients.

Direct projection through the physical strain tensor agrees with the quadratic expression to 1.39×10^{-17} inverse gigapascals in the independent checks. The stored compliance matrices differ from freshly inverted stiffnesses by no more than 1.11×10^{-15} inverse gigapascals. This agreement verifies the convention used for the directional cal-

culation. It does not establish the physical accuracy of the electronic coefficients. Recent discussions of verification in electronic-structure methods distinguish numerical implementation checks from agreement with physical reality [30]. The laboratory makes the same distinction at a scale students can inspect directly.

3.2. Transverse constraint changes the quantity being calculated

Every crystal matrix passes the finite-value, symmetry, and positive-definiteness checks. The smallest Kelvin eigenvalue in the collection is 1.329 GPa. Across the three Cartesian axes of each structure, the constrained coefficient exceeds the freely contracting modulus by more than twenty percent in 2,556 axial cases. At least one axis meets this condition in 926 structures. The median penalty is 35.54 percent, and its ninetieth percentile is 122.88 percent. The axes share one constitutive matrix and are not treated as independent replicates in an inferential test.

For an isotropic solid, the constraint penalty can be expressed directly in terms of Poisson's ratio. It vanishes when transverse contraction is absent, increases as the coupled lateral response becomes more important, and reaches twenty percent at the Poisson ratio used for the exact check. Thus a visually spherical directional-modulus plot does not eliminate the difference between the two loading conditions. This is an especially useful counterexample to the assumption that every difference between elastic numbers must indicate anisotropy. Conversely, a small penalty on one selected axis does not establish a narrow directional range elsewhere. The student should keep the controlled mechanical quantities separate throughout the analysis. A statement about transverse constraints cannot be replaced by a statement about crystal symmetry, even when both are evaluated from the same six-by-six matrix.

Figure 3 shows why a stiffness diagonal cannot be accepted as Young's modulus simply because both have units of pressure. Every point represents one mechanical comparison at a specified axis. The equal-value line marks the special case in which suppressed coupled deformation has no effect. The second line marks the selected twenty-percent difference. For W, the axial stiffness coefficient is 509.815 GPa, whereas the corresponding freely contracting modulus is 396.140 GPa. The resulting penalty is 28.70 percent even though its directional modulus varies only modestly with orientation. Thus a small directional variation does not make the boundary-condition distinction disappear.

For the isotropic test solid, the stiffness diagonal is 120 GPa while Young's modulus remains 100 GPa. That difference is entirely consistent with isotropic elasticity and Poisson contraction. The instructor can therefore distinguish two errors that otherwise lead to similar-looking numerical disagreements. A convention error changes the predicted angular response of a single specified law. A constraint error compares two valid quantities associated with different mechanical experiments. This distinction also matters in indentation, where the indentation response need not equal a directional uniaxial modulus [31]. The laboratory does not infer an indentation modulus from its uniaxial calculations.

3.3. Directional discrepancy is widespread but not uniform

The correctly calculated averaged reference exceeds the selected discrepancy tolerance in at least one tested direction for 863 structures, corresponding to 73.1 percent of the collection. The median largest discrepancy is 32.17 percent, and its ninetieth percentile is 113.06 percent. The median ratio between the largest and smallest directional modulus is 1.6522. Those values describe a complete enumeration of the selected elastic matrices rather than a population estimate with a confidence interval. Their purpose in the laboratory is to show that an orientation statement can materially change the interpretation of a scalar property table.

The frequency changes when the teaching tolerance changes. Differences above ten, thirty, fifty, and one hundred percent occur in 1,069, 634, 365, and 149 structures, respectively. There is consequently no physical discontinuity at twenty percent. A student selecting that value must explain what approximation it permits and which application would justify it. Keeping one entry per composition gives 791 exceedances among 1,087 entries, or 72.8 percent.

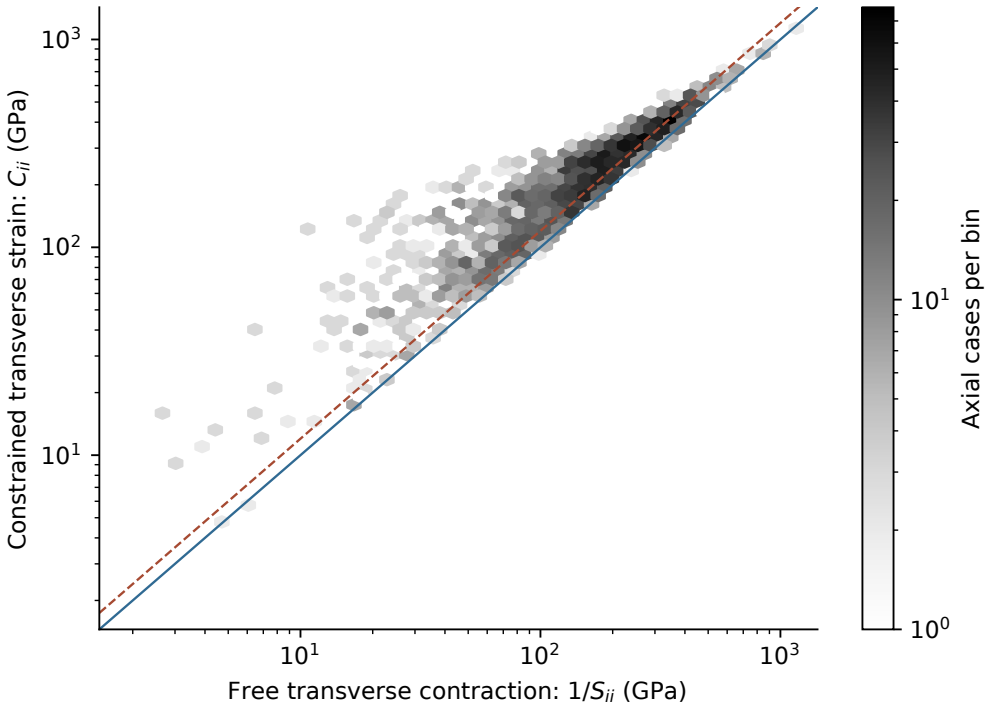


Figure 3: Constrained axial coefficients compared with moduli allowing free transverse deformation for all 3,543 Cartesian axial cases. The solid line denotes equal values; the dashed line denotes a constrained coefficient twenty percent larger. Hexagonal-bin shading represents the number of axial cases, not measurement uncertainty.

The close percentage supports the particular counting conclusion, but it does not make chemically related materials independent or establish that the collection represents every inorganic solid.

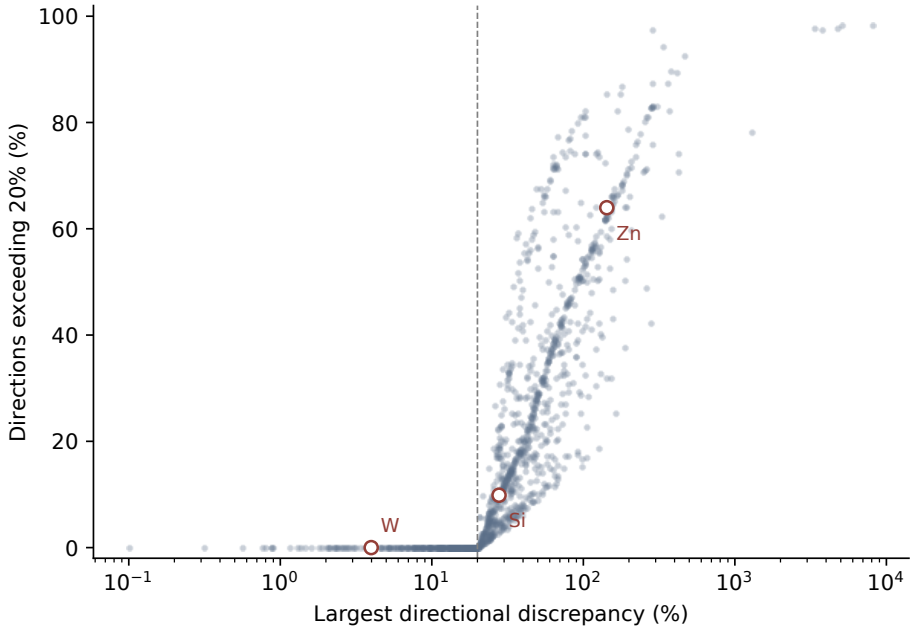


Figure 4: Limiting discrepancy and angular extent for the complete crystal collection. Horizontal position gives the largest tested discrepancy; vertical position gives the fraction of equal-area directions above twenty percent. The dashed line marks the teaching tolerance. Each point represents a crystal structure; outlined points identify W, Si, and Zn for the initial laboratory exercise.

The orientation fraction answers a different question. Its median is 12.92 percent, while 197 structures exceed the tolerance over more than half of the tested sphere. Among the structures with at least one exceedance, 219 have an orientation fraction below ten percent. A limiting direction can therefore matter even when most orientations

satisfy the approximation. Figure 4 places the two quantities together. The vertical spread at a similar largest discrepancy prevents an interpretation in which that single number also measures the breadth of the affected angular region. Directional selection requires both the intended loading orientation and a clearly stated consequence of approximation.

3.4. An equal-modulus pair gives unequal strain intervals

The CaO entry mp-2605 has an averaged reference of 180.111 GPa, whereas the BN entry mp-984 has a reference of 180.028 GPa. Their difference is only 0.0465 percent relative to the latter value. The pair was chosen after the full calculation as a deliberately contrasting teaching example: among references between 50 and 200 GPa, it is the closest match joining a largest discrepancy below eight percent to one above one hundred percent. This selection is not a random sample or a claim that the pair represents typical oxides and nitrides.

The directional ranges are 176.770–182.365 GPa for CaO and 4.748–697.861 GPa for BN on the main search. The large BN range is tied to the identified layered structure and must not be transferred to cubic BN or to a manufactured article specified only by chemical formula. Figure 5 evaluates the longitudinal strain over the entire loading sphere at one megapascal. The equal-area display makes the strong orientation dependence visible without implying that a real specimen has the shape of the projection. Atomic geometry and elastic response are related here through the actual structure and its matrix, not through a photograph of an imagined tensile sample.

At that imposed stress, the scalar approximation predicts about 5.55 microstrain for either material. The directional endpoints instead give 5.48–5.66 microstrain for CaO and 1.43–210.61 microstrain for BN. Figure 6 shows the corresponding elastic strain envelopes as stress increases from zero to one megapascal. Every line and filled interval is calculated; no marker is used to suggest a measured tensile point. Local searches give BN extrema of 4.748159 and 697.871650 GPa, confirming that the fixed angular search captures the scale of the contrast while retaining a small resolution dependence.

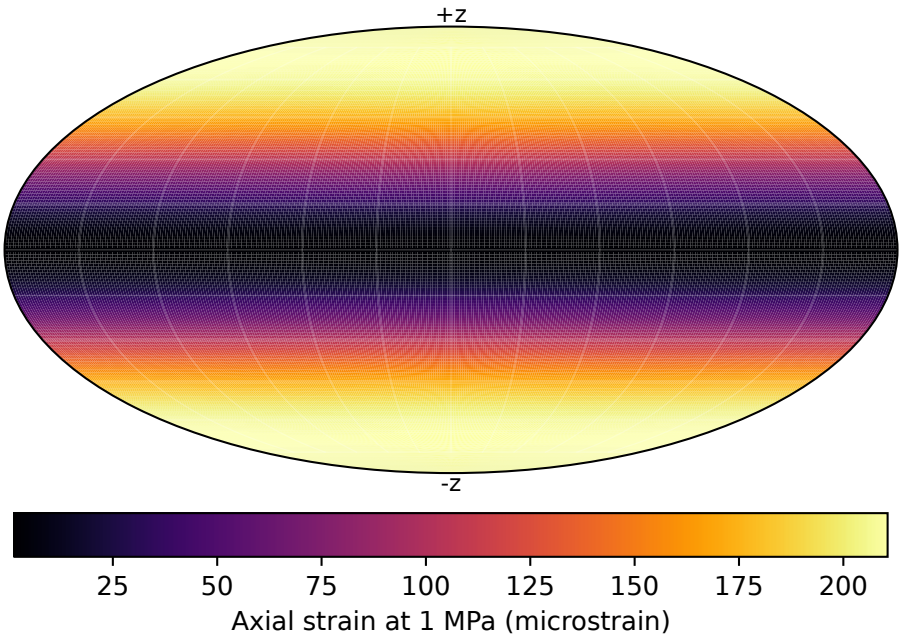


Figure 5: Calculated longitudinal strain of BN mp-984 under one megapascal uniaxial stress over the full loading sphere. The Mollweide projection preserves spherical area. Color expresses strain; projection boundaries do not represent material interfaces or physical specimen edges.

The strain envelopes also expose an asymmetry in how approximation errors should be communicated. A large scalar reference can greatly underpredict the extension of a compliant orientation under a fixed stress, while the same reference may overpredict extension in a much stiffer orientation. Calling the scalar simply conservative is therefore incomplete unless the quantity to be limited has been identified. Under force control, excessive predicted stiffness

can conceal excessive strain. Under imposed deformation, the corresponding question concerns the stress required to sustain that deformation. The laboratory remains in the infinitesimal regime, but the interpretation already depends on which variable is controlled. Students can demonstrate this understanding by stating the consequence of the approximation in words before presenting a percentage. The exercise thereby connects an abstract ratio to the mechanical quantity that would matter in a specified loading arrangement.

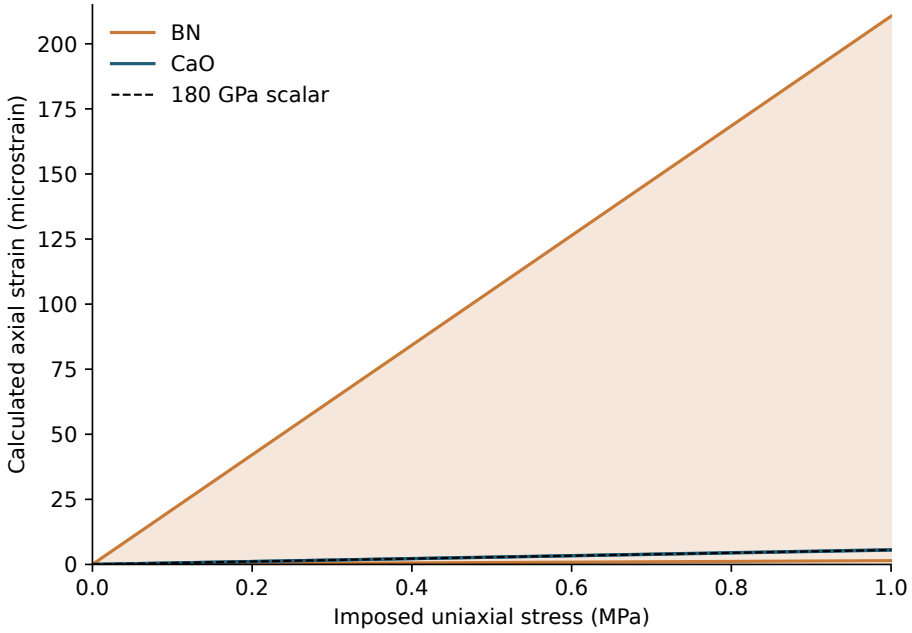


Figure 6: Elastic strain intervals implied by the directional endpoints of the CaO and BN examples. Filled regions span calculated responses at a specified stress, rather than statistical confidence limits. The dashed line uses a common scalar reference near 180 GPa, exposing the information lost when orientation is omitted.

The contrast does not establish a ranking of service performance. Strength, damage tolerance, defects, temperature, and environmental conditions are outside the present linear law. Computational studies of molecular-crystal elasticity emphasize that the chosen electronic treatment can affect elastic predictions [32], while broad code comparisons demonstrate the importance of controlling implementation differences [33]. For a layered structure, weak interlayer interactions deserve particular care. The numerical example is therefore suitable for testing interpretation of the given coefficients, but it is not a substitute for a validated engineering specification.

3.5. Angular resolution and a narrow tolerance crossing

The number of structures exceeding twenty percent is 863 at all three angular resolutions. Between the main and refined searches, the largest relative change in a minimum modulus is 0.1211 percent and that in a maximum is 0.2551 percent. Figure 7 displays the distribution of these changes. The narrow distributions and stable count support the selected numerical comparison. They do not prove exact extrema, establish a universal angular resolution, or replace an error analysis for the underlying elastic coefficients. The sphere points are not nested between resolutions, so a monotone improvement of every approximate endpoint is not assumed.

TiIr mp-1235 provides a useful exception to an overly simple interpretation of angular fractions. Its averaged reference is 216.530 GPa, and the Cartesian reference direction reaches a modulus of 270.668 GPa. The absolute discrepancy there is 20.001683 percent, just beyond the chosen tolerance. None of the equal-area sphere points exceeds the tolerance at any of the three resolutions, so the calculated orientation fraction is zero. Figure 8 resolves the narrow crossing in a plane through that reference direction. Zero sampled fraction therefore does not prove that no continuous direction exceeds the tolerance. Additional reference directions and area estimates have different roles and should remain separate.

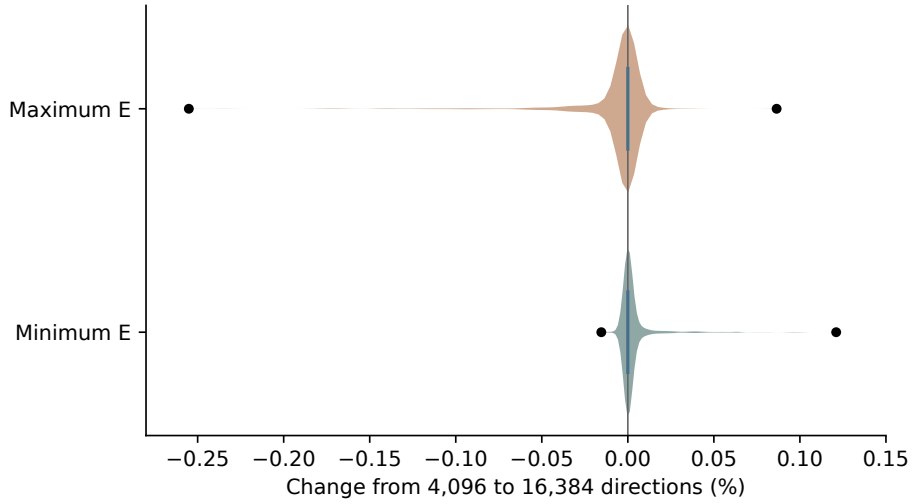


Figure 7: Changes in directional endpoints when the sphere search increases from 4,096 to 16,384 points. Violin widths indicate the distribution across crystal structures, and end dots identify extreme changes. The signed residual is $100(E_{4096}/E_{16384} - 1)$.

4. LABORATORY OPERATION AND INDIVIDUAL INTERPRETATION

4.1. Preparation and the three-hour sequence

The exercise is intended for upper-level undergraduate materials science or mechanical engineering students who have encountered stress, strain, and matrix multiplication. Its three-hour duration is a planning allocation rather than an observed completion time. An instructor prepares the elastic matrices and the isotropic check before the session. Students do not need an electronic-structure calculation or an external service account. A local numerical environment is sufficient for all mechanical operations. The computational task complements physical laboratory work but does not assess specimen preparation, extensometer alignment, machine operation, or experimental safety.

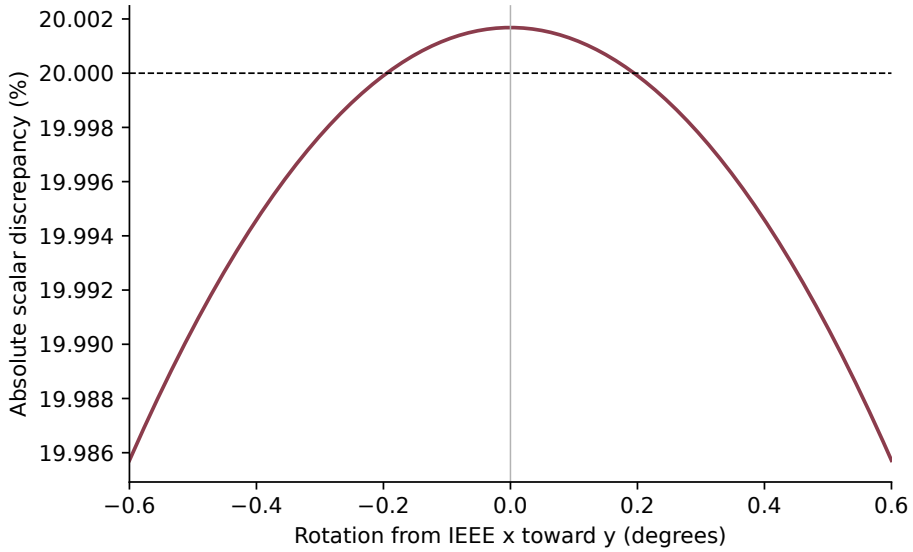


Figure 8: A narrow tolerance crossing for TiIr mp-1235 during rotation from the Cartesian x direction toward y. The curve slightly exceeds twenty percent at the axis, although the equal-area sphere searches give zero sampled angular fraction. The crossing extends approximately 0.194805° on each side of the axis in this plane.

The opening twenty minutes establish the physical question and the distinction between material identity and composition. Students identify the units, matrix order, coordinate frame, and loading assumptions. During the next thirty minutes they evaluate the isotropic solid, inspect a deliberately incorrect shear expression, and explain why coordinate-axis agreement fails to detect it. The following thirty-five minutes compare constrained coefficients with freely contracting moduli for W, Si, and Zn. The instructor asks for a statement of which strain or stress

components vanish in each calculation before accepting a numerical answer. That requirement makes mechanical interpretation visible in the student product.

The next thirty-five minutes use the CaO–BN pair. Students first receive only the two scalar references and commit to a prediction about the similarity of elastic strain. The full matrices and structural information then become available. Each student calculates at least three directions and compares them with the full angular search. The next thirty-five minutes are assigned to numerical refinement and tolerance selection, including the TiIr counterexample. The final twenty-five minutes are individual work on Ti mp-46, followed by a short written explanation of the conditions under which an averaged modulus could be adequate. This order moves from an exact algebraic test to a qualified statement about a real crystal calculation.

4.2. Answers that distinguish different errors

A successful answer to the shear task identifies the duplicated engineering factor and uses Eq. (3) to predict an off-axis result before evaluating it numerically. Simply changing a line until the expected number appears is incomplete. The student should explain why the error vanishes on the axes and why a smooth surface does not establish correctness. For the transverse-constraint task, the answer must specify the suppressed components. Calling a discrepancy an uncertainty is inappropriate because both quantities are defined exactly by the selected matrix under different conditions. These distinctions give the instructor observable reasoning to evaluate alongside numerical output.

The material-pair task requires a statement narrower than saying that the two materials have the same stiffness or that one is better. A defensible conclusion identifies nearly equal aggregate references together with substantially different directional responses in the stated structures. It also distinguishes the sampled strain range from uncertainty in a measurement. The Ti transfer question provides an individual check: the averaged reference is 123.148 GPa, the main directional range is 114.851–146.366 GPa, and the largest discrepancy is 15.86 percent. No tested direction breaches twenty percent, but the nonzero range still excludes exact isotropy. A correct tolerance decision and an incorrect symmetry claim should not be scored as equivalent understanding.

4.3. Assessment evidence and classroom evaluation

The instructor can judge whether the student has demonstrated four distinct decisions: correct shear mapping, correct loading constraints, an explicitly defined discrepancy, and a physically qualified final statement. Each decision can be marked demonstrated, partially demonstrated, or absent. No percentage weighting is essential to the exercise. The supporting evidence is a short derivation, numerical output tied to a material identifier, and an interpretation written without relying on the instructor's preferred wording. Group discussion can assist debugging, but the transfer explanation should be completed individually if it is used to judge individual understanding.

Established uncertainty assessments illustrate the care needed before treating such an explanation as a validated instrument. Development of SPRUCE linked questions to particular measurement-uncertainty objectives [34], and subsequent work examined its validity and reliability [35]. Those properties cannot be assigned to the present transfer task without additional evidence. A classroom study would need a defined cohort, explicit instruction, a scoring procedure, missing-response accounting, and independent checks of scoring consistency. The present paper contains none of those observations and therefore makes no numerical claim about learning improvement, satisfaction, confidence, or course completion.

5. DISCUSSION

The mechanical results support a specific kind of laboratory reasoning. A learner can encounter three disagreements between apparently reasonable elastic numbers and determine that they have different explanations. The shear-factor disagreement is a mathematical implementation error. The stiffness-diagonal disagreement is a change in transverse boundary conditions. The aggregate-reference disagreement is a change in physical scale and orientation description. The same unit, a smooth curve, or a familiar material name cannot resolve those distinctions. Requiring

the student to diagnose them creates a more precise task than asking for a single elastic constant and comparing it with a table.

The exact isotropic check is central because it prevents an instructional circularity. If the student verifies a directional implementation only against a plot made by the same implementation, agreement has little diagnostic value. Eq. (3) supplies a complete angular result that is independent of the numerical projection. It also predicts failures that a small set of coordinate-axis tests will miss. The incorrect expression produces a large and orderly apparent anisotropy, making the error plausible enough to require explanation. Its inclusion should be identified openly as intentional; otherwise an instructor could inadvertently leave students with an incorrect formula that survives beyond the laboratory.

The error diagnosis should remain useful when the numerical environment changes. The same distinction can be tested in a spreadsheet, a short script, or a larger simulation package because its reference is a constitutive identity rather than a particular software interface. An instructor can ask students to exchange only their loading direction and predicted modulus, then explain a disagreement by checking units, shear convention, and controlled components in that order. This exchange does not require a new assessment instrument and should not be interpreted as evidence that peer discussion is effective in every class. Its immediate value is practical: the relevant checks are specific enough to apply to an individual result. The explanation can then be evaluated without rewarding the visual polish of a plot or the familiarity of the software used to produce it.

The boundary-condition comparison adds a physical distinction that the isotropic check alone cannot provide. A well-coded calculation may still answer the wrong question. The large number of constrained penalties above twenty percent demonstrates that this is not an isolated issue restricted to a single example. Nevertheless, the counts are not evidence that particular publications or students made the error. They quantify what would happen if one quantity were substituted for another in the present matrices. The laboratory therefore asks students to state the controlled components before comparing numbers, rather than diagnose correctness from numerical closeness after the calculation.

Worst-direction discrepancy and angular extent also require separate interpretation. An engineering component with a known loading axis may be sensitive to a narrow unfavorable direction, whereas a uniform angular average answers a different question. The TiIr example shows that a finite estimate of zero angular fraction can coexist with a verified reference-direction crossing. That is a useful numerical lesson because the collection-wide count remains stable under refinement. A stable headline count can therefore coexist with unresolved local angular detail. Students should be encouraged to report both what the refinement demonstrates and what it leaves undecided, especially when a decision lies very close to a chosen tolerance.

Uncertainty in the material coefficients remains distinct from all these numerical checks. The reciprocal-space categories describe calculation choices, but they do not provide repeated estimates under every possible setting. Full elastic calculations can be sensitive to the electronic approximation, structural state, magnetism, and interactions between layers. Finite-temperature elastic calculations further show that lattice parameters and stiffness can change together [36]. Increasing the number of loading directions does not correct any of those physical omissions. The appropriate conclusion is that the angular evaluation has become better resolved for a fixed matrix, not that the matrix has become an exact description of a manufactured material.

The distinction between more numerical points and better physical information parallels questions examined in research on uncertainty reasoning. Advanced students can interpret changes in the number or quality of measurements in ways that depend on the particular question [37]. A useful classroom discussion can therefore compare three actions: adding loading directions, improving the electronic calculation, and obtaining independent physical measurements. Only the first is performed here. Their effects differ, so replacing them with a general request for more data would obscure the actual decision. The exercise keeps the independent variable and the purpose of each operation explicit.

The laboratory should also avoid equating access to computations with participation in open research. A prepared activity can have predetermined reference answers and still teach valuable diagnostic reasoning. Computational undergraduate research has additional requirements when students contribute to unresolved scientific questions [3]. Here the expected elastic answers are supplied for instruction, while a future educational evaluation would investigate a separate unresolved question about student reasoning. That separation prevents a numerical materials exercise from being presented as an empirical comparison of teaching methods. Its educational value must be tested rather than inferred from the sophistication of the graphics.

Several practical choices can help maintain that distinction. The prediction preceding the CaO–BN reveal gives students a statement that they can reconsider using calculations. The intentionally faulty isotropic expression makes successful debugging depend on reasoning about notation. The individual Ti problem checks whether a learner transfers the tolerance distinction without repeating the paired example. These choices are specific teaching arrangements, not established causes of improved performance. Studies of laboratory-course transformation show that aligned instruction can change how students articulate uncertainty [38], but the extent of change depends on actual instruction and assessment. The present paper supplies the task and reference answers needed to examine such change directly.

The reference literature also places limits on the scientific novelty. Directional elastic extrema, anisotropy visualization, and aggregate averaging are established topics, and extensive software already evaluates them. The present work does not replace those methods or introduce a new constitutive law. Its contribution lies in joining exact convention diagnostics, loading-condition distinctions, and a complete instructional exercise with actual crystal calculations. This positioning is narrower than a claim of discovering that averaged stiffness can hide directional compliance. It is also more useful for a laboratory-module article because it specifies what a learner does, what a correct answer contains, and which mistaken explanations can be distinguished.

Connection to a physical laboratory would require an additional experimental design. A suitable extension could compare orientations in a material whose symmetry, texture, dimensions, and temperature are independently characterized. The loading machine would need to distinguish axial displacement from apparatus compliance, while transverse measurements would establish whether the intended mechanical constraint had actually been achieved. Those requirements cannot be satisfied by adding a realistic-looking specimen image to a numerical paper. They require real specimens, instrument records, and documented observations. The present visual material therefore remains confined to atomic coordinates and computed response. This limit preserves the distinction that students are being asked to learn: a calculation can be correct for its assumptions without supplying the observations needed to validate those assumptions in a particular manufactured specimen.

Further work can evaluate how different levels of preparation affect completion and interpretation. Students with limited linear algebra may need an initial exercise that converts one engineering-strain vector into a physical tensor. Students comfortable with tensors can instead test rotational invariance or examine the Schur-complement argument. Neither adaptation requires changing the physical distinctions. A classroom investigation should preserve separate outcomes for notation, boundary conditions, tolerance reasoning, and claims about uncertainty, since success in one does not establish success in another. Instructional decisions should then follow the observed student work rather than an assumed benefit of computational presentation.

6. CONCLUSION

A crystal-elasticity laboratory can make the interpretation of a material property as visible as the calculation itself. An exact isotropic check reveals large false directional variations caused by incorrect shear mapping. A separate analysis shows that constrained stiffness diagonals and freely contracting tensile moduli differ substantially for many crystal axes. Correct directional calculations then connect averaged references with loading-dependent strain, angular extent, and finite-resolution limits. The CaO–BN pair supplies a strong contrast, while Ti and TiIr provide different transfer questions about tolerance and angular sampling. The resulting exercise has complete numerical

answers and eight scientific visualizations. Its effect on student learning remains to be established through classroom evidence.

Conflict of Interests

The author declares that they have no conflicts of interest.

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Data Availability

The data supporting the findings of this study are available from the author upon reasonable request.

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