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Learning to Defend Material-Property Claims through Open Elasticity Resources

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ABSTRACT

Elasticity resources allow students to calculate a material property quickly, yet a correct numerical answer can conceal an incorrect physical interpretation. This study examines the explanation of structure, directional response, aggregate averaging, and the limits of inference. The appraisal combines inspection of resource capabilities with calculations for crystal records. Every stiffness matrix is positive definite, and the largest stiffness–compliance inverse residual is approximately 8.0×10^{-13}. These internal checks establish algebraic consistency without establishing measurement accuracy. Shear averaging bounds differ by more than one tenth of their Hill mean in 37.76% of records; the corresponding proportion for bulk modulus is 4.91%. Giving each composition equal weight changes these proportions only modestly. Directional calculations expose additional distinctions that scalar averages cannot express: the largest to smallest Young-modulus ratio is about eight for the selected copper record, whereas two carbon structures with the same space-group number have ratios near 132 and 1.16. The resource collection therefore supports demanding explanation tasks when identifiers, tensor conventions, units, and calculation conditions remain visible. Matminer assists numerical inspection, while ELATE supports interpretation of directional elasticity; neither capability establishes educational effectiveness by itself. The study identifies adoption requirements and assessable student work without assigning untested learning gains. Its central judgment is that useful educational access preserves the information needed to defend a material-property claim, rather than merely supplying an attractive display or a convenient average.

KEYWORDS

materials education; education resources; elastic constants; crystal structure; directional stiffness; data literacy

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1. INTRODUCTION

A learner who encounters a tabulated elastic modulus faces a scientific question before performing any arithmetic: what physical object and loading assumption does the number describe? A crystal, an ideal aggregate, and a manufactured component do not have interchangeable elastic descriptions. Likewise, a calculated constant at a relaxed reference state does not automatically represent a measurement at room temperature. Open materials resources make these distinctions unusually teachable because a student can move between atomic coordinates, stiffness coefficients, compliance, and scalar summaries. Their educational merit depends on whether that movement

remains understandable. A resource that conceals the meaning of its variables can simplify calculation while making the resulting explanation less defensible.

Recent discussion of undergraduate materials education emphasizes active engagement, realistic disciplinary problems, and accessible entry points for students with different preparation [1]. Materials-informatics workshops connect scientific questions with computational practice, including the interpretation of numerical material descriptions [2]. A polymer-science workshop similarly demonstrates how undergraduate teaching can introduce modern information analysis through subject-specific activities [3]. These contributions support bringing authentic materials information into teaching. They do not establish that every available collection or software interface is ready for unaided classroom use. Choosing a resource still requires attention to prerequisite knowledge, scientific assumptions, and the evidence through which an instructor can judge students' reasoning.

Working with open numerical information can join disciplinary learning with critical interpretation, but the activity requires deliberate support for both subject knowledge and digital practice [4]. Studys of data-literacy education identify variation in the competencies taught and the methods used to develop them [5]. Assessment research further distinguishes competence definitions, response formats, reliability, and validity [6]. Consequently, a materials exercise should not treat successful software execution as a complete demonstration of understanding. Explaining why a quantity has particular units, why a formula identifies more than one structure, and why an average differs from a directional property provides more specific evidence of what the learner knows.

Science-focused assessment work connects data interpretation with the construction and evaluation of explanations [7]. Undergraduate discussion also emphasizes the distinction between inference and prediction, the possibility of misleading presentations, and responsible communication [8]. Elasticity offers concrete versions of these issues. A stiffness matrix may be internally consistent but physically inaccurate. Many crystal records may describe relatively few compositions. A smooth directional surface may communicate anisotropy clearly while encouraging unwarranted confidence in the underlying calculation. These are not merely technical obstacles to remove before teaching begins; they are substantive matters that a well-chosen resource can help students investigate.

The literature on open educational resources provides a necessary caution about equating availability with achievement. Studies of student outcomes and perceptions cover diverse settings and instructional arrangements [9]. A meta-analysis of open-textbook adoption found no overall difference in learning performance between open and commercial textbooks across its included comparisons [10]. More recent analyses examine broader educational practices and student achievement rather than assuming that the access model determines the outcome [11, 12]. These findings justify examining resources carefully while withholding a causal judgment about learning until an appropriate educational comparison has been conducted. A scientific resource can be promising without yet having demonstrated instructional superiority.

Affordability, perceived quality, technical support, and institutional conditions influence adoption alongside educational outcomes [13]. Analysis of open educational practices also indicates that the way resources are used matters, especially when students mainly receive information rather than interrogate it [14]. Faculty perceptions and qualitative accounts of resource assessment show why teachers need material that fits their instructional purposes [15, 16]. For elasticity, such fit is specific. A useful activity might require a student to distinguish elastic stability from phase stability, justify a homogenization assumption, or explain an apparent inconsistency between two summaries. General enthusiasm for openness cannot answer these instructional questions.

Materials research already provides substantial technical support for this kind of inquiry. Open computational infrastructures organize electronic-structure calculations and their associated descriptions, making relationships between quantities available for inspection [17, 18]. Materials Cloud connects computational results with the operations that produced them, while JARVIS combines several routes to materials-property calculation and analysis [19, 20]. These developments create educational opportunities, but their scientific purpose is broader than classroom instruction. An instructor must still determine which information students should inspect, which operations they should perform independently, and which claims require evidence that the selected resource cannot supply.

The elastic-constant collection considered here is particularly useful because it retains more than final scalar answers. It contains structural descriptions, material identifiers, stiffness and compliance arrays, aggregate moduli, and calculation settings [21, 22]. Matminer provides a route to manipulating materials information within numerical workflows, while ELATE supports analysis and visualization of elastic anisotropy [23, 24]. Together, these resources permit a close examination of how scientific meaning changes when a tensor is reduced to a few moduli or converted into a visual surface. Their value can therefore be judged through explicit tasks rather than through an unsupported ranking of attractive interfaces.

The question guiding this study is how well these resources preserve the information required for a defensible explanation of elastic response. The analysis examines identity, unit conventions, internal mathematical relationships, averaging spread, directional variation, and the treatment of repeated compositions. These aspects are connected to instructional demands rather than combined into an arbitrary overall score. Numerical checks establish what the available material permits a learner to verify. Literature on teaching and assessment establishes why such verification should be distinguished from evidence of learning. The resulting judgment concerns suitability for specified educational work, with transparent boundaries around what the calculations and resource descriptions can establish.

An explanation-centered study differs from a catalogue of available features. The presence of a rotation control, a calculator, or a large property table says little about whether a student can justify a conclusion. A feature becomes educationally relevant when it enables a specific intellectual action, such as testing a unit convention or comparing two structures without losing their identities. Conversely, an omitted field matters when its absence prevents an intended explanation. This approach keeps the appraisal close to the discipline while avoiding a claim that a resource's technical sophistication predicts its instructional value. It also makes the recommendations open to inspection and disagreement.

Elasticity is particularly appropriate for this purpose because several sources of ambiguity are mathematically accessible. Students can inspect an inverse, distinguish a directional function from a scalar, and examine how an averaging assumption changes a value without needing to complete a demanding electronic-structure calculation. The available numerical relationships are rich enough to expose errors of interpretation even when arithmetic is correct. That combination permits an educational study with substantive calculations while keeping its claim separate from a trial of teaching effectiveness. The distinction matters for institutions choosing resources under limited computing capacity, where a manageable exercise must still preserve scientific meaning.

A further concern is the transfer of confidence from research software to a learner's answer. A respected scientific tool may correctly perform an operation whose meaning the user has misunderstood. The resulting figure can look authoritative even when the chosen input, convention, or inference is inappropriate. Resource appraisal should therefore examine how a student can question the output as well as obtain it. The present study uses elasticity to make that requirement concrete, connecting structural identity and mathematical checking with the language of a defensible conclusion. The aim is an inspectable educational judgment, rather than an assertion that access alone transforms learning.

2. STUDY DESIGN AND MATHEMATICAL PROCEDURE

2.1. Selection and Scope of the Appraisal

The elastic properties of inorganic crystalline materials were investigated using first-principles calculations, providing a comprehensive foundation for understanding the relationships between crystal structure, elastic stiffness, compliance, and mechanical response [21, 22]. The investigation considered crystallographic information, atomic positions, elastic stiffness and compliance tensors, and related mechanical properties, enabling quantitative comparisons across different material representations. Particular attention was given to the consistency of calculated elastic quantities, their physical interpretation, and the computational conditions required to characterize mechanical behavior. These findings established a valuable basis for examining how crystallographic geometry and tensor-based descriptions contribute to understanding the elastic response of inorganic materials.

The present appraisal focuses on the scientific and educational suitability of elastic-property information for materials science instruction. Particular emphasis is placed on the mathematical relationships between stiffness and compliance tensors, the interpretation of elastic constants, and the connection between atomic arrangements and macroscopic mechanical behavior. The analysis considers the completeness of material descriptions, consistency of physical units, clarity of computational conventions, and accessibility of numerical information. These considerations support the development of instructional activities in which students can examine relationships among elastic quantities, verify mathematical consistency, and interpret the physical significance of crystallographic and mechanical properties.

Scientific interpretability, inspectability, computational requirements, and suitability for educational assessment provide the principal criteria for evaluating instructional applications. Scientific interpretability concerns the physical meaning of material properties, their units, reference conditions, and mathematical conventions. Inspectability addresses the extent to which numerical results can be examined, reproduced, and connected to underlying crystallographic information. Computational requirements concern the technical preparation and analytical procedures necessary to perform meaningful calculations. Educational suitability emphasizes opportunities for students to demonstrate conceptual understanding, quantitative reasoning, and the ability to connect mathematical representations with physical material behavior. The corresponding evaluation criteria are presented in Table 1.

Table 1: Evidence tests used to judge suitability for specified educational tasks.

Criterion	Evidence available for inspection	Instructional consequence
Scientific interpretability	Material identity, units, reference state, and tensor convention	A learner can specify the object and quantity before calculating.
Inspectability	Coefficient arrays, structural positions, aggregate bounds, and identifiers	A conclusion can be checked against particular numerical information.
Execution burden	Required operations, software preparation, and retained variables	Work can be matched to mechanics and programming preparation.
Assessed explanation	Calculation, justification of assumptions, and limits of inference	A correct answer is distinguished from a defensible explanation.
Access alternatives	Numerical values and text accompanying spatial graphics	Essential meaning need not depend on colour or rotation controls.

Related research on materials education, open educational resources, computational learning, and scientific data literacy provides additional context for interpreting these instructional opportunities. Studies of educational resource adoption, student achievement, and assessment practices highlight the importance of connecting technical information with clearly defined learning objectives and observable reasoning processes. Within materials science education, the integration of crystallographic descriptions, elastic-property calculations, and comparative analysis can support the development of analytical skills and a deeper understanding of structure–property relationships. However, the educational effectiveness of these applications requires independent classroom evaluation, since the availability of scientifically reliable material information does not, by itself, establish improvements in student learning.

2.2. Physical conditions and tensor convention

The crystal constants describe a relaxed, static reference state at zero temperature and zero pressure. The electronic-structure procedure uses the projector augmented-wave method in VASP, principally with PBE, together with selected oxide treatments incorporating a Hubbard correction. The nominal plane-wave cutoff is 700 eV. The initial strain amplitudes are -1%, -0.5%, $+0.5\%$, and $+1\%$, with additional checks where convergence or the linear fitting range requires attention [21]. These are essential conditions for interpretation, although the collection does not contain complete strain–stress trajectories, finite-temperature series, or individual uncertainty intervals. Stiffness and elastic moduli are expressed in GPa; compliance is expressed in inverse GPa.

The stiffness matrix C relates the six-component stress vector to an engineering-strain vector (Eq. (1)), whose shear entries are twice the corresponding tensor strains. The index order is $11, 22, 33, 23, 13, 12$, and the compliance matrix is $S = C^{-1}$. This convention controls the factors that appear when aggregate or directional properties are

calculated. An unnoticed substitution of tensor shear strain for engineering shear strain changes the calculation without necessarily producing an obviously invalid matrix. The unstressed stiffness was checked for symmetry and positive definiteness, consistent with the distinction between a stable elastic quadratic form and broader questions of structural stability [25]. The stiffness–compliance product was examined element by element.

$$\begin{cases} \boldsymbol{\sigma}_{\mathrm{V}} = C\boldsymbol{\varepsilon}_{\mathrm{V}}, \qquad S = C^{-1}, \\ \boldsymbol{\varepsilon}_{\mathrm{V}} = (\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{33}, 2\varepsilon_{23}, 2\varepsilon_{13}, 2\varepsilon_{12})^{\mathsf{T}}. \end{cases} \tag{1}$$

2.3. Aggregate calculations and composition weighting

For a compact statement of the aggregate calculations, let $A_C = C_{11} + C_{22} + C_{33}$, $B_C = C_{12} + C_{13} + C_{23}$, and $D_C = C_{44} + C_{55} + C_{66}$, with corresponding definitions for compliance. The Voigt and Reuss quantities were calculated using Eq. (2), and compared with the scalar entries retained for each crystal. Hill means were checked separately. The universal anisotropy index and isotropic Poisson ratio were also calculated from the aggregate quantities. These operations share mathematical ingredients and are therefore consistency checks rather than independent evidence that a constant agrees with physical measurements. Similar distinctions are relevant when elastic-analysis software supplies several derived quantities from a single coefficient matrix [26, 27].

$$\begin{cases} K_{\mathrm{V}} = (A_C + 2B_C)/9, \\ K_{\mathrm{R}} = (A_S + 2B_S)^{-1}, \\ G_{\mathrm{V}} = (A_C - B_C + 3D_C)/15, \\ G_{\mathrm{R}} = 15\,[4(A_S - B_S) + 3D_S]^{-1}. \end{cases} \tag{2}$$

Relative separation of the two averaging bounds was evaluated through Eq. (3). The thresholds used for displaying that separation are descriptive choices, not engineering acceptance rules. The arithmetic retains zero widths; only the logarithmic display places very small bulk widths at a lower plotting limit. Every crystal record was retained. For composition-sensitive summaries, atomic occupancies were reduced to integer element ratios, and records sharing that ratio were grouped. The composition-weighted percentage (Eq. (5)) averages the threshold indicator within each group and then gives every composition equal weight. This changes the counting unit while preserving legitimate structural alternatives. It does not establish independence among related compounds or turn a selected collection into a representative materials survey.

$$M_{\mathrm{H}} = \frac{M_{\mathrm{V}} + M_{\mathrm{R}}}{2}, \qquad \Delta_M = \frac{M_{\mathrm{V}} - M_{\mathrm{R}}}{M_{\mathrm{H}}}, \qquad M \in \{K, G\}. \tag{3}$$

$$A^{\mathrm{U}} = 5\frac{G_{\mathrm{V}}}{G_{\mathrm{R}}} + \frac{K_{\mathrm{V}}}{K_{\mathrm{R}}} - 6, \qquad \nu_{\mathrm{H}} = \frac{3K_{\mathrm{H}} - 2G_{\mathrm{H}}}{6K_{\mathrm{H}} + 2G_{\mathrm{H}}}. \tag{4}$$

$$p_{\mathrm{c}}(t) = \frac{100}{N_{\mathrm{c}}} \sum_{i=1}^{N_{\mathrm{c}}} \frac{1}{n_i} \sum_{j=1}^{n_i} \mathbb{1}(\Delta_{ij} > t). \tag{5}$$

2.4. Directional stiffness and structural geometry

Directional Young modulus was calculated directly from compliance rather than inferred from aggregate shear spread. For a unit loading vector n, the contracted vector in Eq. (6) contains no additional factor of two in its shear entries, because it is paired with engineering compliance. This is consistent with applying uniaxial stress and projecting the resulting strain onto the same direction. A 91×181 angular grid supplied eight candidates at

each extreme. Together with coordinate-axis directions, these initialized BFGS refinements allowing five hundred iterations; the smallest and largest values were retained. Values in the figures are independent calculations from the retained matrices, not a test of ELATE execution or a new measurement of anisotropy.

$$E(n)^{-1} = q(n)^{\mathsf{T}} S q(n), \qquad q(n) = (n_x^2, n_y^2, n_z^2, n_y n_z, n_x n_z, n_x n_y)^{\mathsf{T}}, \qquad \|n\| = 1. \tag{6}$$

Carbon structures were chosen to examine the information omitted by a formula and space-group number. Local coordination was determined by counting periodic neighbours within a declared distance of 1.8 Å, with adjacent cells included. This distance rule describes geometric proximity; it is not an electronic bonding calculation or a measurement of bond strength. Structural images display expanded atomic coordinates with connections determined by the same distance rule. Directional plots use the stated IEEE tensor axes, whereas structural renderings retain their crystallographic coordinates. The figures are calculated representations of atomic arrangements and elastic response. They are not photographs, microscopy images, or records of fabricated specimens.

For the numerical checks, absolute residuals retain the units of the quantity being compared, whereas the stiffness–compliance product and normalized spreads are dimensionless. Relative residuals were calculated against the retained scalar value only where its denominator is nonzero. Residual magnitudes are presented directly rather than converted into a pass rate by choosing a tolerance after inspection. Structural and directional examples were selected for their diagnostic properties, and their selection rules are stated alongside the corresponding discussion. These controls keep visual prominence separate from statistical representativeness and prevent a highly legible example from becoming an unsupported claim about every material.

3. TEACHING RESOURCES AND REPRESENTATION CHOICES

The collection's main educational strength is the coexistence of related representations. An instructor can ask a learner to explain why a material identifier matters, inspect an atomic arrangement, calculate a modulus from a coefficient matrix, and compare the answer with an aggregate summary. This allows the scientific question to precede the software command. It also exposes omissions: complete numerical fields do not provide a full record of every electronic-structure operation, repeated specimen measurements, or uncertainty intervals. The FAIR principles address discoverability and interpretability of research information, but an educational task must additionally specify which reasoning the learner should make explicit [28]. A convenient property table alone does not meet that requirement.

Matminer supports tabular manipulation and materials-specific numerical analysis [23]. Its educational role is strongest when students inspect the returned variables before computing summaries. In the inspected elastic-constant loader, the default metadata option omits the structural text descriptions and the reciprocal-space sampling setting. A general table reader can preserve every field, while the convenience function requires an explicit choice to retain them. The study therefore treats column visibility as an instructional decision. Successful loading demonstrates access to values; it does not demonstrate that a learner understands their calculation conditions. This distinction is especially important when a brief notebook conceals preparatory decisions that an experienced instructor takes for granted.

ELATE offers a complementary opportunity to interrogate directional elasticity through a matrix-based interface and graphical output [24]. Its display can connect an anisotropic coefficient array to a spatial response that is difficult to infer by inspecting numbers alone. Nevertheless, a student needs to distinguish a directional function from an isotropic aggregate estimate before interpreting the shape. A surface radius that represents Young modulus cannot be read as a fracture load, yield strength, or hardness. A change of tensor axes also changes the displayed orientation without changing the physical material. The interface is consequently most useful when accompanied by a declared loading direction and a written explanation of the quantity being visualized.

MechElastic and ElATools illustrate the wider range of quantities that can be calculated from elastic coefficients [26, 27]. Their relevance to this study is not a claim that their execution was compared with ELATE. Rather, their scientific descriptions clarify how one matrix can generate many apparently different answers. An instructor should avoid treating this abundance as a sequence of independent confirmations. Aggregate moduli, anisotropy indices, and directional extrema are related transformations of a common elastic description. Table 2 separates the educational roles of the collection, numerical access, and directional visualization, while identifying the preparation each role requires. No software receives an overall superiority score.

Technical openness also matters to what students can investigate. A resource that can only be viewed offers a different educational opportunity from one whose quantities can be inspected and recalculated. Study of open educational resources distinguish these technical possibilities from permission to access material [29]. Practical accounts of adoption emphasize the value of experience, support, and teaching context [16, 30]. For the present subject, technical openness means that a student can inspect the coefficient matrix, keep the material identifier attached to the result, and explain an operation without relying entirely on a hidden interface. It does not require every class to install an electronic-structure code or perform expensive calculations.

Resource selection should also distinguish intended scientific functionality from tested learner usability. Instructors' beliefs about open resources vary across perceived professional value, instructional value, and opportunities for student participation [31]. The appropriate response is to state what the learner will actually do with the elasticity resource. A calculator task, a structural comparison, and a critique of a misleading property claim impose different demands. The same software may support all three while requiring different preparation. The study accordingly judges fit for specified activities instead of attributing a general educational benefit to a resource's reputation, computational sophistication, or number of available outputs.

Accessibility requires an equally specific treatment. Evidence from online courses shows that widespread availability and an accessibility policy can coexist with barriers encountered by users with disabilities [32]. That evidence concerns those courses, not the elasticity tools examined here, and cannot be transferred as an accessibility rating. It does justify requiring numerical alternatives to interactive surfaces, readable descriptions of loading direction, and figures whose interpretation does not depend on colour alone. Keyboard access, assistive-technology compatibility, and the clarity of an instructor's alternative explanations would need direct evaluation with the intended users. They are adoption requirements in this study, not tested properties of the three resources.

Table 2: Task-specific appraisal of the connected resources.

Resource	Scientific work it supports	Support required for educational use
Elastic-constant collection	Identify a crystal; inspect structure; compare stiffness, compliance, and aggregate quantities	Retain identity, units, reference conditions, and the distinction between records and specimens.
Matminer	Manipulate numerical descriptions and inspect the variables passed to an analysis	Check the returned fields; choose metadata retention deliberately; make preparatory decisions visible.
ELATE	Examine directional elastic response for a specified stiffness matrix	Declare units and orientation; distinguish a directional function from an aggregate property; provide numerical alternatives.

4. RESULTS AND DISCUSSION

4.1. Crystal identity survives only if structure remains visible

The examined material descriptions contain distinct identifiers for every record and complete entries for all twenty retained fields. Composition grouping gives 1,007 compositions represented once, 69 represented twice, nine represented three times, and one each represented four and five times. Thus, repeated chemistry is a meaningful feature of the collection rather than a reason to delete records automatically. The grouping also changes the interpretation of sample size. Counting identifiers answers how many crystal descriptions were inspected; counting compositions

answers how many reduced chemical ratios occur. Neither count is the number of independent laboratory specimens or the number of participants in an educational evaluation.

The two carbon structures in Figure 1 demonstrate why this distinction matters physically. Their common formula and space-group number do not specify identical atomic geometry. Under the stated distance rule, every atom in the first arrangement has three neighbours, with separations close to 1.424 Å. Every atom in the second has four neighbours, with separations approximately between 1.544 and 1.569 Å. The calculated images preserve those positional differences without assigning an experimentally verified phase name. They make a useful demand on explanation: a learner must connect the particular structural description to the elastic calculation rather than assuming that a chemical label determines a unique mechanical response.

This comparison should not be reduced to a visual recognition exercise. Seeing a layered arrangement is not sufficient to determine its elastic constants, and the neighbour cutoff does not establish electronic bond character. The scientific explanation requires the structural coordinates and the compliance calculation together. The images support checking whether two records describe the same arrangement; the elastic quantities support checking how their responses differ. Materials information infrastructures emphasize the importance of retaining such relationships between descriptive objects and calculations [18, 19, 33]. In teaching, the equivalent requirement is that a student's conclusion retain enough identity information for another reader to establish which crystal was actually considered.



(a) Carbon record mp-48.

(b) Carbon record mp-611426.

Figure 1: Atomic arrangements that share a formula and space-group number but retain different local geometries. Both panels are crystallographic renderings from atomic coordinates, with proximity connections below 1.8 Å and a $3 \times 3 \times 1$ cell expansion. Periodic coordination is three in (a) and four in (b). The connections indicate the stated geometric rule, not measured bond strength.

4.2. Internal consistency and physical accuracy answer different questions

Every retained stiffness matrix is positive definite in the unstressed reference description. The smallest matrix eigenvalue across the collection is about 0.667 GPa, and symmetry differences are close to numerical precision. The largest elementwise difference between the stiffness–compliance product and the identity matrix is approximately 8.0×10^{-13}. These observations establish a coherent numerical relationship between two stored descriptions. They do not show that either description matches a measured crystal, that every material is thermodynamically stable, or that the same response persists at another temperature. An educational explanation should state which of these questions has actually been checked instead of treating a successful matrix operation as universal validation.

The scalar comparisons offer a particularly instructive counterpoint. Differences between recalculated and retained Voigt quantities remain below approximately one thousandth of a gigapascal, whereas the largest Reuss shear difference is about 0.0172 GPa. The corresponding maximum relative difference is small, below 0.066%, but it is much larger than the inverse residual. Figure 2 displays the six records with the largest absolute scalar discrepancies, selected by the maximum difference across the four aggregate bounds. The selection rule identifies diagnostic cases rather than a representative subset. Table 3 gives the collection-wide checks without interpreting those small discrepancies as measured errors.

Mixed numerical precision is consistent with the scalar differences, especially where compliance contraction involves cancellation, but the retained values do not reveal every unrounded intermediate. The appropriate conclusion is therefore limited: the identities agree closely, with distinguishable numerical residuals across different transformations. A learner who observes close agreement should still explain the tolerance and the quantities being compared. Conversely, a small nonzero residual should not automatically be classified as a defective material record. The precision map is useful because it turns a numerical imperfection into a question about calculation and interpretation. It encourages students to evaluate the significance of a discrepancy rather than hide it or exaggerate it.

The residual comparison can also expose a difference between a check that is easy to automate and one that is scientifically informative. Multiplying two matrices is straightforward, but its result addresses a narrow internal relationship. Comparing an aggregate scalar with the contraction that defines it addresses a different relationship and may reveal precision effects that the inverse check cannot detect. A learner should therefore explain why each check was chosen. Repeating many checks of the same dependency increases the volume of output without necessarily increasing the independent support for a conclusion. This is a useful discipline when scientific software makes additional outputs inexpensive.

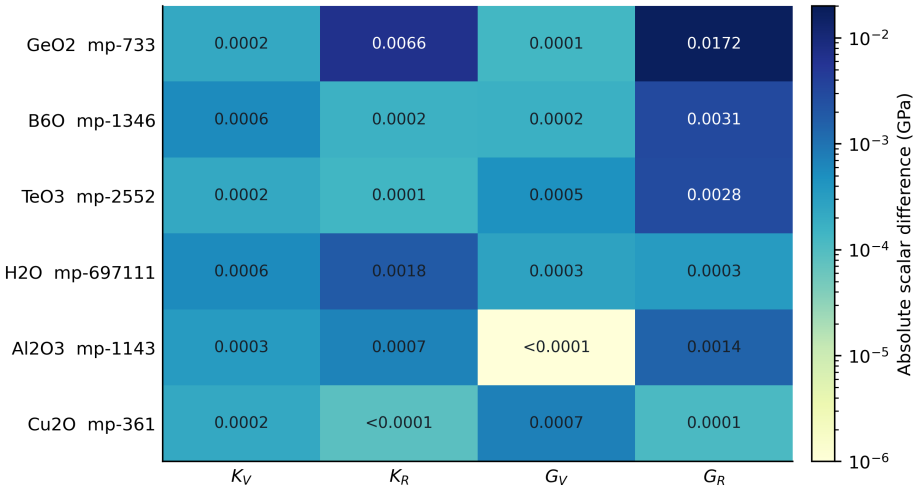


Figure 2: Absolute differences between calculated aggregate contractions and retained scalar values for the six largest diagnostic discrepancies. Selection uses each record's largest difference among the four bounds. The colour scale is logarithmic and saturates below 10^{-6} GPa; cell labels retain the numerical scale. These small differences concern precision within a crystal description and do not express measurement errors or confidence intervals.

4.3. Aggregate averaging suppresses different amounts of information

The joint distribution in Figure 3 shows that bulk and shear averaging spreads occupy very different ranges. Shear spread has a median of about 6.65%, whereas the bulk median is approximately 0.048%. The prevalence contrast remains clear at several descriptive thresholds, as shown in Table 3. At the one-tenth threshold, 52 records exceed the threshold in both properties, 394 exceed it only in shear, and six exceed it only in bulk; the remaining records exceed it in neither. A lesson built solely around bulk modulus would therefore expose fewer large averaging differences than a lesson that also examines shear response in this particular collection.

This observation is specific to the selected calculations. It does not estimate how commonly real manufactured materials have large averaging spreads, nor does it establish that shear modulus is intrinsically less reliable. The distinction arises from different contractions of stiffness and compliance and from the crystals included in the collection. The graphic deliberately retains this joint structure rather than turning the two quantities into competing quality scores. A student can examine where a record lies, determine which bounds differ, and relate that difference to the averaging assumptions. The educational outcome being sought is a defensible explanation of information loss, not the memorization of a universal spread threshold.

The averaging interval is also different from a measurement confidence interval. Voigt and Reuss treatments embody different idealized constraints on the aggregate response. Their separation expresses disagreement between those

homogenization assumptions for an anisotropic crystal description. A narrower interval does not establish that the underlying electronic calculation is more accurate, and a wider interval does not establish that the material is defective. Similarly, a Hill value is a specified mean, not an independently observed property. These distinctions make elasticity a useful subject for teaching why numerical intervals acquire meaning from how they were constructed. The interpretation must accompany the displayed number rather than be inferred from the familiar appearance of an interval.

Table 3: Finite-collection numerical checks.

Check	Result	Interpretation
Distinct identities / compositions	1,181 / 1,087	Different counting units
Positive-definite stiffness matrices	All retained matrices	Unstressed elastic quadratic form
Largest $\lvert CS - I \rvert$ element	8.0×10^{-13}	Internal inverse consistency
Largest K_{V} / G_{V} residual (GPa)	0.000667 / 0.000734	Scalar contraction agreement
Largest K_{R} / G_{R} residual (GPa)	0.00656 / 0.0172	Small precision-sensitive differences
Largest Hill-mean residual (GPa)	0.000501	Mean calculated from retained bounds
Largest A^{U} / ν_{H} residual	0.000594 / 0.000495	Dimensionless derived quantities
Spread threshold	Shear, count (%)	Bulk, count (%)
$\Delta > 5\%$	709 (60.03)	99 (8.38)
$\Delta > 10\%$	446 (37.76)	58 (4.91)
$\Delta > 20\%$	236 (19.98)	27 (2.29)
$\Delta > 50\%$	77 (6.52)	9 (0.76)
$\Delta > 100\%$	13 (1.10)	6 (0.51)

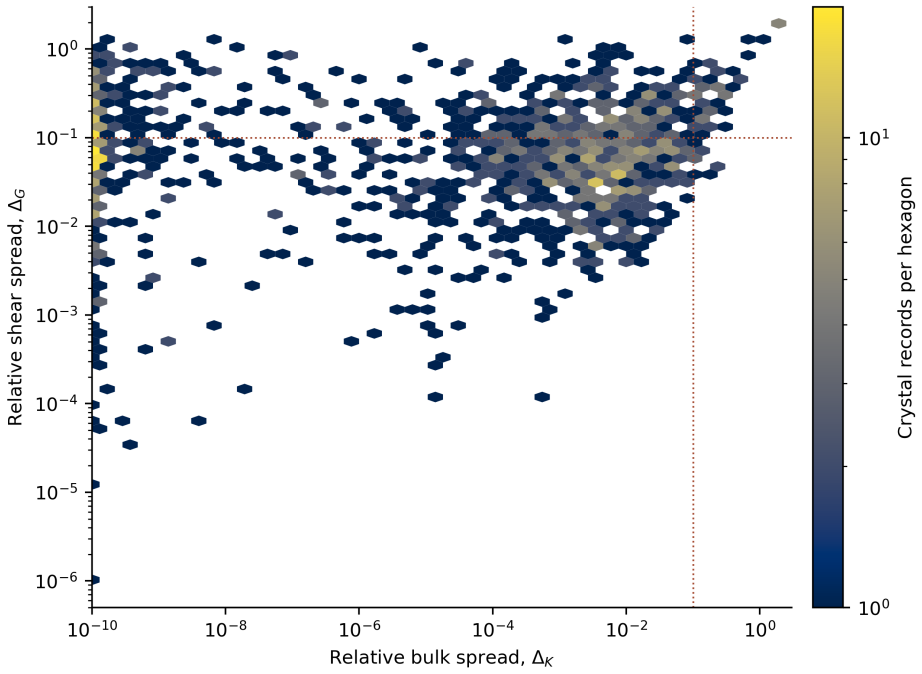


Figure 3: Joint distribution of relative bulk and shear averaging spreads. Hexagon colour gives the number of crystal records, with logarithmic axes and a logarithmic count scale. Dotted lines mark a relative spread of 0.1 for each property. Bulk widths below 10^{-10} are placed at that plotting limit, including exact zeros; arithmetic summaries use the unmodified values. The concentration near small bulk widths contrasts with the wider range of shear separation.

The anisotropy index in Eq. (4) adds another opportunity to examine dependent quantities. Its reconstruction agrees closely with the retained values, yet a correlation between that index and aggregate spread would partly reflect their common definitions. A strong numerical association could therefore be a mathematical consequence rather than a new materials discovery. This is an important transition to advanced information analysis: before fitting an association, a learner should identify whether the variables were generated from the same ingredients. Work on materials-property prediction and scientific model evaluation warns that favourable numerical comparisons can depend strongly on how information is organized and evaluated [34–36]. Here the dependence can be inspected directly.

The averaging results also illustrate why educational resources should retain intermediate quantities when possible. If only the Hill mean remains, a student cannot recover how far apart the two bounds were. Different pairs of bounds can have the same mean, so the missing information cannot be restored by more precise arithmetic on that mean. The limitation is representational rather than a failure of calculation. An effective exercise can make that loss explicit by asking students to compare what can be concluded from a scalar-only description with what can be concluded when its constituent bounds remain available. The answer depends on retained information, not display quality.

4.4. Directional stiffness changes the question, not just the display

Directional Young modulus asks how a particular crystal resists uniaxial deformation along a stated direction. It is therefore not another label for the aggregate bulk or shear mean. Figure 4 represents the function obtained from the selected copper compliance. Its radial variation is substantial: the largest to smallest modulus ratio is approximately eight. The smooth appearance of the surface follows from evaluating the elastic expression over direction, not from collecting a dense set of physical measurements. The surface is useful educationally precisely when students can distinguish those two origins of smoothness. It makes directional dependence visible while retaining the mathematical operation that produced the image.

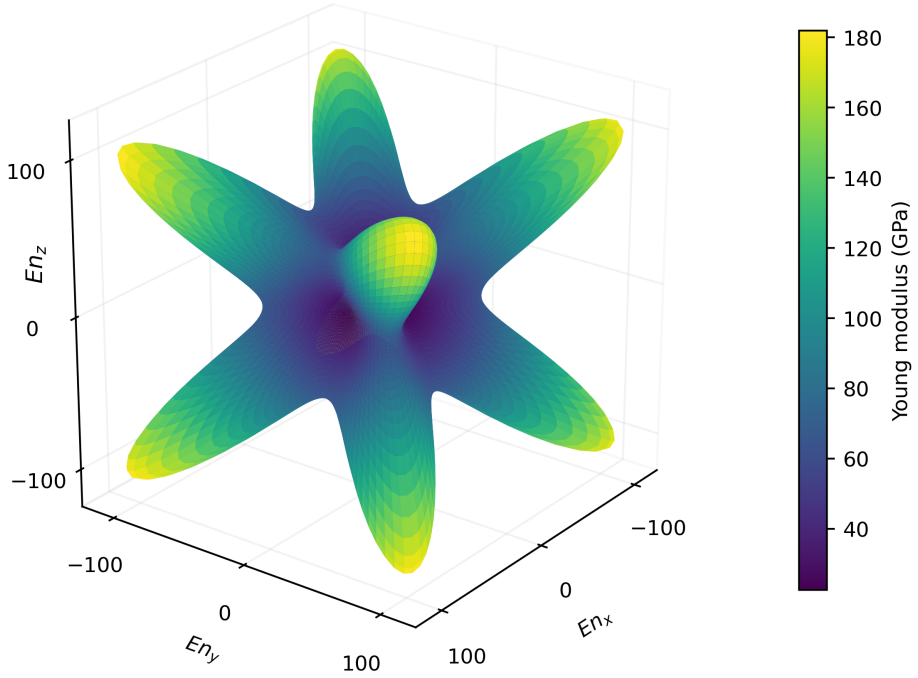


Figure 4: Directional Young modulus for copper record mp-30.

The copper example also shows why crystal symmetry should be distinguished from elastic isotropy. Cubic symmetry constrains the coefficient relationships but does not force the directional Young modulus to be constant. The selected sodium chloride record provides a contrasting cubic case with a much smaller, though still nonunit, directional ratio.

Table 4 places the extrema alongside those of the other diagnostic crystals. The comparison is between individual calculated records, not a ranking of all copper and sodium chloride specimens. Mechanical stability criteria and elastic-analysis tools supply the mathematical context for making this distinction [25–27]; they do not remove the need to identify the crystal and reference state.

Table 4: Numerical directional Young-modulus extrema for diagnostic crystal records.

Formula	Identifier	Space group	$E_{\min}$ (GPa)	$E_{\max}$ (GPa)	$E_{\max}/E_{\min}$
NaCl	mp-22862	225	31.24	42.33	1.355
Si	mp-149	227	115.28	172.26	1.494
Al	mp-134	225	43.75	84.76	1.937
Cu	mp-30	225	22.60	181.86	8.047
C	mp-48	194	6.65	876.24	131.864
C	mp-611426	194	1070.36	1239.80	1.158

The carbon section in Figure 5 changes the visual and scientific emphasis. Instead of displaying every direction for one crystal, it compares the same angular path for two structural alternatives. One arrangement changes strongly with loading direction, while the other remains comparatively uniform on the common radial scale. Over the full sphere, their largest to smallest Young-modulus ratios differ by more than two orders of magnitude. This comparison shows that shared chemical composition and space-group classification do not determine the extent of elastic anisotropy. The structure images and directional calculations answer complementary questions, and neither can replace the other in a complete explanation.

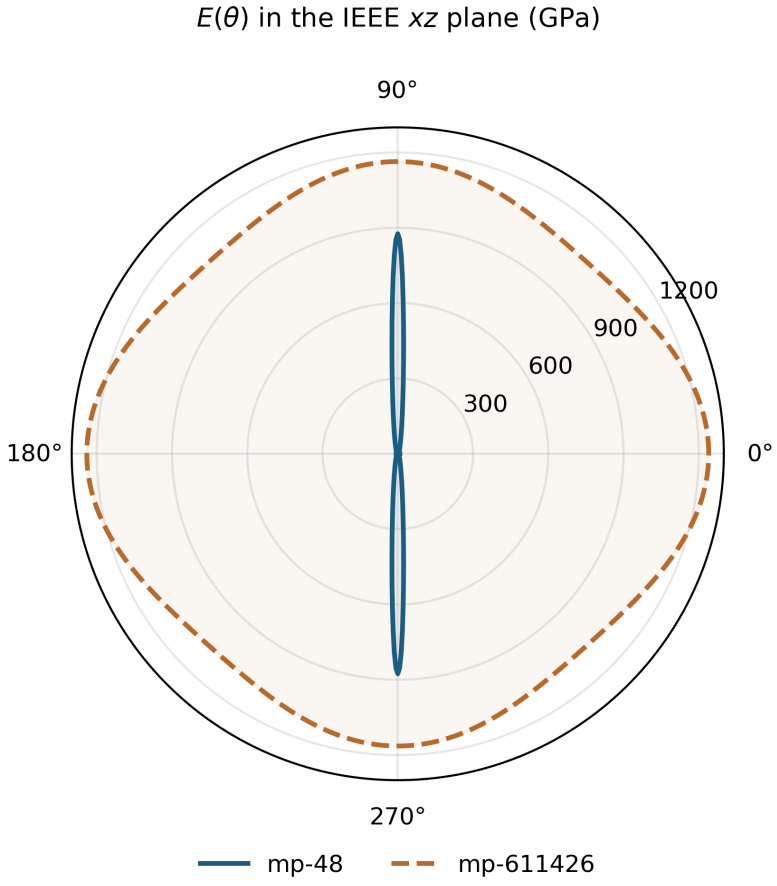


Figure 5: Young modulus along a common angular path for the two carbon records in Figure 1.

Care is needed when moving between the polar section and the full directional extrema. A plane samples only the directions contained within it, whereas the extrema in Table 4 are sought across the full sphere. A polar maximum is not automatically the global maximum for a lower-symmetry record. Plot orientation likewise concerns the declared tensor axes rather than the camera angle used to render atomic coordinates. These distinctions allow an

instructor to ask a precise question about representation: which information is retained by this particular view, and which directions remain unexamined? A technically correct visual answer can then be judged alongside a written statement of its limits.

The engineering-shear convention provides a further test of genuine understanding. If the directional contraction is implemented with an incorrect shear factor, the resulting surface may still appear smooth and plausible. Appearance alone cannot reveal the mistake. A defensible explanation therefore connects the stress vector, engineering strain, compliance, and axial projection used in Eq. (6). Software can support this connection by exposing inputs and values for selected directions. It should not be expected to supply the learner's reasoning automatically. This point distinguishes a study of teaching suitability from a catalogue of visualization features: the resource is evaluated through the explanation it permits a student to construct and check.

The structural contrast gives an additional reason to avoid interpreting a visual resemblance as a physical equivalence. Two renderings can look similar from a selected viewpoint while representing different periodic arrangements, and two directional sections can appear similar while omitting different directions. Explicit identifiers and coordinate conventions make those ambiguities tractable. The aim is not to ask students to distrust images in general, but to require that an image answer a stated question. When a view is chosen to reveal coordination, it should be evaluated as a structural view; when a radius represents stiffness, its mathematical meaning should remain explicit.

4.5. Composition weighting tests a counting choice

Equal weighting of compositions leaves the principal bulk–shear contrast intact. Figure 6 shows the signed percentage-point change at each display threshold rather than repeating the prevalence curves. The changes remain below one percentage point in magnitude. This is evidence that repeated compositions do not dominate the particular descriptive contrast, but it is not evidence that the records are independent or that the collection represents all chemistries equally. Weighting resolves one specified counting choice. It does not correct an unknown selection process, balance every element, or remove relationships among chemically similar solids. The interpretation should remain aligned with that limited operation.

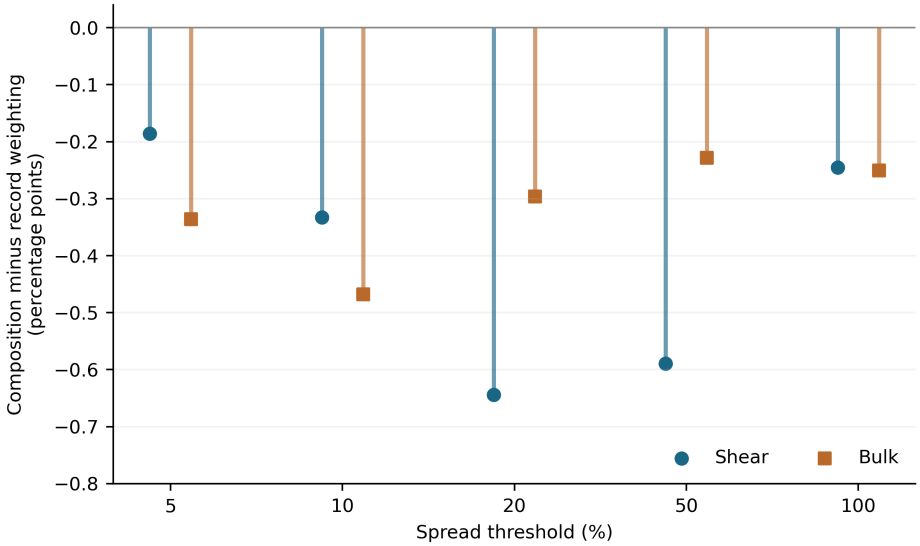


Figure 6: Effect of the counting unit on threshold summaries.

This makes weighting a useful topic even in a course without machine-learning content. A learner can calculate a record-weighted proportion, identify repeated chemistry, calculate a composition-weighted alternative, and explain what changed. An advanced class can connect the same reasoning to evaluation of predictive materials models, where distinctions among known compositions, new structures, and genuinely unfamiliar chemical systems can affect apparent performance [34, 35]. The present calculations do not train such a model. They provide a concrete, inspectable example of why the question and the counting unit should be settled before a large number of records is treated as persuasive evidence.

4.6. Educational conclusions must follow the kind of evidence available

The numerical checks support a practical resource judgment: the collection can sustain tasks that require students to examine identity, convention, averaging assumptions, and directional response. They do not show that students will complete those tasks successfully or retain the underlying ideas. Research on data-literacy assessments emphasizes the need to define the intended competence and obtain evidence appropriate to the responses being evaluated [6, 7]. For this subject, a correct modulus can be one component of a response, but the assessment should also reveal why the quantity applies to the stated object and loading assumption. Otherwise, an instructor may reward execution while overlooking a serious interpretive mistake.

The contrast between resource capability and learning evidence is consistent with recent open-education research. Different forms of instruction, participant characteristics, and implementation conditions complicate attempts to attribute educational effects to resource access alone [11, 12, 14]. The present study consequently makes a bounded recommendation rather than an effectiveness claim. It recommends the resources for specific explanation tasks when scientific context and instructional support are supplied. It does not attach an effect size, predict examination gains, or describe a comparative classroom trial. Such evidence would require participants, assessments, and a study design that are absent from the numerical collection and from this appraisal.

An important implication is that the resource can support disagreement that is scientific rather than procedural. Students may obtain different answers because they selected different averaging assumptions, directions, or counting units, even when both calculations are correct. Asking them to resolve the disagreement requires identifying the question each answer addresses. This is more demanding than finding the command that produces a preferred number. It also provides a precise route from numerical work to scholarly explanation: students must state an assumption, show its consequence, and delimit the conclusion. Whether that activity improves learning remains an empirical educational question, distinct from its demonstrable scientific content.

5. CLASSROOM ADOPTION AND ASSESSMENT

Adoption should begin with the scientific explanation that students are expected to produce. An instructor can require an identified crystal, a statement of the reference state, a calculation with units, and an interpretation of the result's limits. This is a compact but demanding submission because each component constrains the others. A modulus without a crystal identity is ambiguous; an identity without a loading assumption is incomplete; a calculation without units can conceal an error; and a conclusion without scope can overstate what has been established. None of these requirements depends on a particular commercial platform. They depend on the information a resource preserves and on the questions asked of the learner.

Preparation should separate essential mechanics from optional programming complexity. Students who already know matrix multiplication can inspect a small set of coefficient arrays before analysing the full collection. Students with stronger computational preparation can examine composition grouping, precision differences, and directional optimization. Both routes should lead to the same standards of explanation. Providing a shorter numerical task should not mean removing identifiers, units, or reference-state information. Evidence concerning teachers' adoption decisions supports attention to practical fit and assistance rather than assuming that a technically capable resource can enter any course unchanged [15, 16, 30]. The instructor remains responsible for matching the exercise to prior preparation.

Assessment can distinguish arithmetic, interpretation, and transfer without assigning an unsupported overall quality score. An arithmetic response demonstrates a calculation and its units. An interpretive response explains why an aggregate interval differs from uncertainty and why a directional quantity depends on orientation. A transfer response recognizes the same problem when it appears in a different crystal or a differently organized resource. These are proposed assessment demands, not validated dimensions of a new test. Research on instructors' value beliefs and undergraduate data-literacy priorities helps justify making the demands explicit [8, 31]. Student responses and evaluation criteria would still need to be examined in an actual course before conclusions about attainment are drawn.

Instructor preparation also needs to address evidence quality. Reviews of teaching for statistical and data literacy show that teacher knowledge, professional learning, and classroom implementation remain connected issues [37]. That research concerns a different educational level and cannot establish outcomes in undergraduate materials courses. It does support the modest recommendation that the instructor rehearse the scientific interpretation before assigning the exercise. For example, the instructor should be able to explain why positive definiteness does not establish phase stability and why a small inverse residual does not prove measurement accuracy. Without that preparation, open numerical access can propagate a confident misunderstanding as efficiently as it can support a correct explanation.

Practical support should preserve alternatives to the most visually elaborate representation. A table of directional values and a written description can accompany a rotating surface; a clearly identified structural rendering can accompany atomic coordinates. Students should not have to infer units from colour or manipulate an inaccessible interface to understand the scientific claim. Accessibility findings from online learning provide a reason to investigate these arrangements directly with intended users [32]. Broader adoption research likewise shows that positive perceptions coexist with technical and institutional obstacles [13]. These considerations strengthen the recommendation for deliberate local preparation while leaving resource-specific usability and accessibility outcomes open to direct evaluation.

Feedback should address the explanation at the point where an unsupported step occurs. A student who calculates an aggregate spread correctly but calls it uncertainty needs a different response from a student who selects an incorrect compliance convention. Likewise, a missing crystal identifier is not the same difficulty as an unjustified population claim. Keeping these errors separate helps the instructor give specific feedback and helps students revise their reasoning rather than merely replace a number. This is a recommendation about assessment practice, not evidence that a particular marking rubric has been validated or that the proposed distinctions describe independent psychological abilities.

6. CONCLUSIONS

Open elasticity resources are most useful for materials education when they preserve the information needed to explain a result. Atomic coordinates and identifiers distinguish structural alternatives; coefficient matrices expose conventions; aggregate bounds reveal the consequences of averaging; and directional calculations show what an isotropic summary cannot express. The examined collection supports all of these operations, with small internal numerical residuals and substantial differences between bulk and shear averaging behaviour. Matminer and ELATE provide complementary routes to inspection and interpretation, subject to explicit preparation. The resulting recommendation concerns well-defined explanation tasks, not untested learning gains. A defensible material-property claim remains the appropriate standard for judging educational use.

These distinctions also define a practical limit on simplification. Shortening an exercise can reduce computational effort, but it should preserve the material identity, physical state, and meaning of the requested quantity. An educational resource is then judged through the claim a learner can support, rather than through the number of outputs available. Direct classroom evaluation can test whether this emphasis develops the intended understanding without confusing a resource appraisal with evidence of instructional effectiveness. Assessment should therefore examine whether learners can identify assumptions before accepting a convincing numerical answer.

Conflict of Interests

The authors declare that they have no conflicts of interest.

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Data Availability

The data supporting the findings of this study are included within this manuscript.

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