DALHOUSIE UNIVERSITY

Seminar 1: What The Flip Are Stress Tensors?

How do I use them, and why do I care?

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February 09, 2021
PHYC6802: Phys&Atmos PhD Seminar Series

First-Principles Calculation of Third-Order Elastic Constants via Numerical Differentiation of the Second Piola-Kirchhoff Stress Tensor

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(Received 9 September 2018; published 21 November 2018)

A general method is presented to calculate from *first principles* the full set of third-order elastic constants of a material of arbitrary symmetry. The method here illustrated relies on a plane-wave density functional theory scheme to calculate the Cauchy stress and the numerical differentiation of the second Piola-Kirchhoff stress tensor to evaluate the elastic constants. It is shown that finite difference formulas lead to a cancellation of the finite basis set errors, whereas simple solutions are proposed to eliminate numerical errors arising from the use of Fourier interpolation techniques. Applications to diamond, silicon, aluminum, magnesium, graphene, and a graphane conformer give results in excellent agreement with both experiments and previous calculations based on fitting energy density curves, demonstrating both the accuracy and generality of our new methodology to investigate nonlinear elastic behaviors of materials.

DOI: 10.1103/PhysRevLett.121.216001

The Cauchy Stress Tensor

$$\boldsymbol{\sigma} = \begin{pmatrix} \sigma_{xx} & \sigma_{xy} & \sigma_{xz} \\ \sigma_{yx} & \sigma_{yy} & \sigma_{yz} \\ \sigma_{zx} & \sigma_{zy} & \sigma_{zz} \end{pmatrix}$$

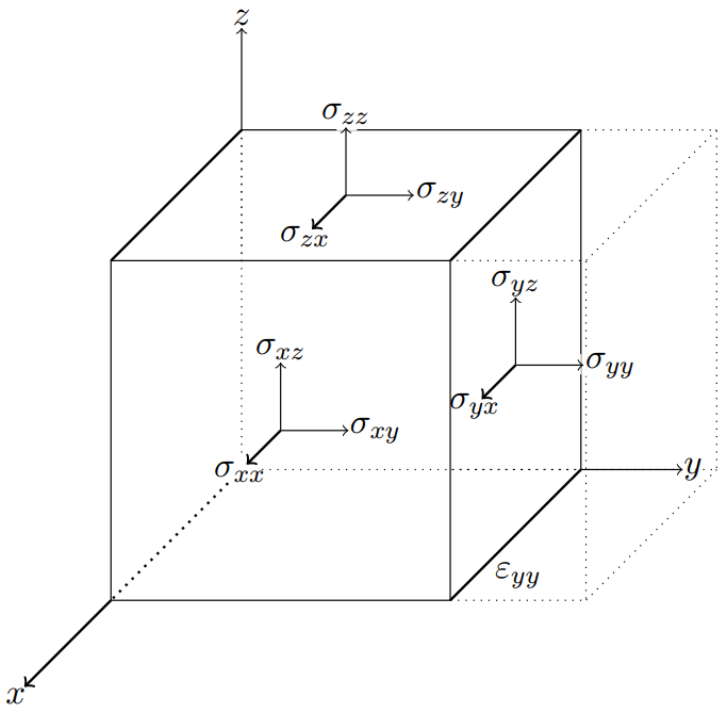

Figure 2.1.: Components of the stress tensor. On each face of the cube, stress can act perpendicular to the surface normal or parallel to it. E.g. the stress component σ_{yy} causes the cube to expand or to shrink by ε_{yy}.

D. A. Klüppenberg, *Calculation of stress tensor within the ab-initio full-potential linearized augmented plane wave method*. Dissertation, Peter Grünberg Institute, Jülich, (2012). pp7

Types of Stress Measures

Conversion Formulae

	$\boldsymbol{\sigma}$	$\boldsymbol{\tau}$	$\boldsymbol{N}$	$\boldsymbol{P}$
$\boldsymbol{\sigma} =$	$\boldsymbol{\sigma}$	$J^{-1}\boldsymbol{\tau}$	$J^{-1}\boldsymbol{N}F^T$	$J^{-1}\boldsymbol{F}\boldsymbol{P}\boldsymbol{F}^T$
$\boldsymbol{\tau} =$	$J\boldsymbol{\sigma}$	$\boldsymbol{\tau}$	$\boldsymbol{N}\boldsymbol{F}^T$	$\boldsymbol{F}\boldsymbol{P}\boldsymbol{F}^T$
$\boldsymbol{N} =$	$J\boldsymbol{\sigma}\boldsymbol{F}^T$	$\boldsymbol{\tau}\boldsymbol{F}^{-T}$	$\boldsymbol{N}$	$\boldsymbol{F}\boldsymbol{P}$
$\boldsymbol{P} =$	$J\boldsymbol{F}^{-1}\boldsymbol{\sigma}\boldsymbol{F}^{-T}$	$\boldsymbol{F}^{-1}\boldsymbol{\tau}\boldsymbol{F}^{-T}$	$\boldsymbol{F}^{-1}\boldsymbol{N}$	$\boldsymbol{P}$

$\boldsymbol{\sigma}$:	Cauchy stress tensor	$\boldsymbol{\tau}$:	Kirchhoff stress tensor
$\boldsymbol{N}$:	First Piola-Kirchoff stress tensor	$\boldsymbol{F}$:	Deformation gradient tensor
$\boldsymbol{P}$:	Second Piola-Kirchhoff stress tensor	J:	$\det(\boldsymbol{F})$

https://en.wikipedia.org/wiki/Stress_measures

Types of Stress Measures

Is your system simple and linear?

Stick with the *Cauchy* or *Kirchhoff Stress Tensors*: $\boldsymbol{\sigma}$, $\boldsymbol{\tau}$

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	$\boldsymbol{\sigma}$	$\boldsymbol{\tau}$	$\boldsymbol{N}$	$\boldsymbol{P}$
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Types of Stress Measures

Is your system more complicated than that?

You will at least need the *First Piola-Kirchhoff Stress Tensor*: $\boldsymbol{N}$

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Types of Stress Measures

Is your work computationally intense?

You want symmetry, use the *Second Piola-Kirchhoff Stress Tensor*: $\boldsymbol{P}$

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Types of Stress Measures

Are there others besides what's listed here?

Many.

Conversion Formulae

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Types of Stress Measures

Why so many?

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Types of Stress Measures

Why so many?

I blame engineers.

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The Deformation Gradient Tensor

We need to get from $\boldsymbol{\sigma}$ to $\boldsymbol{S}$. To do that we need to use the *Deformation Gradient Tensor*. Let X and Y represent the undeformed reference configuration with x and y are the deformed current configuration. Then $\boldsymbol{F}_{ij} = \frac{\partial x_i}{\partial X_j}$, and the weight function is given by $J = \det(\boldsymbol{F})$.

- Displacement
- Rotations
- Stretching
- Shear (with rotation)
- Pure Shear

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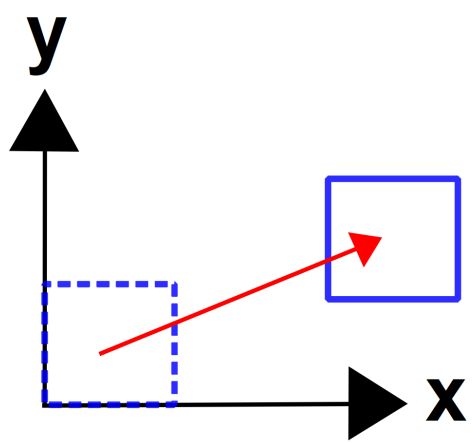
$$x = X + 5$$

$$y = Y + 2$$

$$\boldsymbol{F} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$



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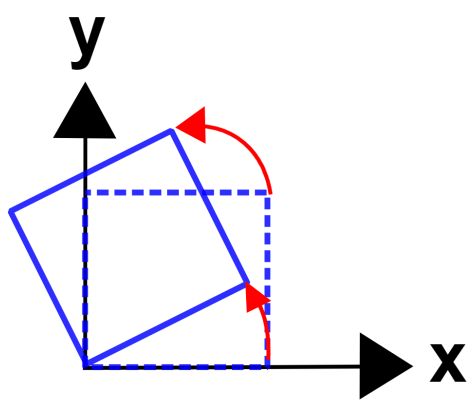
$$x = X\cos\theta - Y\sin\theta$$
$$y = X\sin\theta + Y\cos\theta$$
$$\boldsymbol{F} = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$



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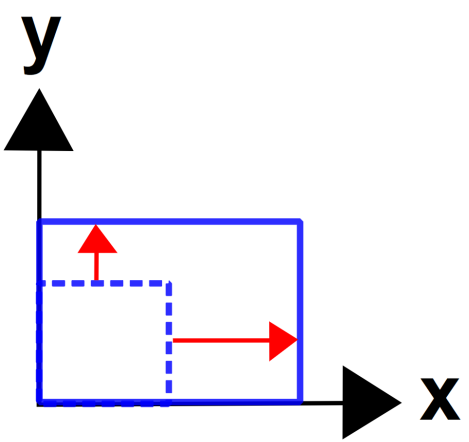
$$x = 2.0X + 0.0Y$$
$$y = 0.0X + 1.5Y$$
$$\boldsymbol{F} = \begin{pmatrix} 2.0 & 0.0 \\ 0.0 & 1.5 \end{pmatrix}$$



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$$x = 1.0X + 0.0Y$$
$$y = 0.5X + 1.0Y$$
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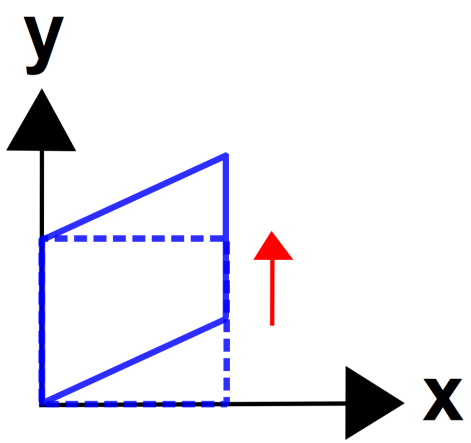

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$$x = 1.0X + 0.5Y$$

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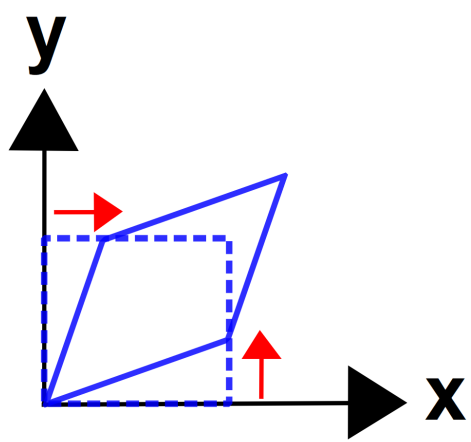

The Second Piola-Kirchhoff (2nd-PK) Stress Tensor

Now that we understand what the Deformation Gradient Tensor is, we can derive the 2nd-PK Stress Tensor $\boldsymbol{P}$.

$$\boldsymbol{P} = J\boldsymbol{F}^{-1}\boldsymbol{\sigma}\boldsymbol{F}^{-T}$$

With this, we can examine *Non-Linear Elastic* behaviour.

What do you mean "Non-Linear" Elasticity?

- **Linear Elastics**
  - Steel
  - Glass
  - Wood
- **Hypoelastics**
  - Elastin
  - Fat
  - Tendons
- **Hyperelastics**
  - Rubbers
  - Elastomers
  - Silicone
- **Plastics**
  - Well... Plastics
  - PVC Pipe
  - Sheet Metal
- **Brittle Material**
  - Ceramics
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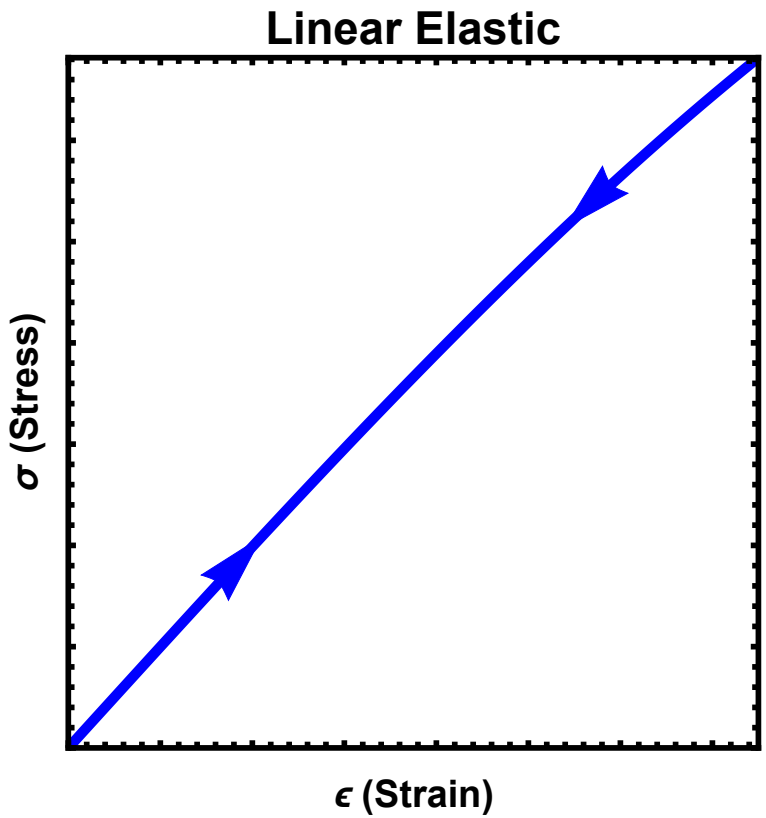

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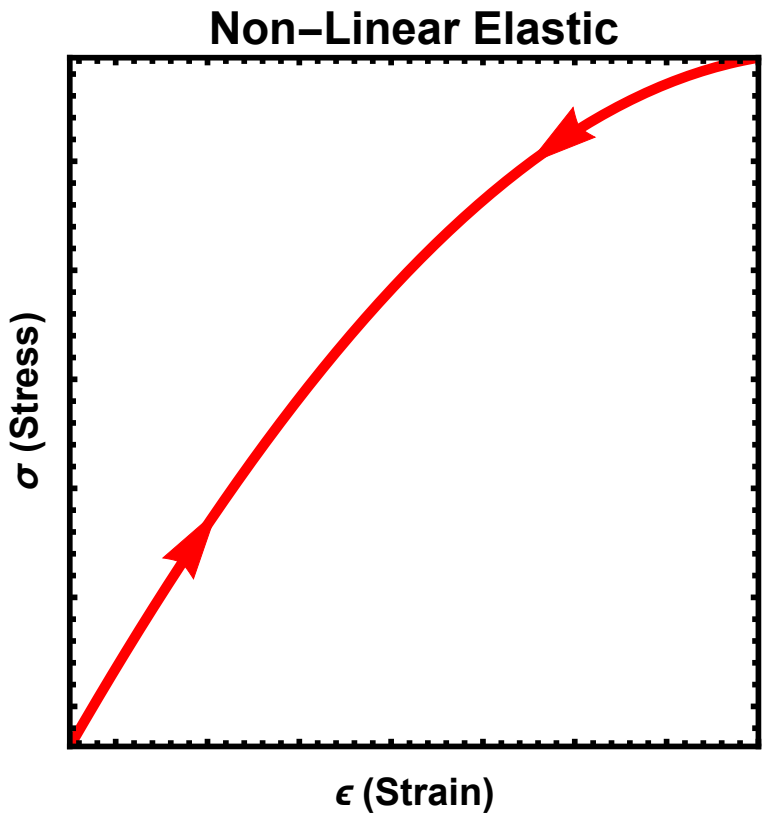

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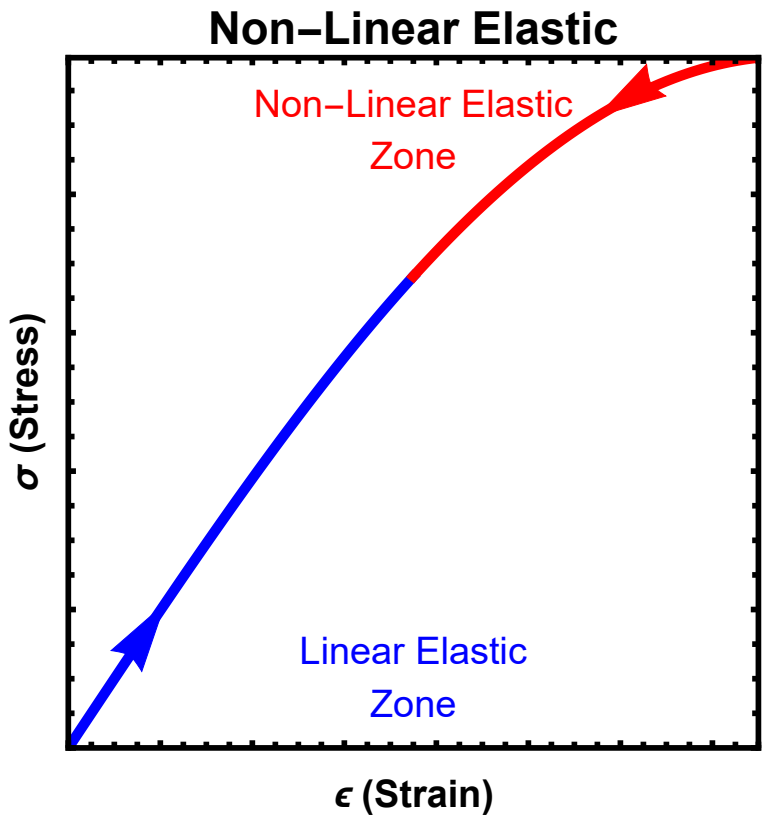

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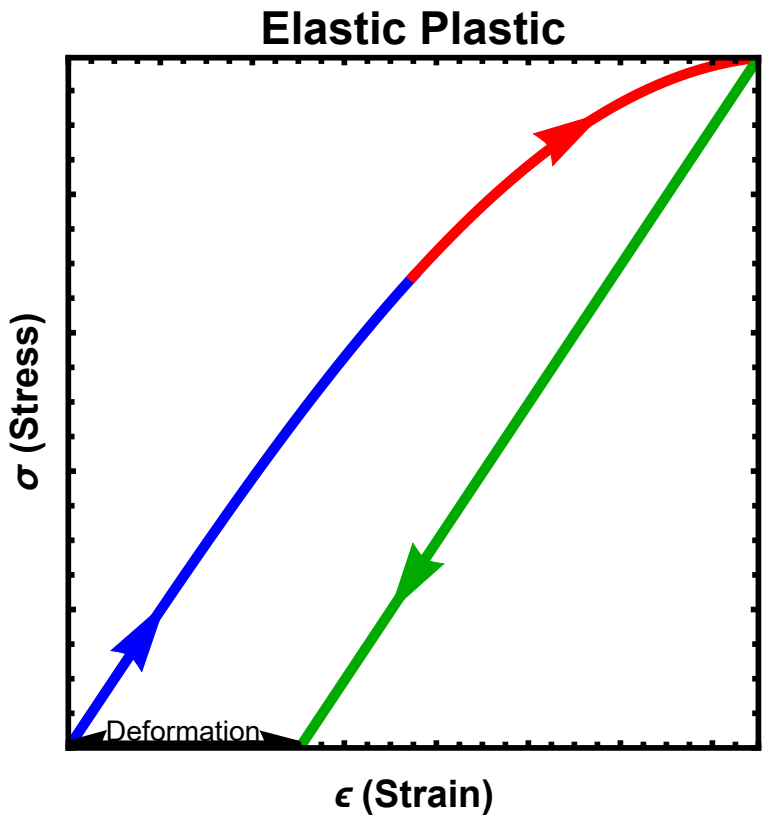

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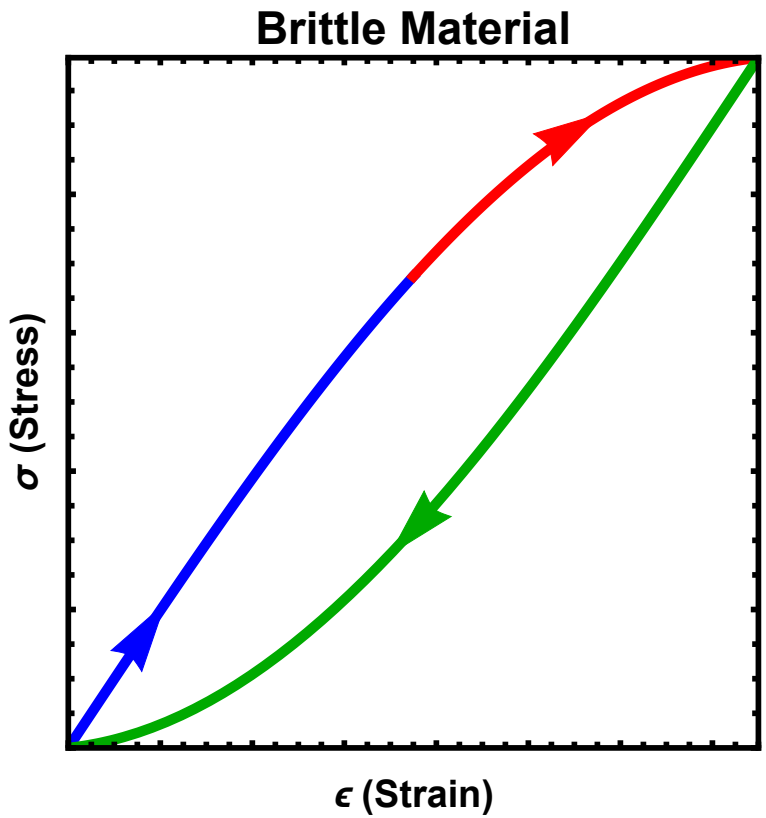
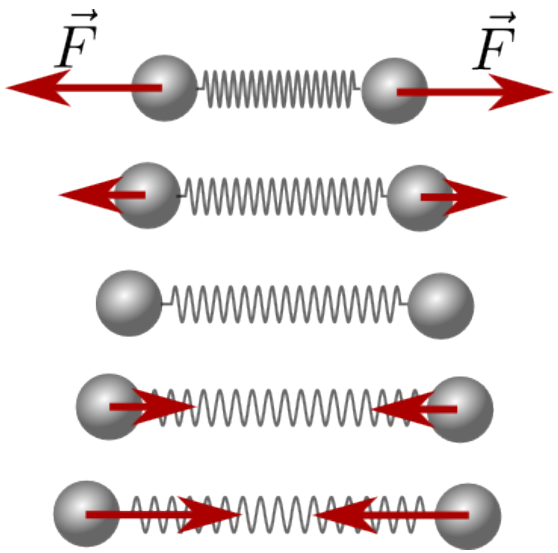
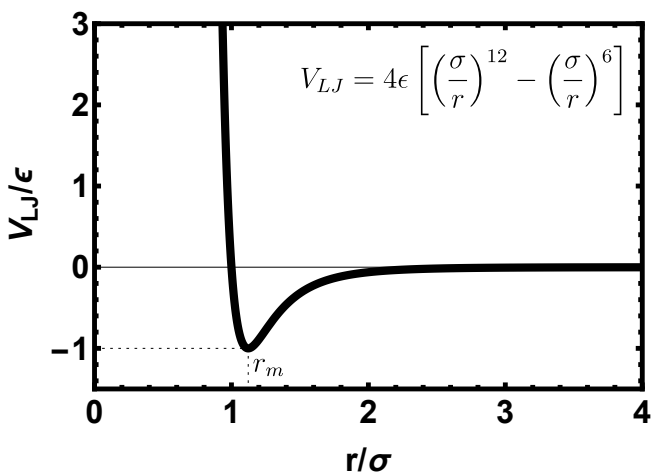


What Are Force Calculations?

- Electronic-structure theory software has a process called a geometry optimization.
- The forces on each atom are calculated in each geometry optimization step.
- The atom positions will be adjusted in the direction of the largest gradient.
- Once the atoms are moving sufficiently small within each step, they are said to be relaxed and the geometry is optimized.
- The system will adjust itself until it settles into a minimum in the potential energy surface.





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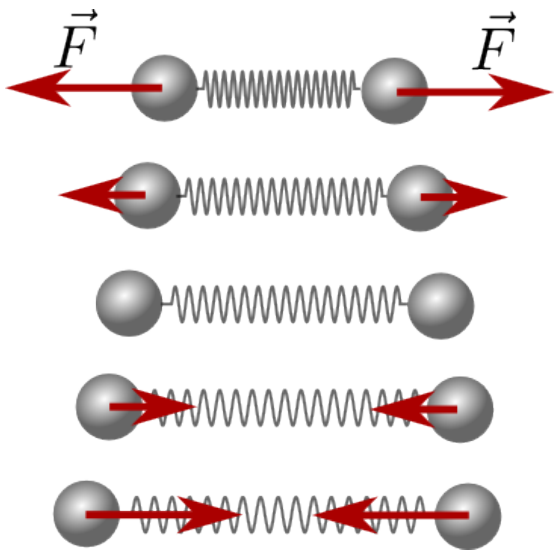

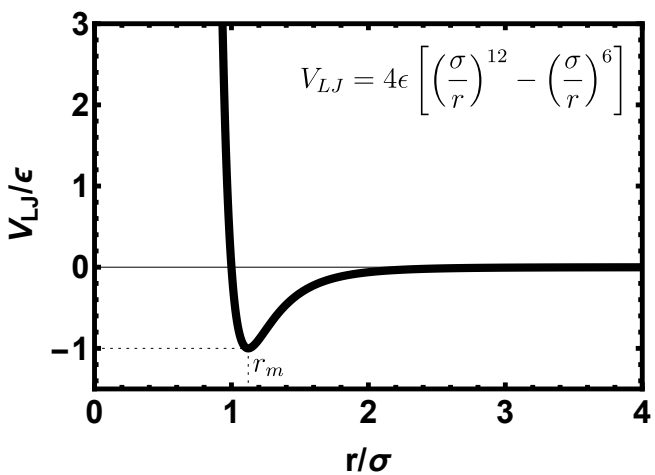

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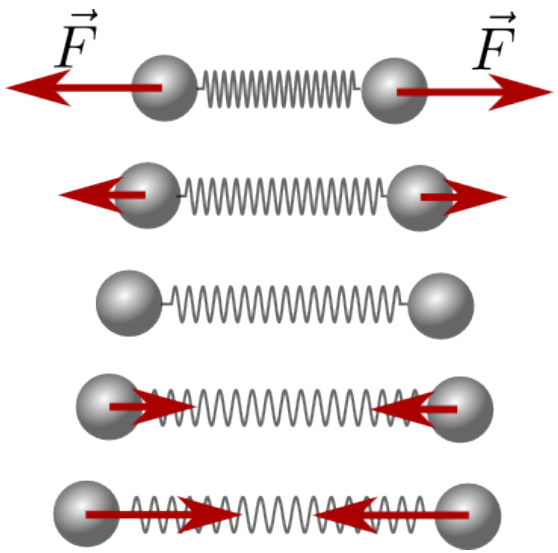

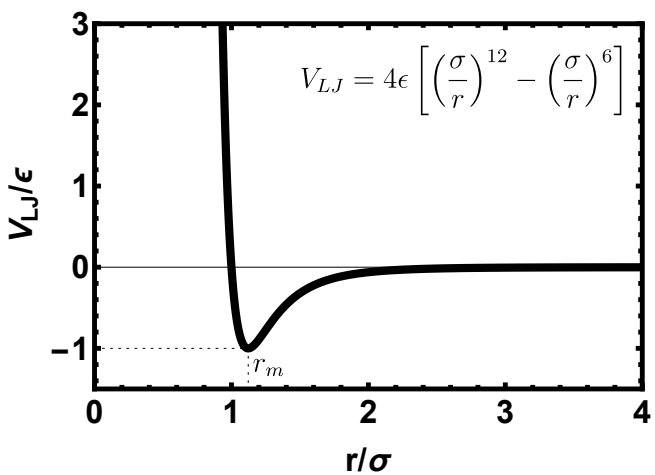

https://msuperl.org/wikis/pcubed/doku.php?id=183_notes:model_of_solids

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- Electronic-structure theory software has a process called a geometry optimization.
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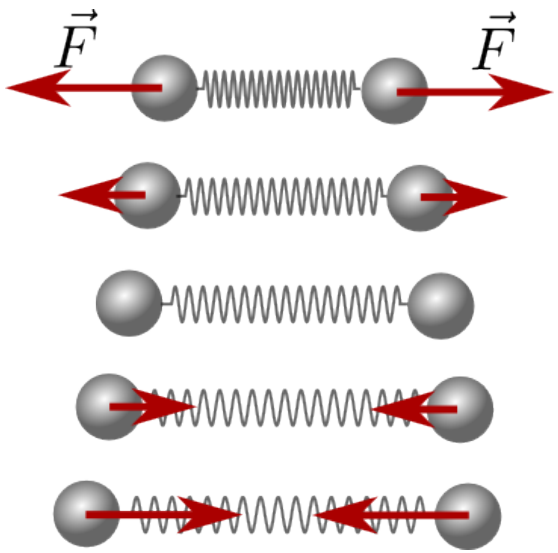

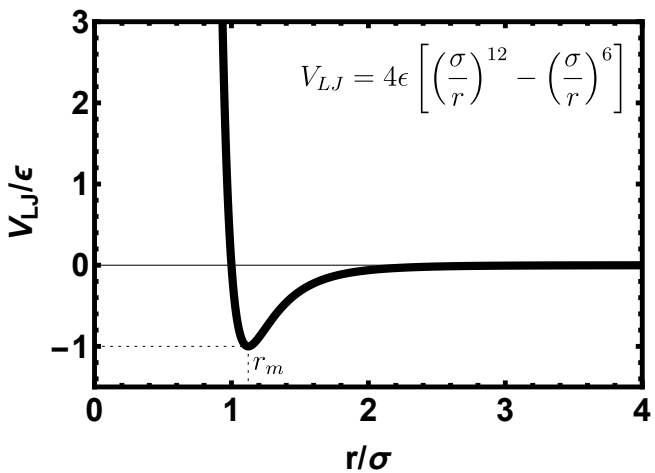

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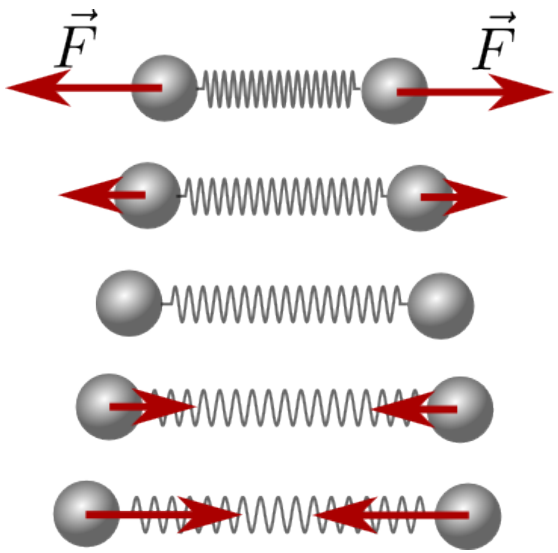

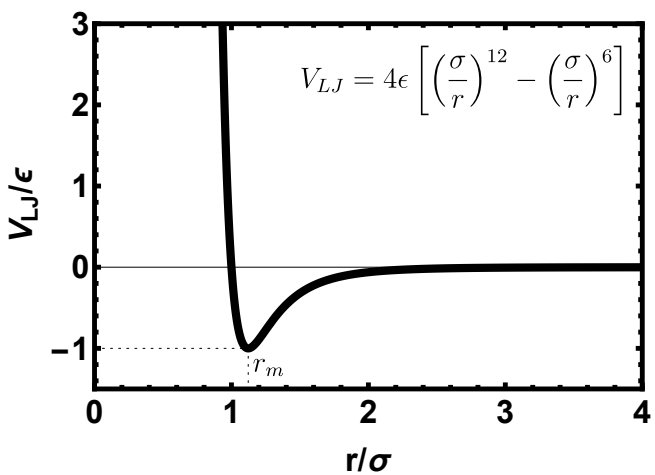

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Two Sides of the Same Coin?

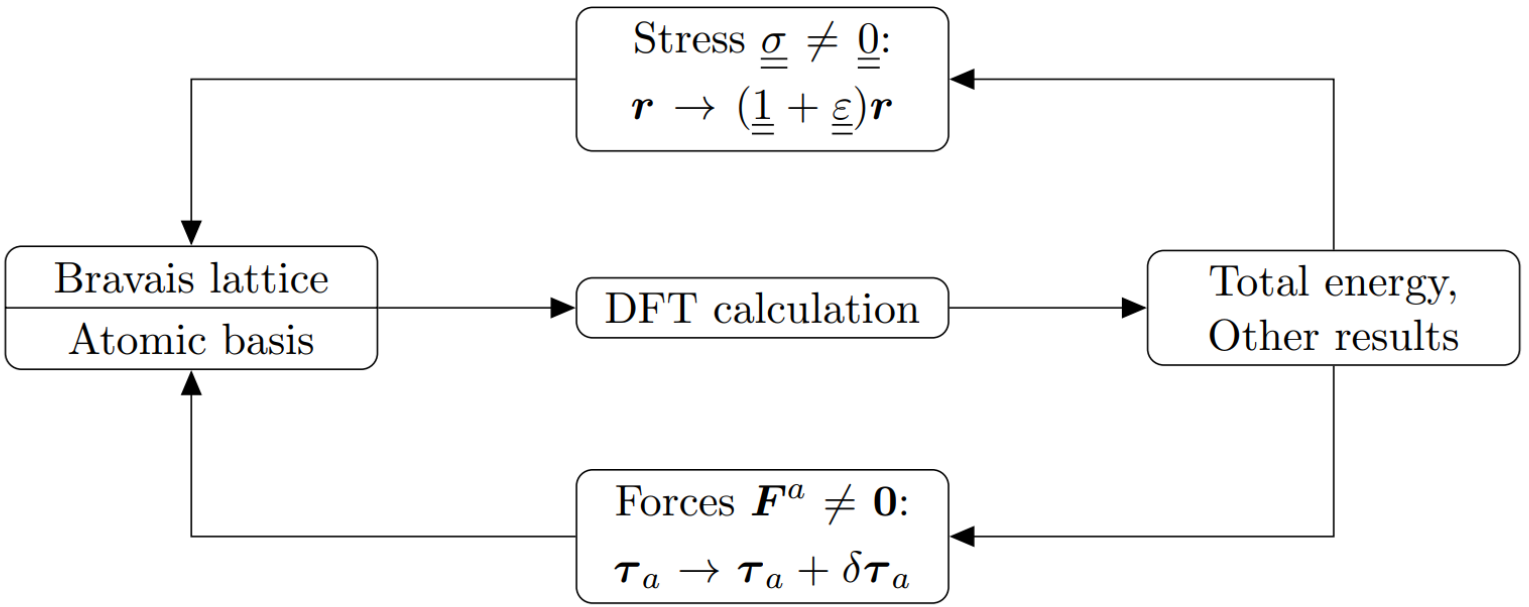
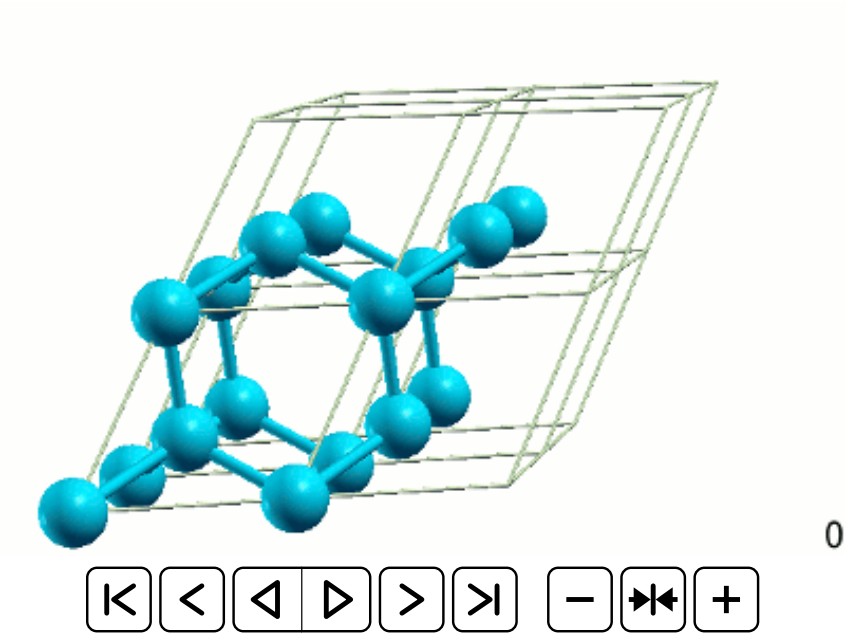


Figure 1.3.: Lattice structure optimization: Start with a guessed lattice geometry. If the resulting atomic forces are non-zero, shift the atoms in the unit cell and continue the optimization until the forces are sufficiently small. If the stress is non-zero, change the Bravais lattice vectors accordingly and continue the optimization until the stress vanishes.

D. A. Klüppenberg, *Calculation of stress tensor within the ab-initio full-potential linearized augmented plane wave method*. Dissertation, Peter Grünberg Institute, Jülich, (2012). pp5

Geometry Optimization of a Silicon Lattice



http://jdftx.org/LatticeOpt.html

"So... what's an elastic constant?"

There are two types of elastic constants we're considering:

- SOECs: Second-order elastic constants
- TOECs: Third-order elastic constants

These elastic constants are important parameters for characterizing nonlinear elastic material behaviour. Through them we can predict:

- Interactions of thermal and acoustic phonons
- Long-wavelength phonon anharmonicities
- Intrinsic mechanical strength of a material
- Thermal expansion
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Internal Energy, SOECs, and TOECs,

Within the framework of finite (or large) strain theory, the symmetric Lagrangian elastic strain is given by

$$\varepsilon_{ij} = \frac{1}{2}\left(F_{ki}F_{kj} - \delta_{ij}\right) .$$

Then the internal energy is given by

$$\begin{aligned} U &= \frac{1}{2!}\frac{\partial^2 U}{\partial\varepsilon_{ij}\,\partial\varepsilon_{lm}}\varepsilon_{ij}\varepsilon_{lm} + \frac{1}{3!}\frac{\partial^3 U}{\partial\varepsilon_{ij}\,\partial\varepsilon_{lm}\,\partial\varepsilon_{pq}}\varepsilon_{ij}\varepsilon_{lm}\varepsilon_{pq} \\ &= \frac{1}{2}C^{(2)}_{ijlm}\varepsilon_{ij}\varepsilon_{lm} + \frac{1}{6}C^{(3)}_{ijlmpq}\varepsilon_{ij}\varepsilon_{lm}\varepsilon_{pq} . \end{aligned}$$

- $C^{(2)}_{ijlm}$ is a second-order elastic coefficient (SOEC)
- $C^{(3)}_{ijlmpq}$ is a third-order elastic coefficient (TOEC)

The Second Piola-Kirchhoff Stress Tensor and Voigt's Notation

The elements of the 2nd-PK Stress Tensor may be written as

$$P_{ij} = C^{(2)}_{ijlm}\varepsilon_{lm} + \frac{1}{2}C^{(3)}_{ijlmpq}\varepsilon_{lm}\varepsilon_{pq}\,.$$

However, the coefficients as they are now are very cumbersome. We will shift to *Voigt's Notation* where

$$C^{(2)}_{ijlm} \to C^{(2)}_{\alpha\beta}$$
$$C^{(3)}_{ijlmpq} \to C^{(3)}_{\alpha\beta\gamma}$$

and $\alpha, \beta, \gamma \in \{1, 2, 3, 4, 5, 6\}$, with

$$xx \to 1\,, \qquad yy \to 2\,, \qquad zz \to 3\,,$$
$$yz \to 4\,, \qquad xz \to 5\,, \qquad xy \to 6\,.$$

"... So what's the catch?"

These constants are typically determined experimentally, and doing so is very difficult.

- TOECs are typically obtained from ultrasonic velocity measurements.
- These experiments produce data with large error margins, as high as 50%.
- TOECs are far more structure sensitive than SOECs.
- Sample quality drastically effects experimental data.
- Some materials are prohibitively difficult to measure.
- TOECs have only been measured for a small number of bulk materials.

Researchers have tried to move to computational methods. Many of these methods are onerous, inaccurate, and only applicable to highly symmetric crystals. The present finite-difference method calculates these coefficients from first-principles. Using It is efficient, accurate, and general. It can be used in 3D and 2D low-symmetry crystals, as well as defected or inhomogeneous materials.

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Finite Difference Method for SOECs

Now that the framework has been set, we can now show how SOECs and TOECs can be calculated with finite difference methods. This was motivated because finite-difference methods have the added benefit of leading to the cancelling out of finite basis set errors. Consider a 2nd-PK tensor element P_α and a strain element ε_β,

$$C^{(2)}_{\alpha\beta} = \frac{\partial P_\alpha}{\partial \varepsilon_\beta} = \frac{P_\alpha^{(+\Delta\varepsilon_\beta)} - P_\alpha^{(-\Delta\varepsilon_\beta)}}{2\Delta\varepsilon_\beta}\,.$$

For clarity, $P_\alpha^{(\pm\Delta\varepsilon_\beta)}$ is the αth component of the 2nd-PK tensor of the supercell that accommodates the finite strain $\pm\Delta\varepsilon_\beta$.

Finite Difference Method for TOECs

For TOECs we use two formulas for efficiency. For TOEC elements with a symmetric index (e.g. $\beta = \gamma$)

$$C^{(3)}_{\alpha\beta\beta} = \frac{\partial^2 P_\alpha}{\partial^2 \varepsilon_\beta} = \frac{P_\alpha^{(+\Delta\varepsilon_\beta)} + P_\alpha^{(-\Delta\varepsilon_\beta)} - P_\alpha^{(0)}}{\Delta\varepsilon_\beta^2},$$

and otherwise

$$C^{(3)}_{\alpha\beta\gamma} = \frac{P_\alpha^{(+\Delta\varepsilon_\beta\,,+\Delta\varepsilon_\gamma)} - P_\alpha^{(-\Delta\varepsilon_\beta\,,+\Delta\varepsilon_\gamma)} - P_\alpha^{(+\Delta\varepsilon_\beta\,,-\Delta\varepsilon_\gamma)} + P_\alpha^{(-\Delta\varepsilon_\beta\,,-\Delta\varepsilon_\gamma)}}{4\Delta\varepsilon_\beta\,\Delta\varepsilon_\gamma}.$$

Here $P_\alpha^{(0)}$ refers to the component of the 2nd-PK stress tensor of the unstressed reference material, and $P_\alpha^{(\pm\Delta\varepsilon_\beta\,,\pm\Delta\varepsilon_\gamma)}$ are components that accommodate two types of finite deformation.

Calculating SOECs and TOECs

When validating and implementing the finite difference method, the researchers used the following methodology:

Roadmap

- Density-functional theory
- Geometry optimization
- Strain the cell
- Stress tensor
- 2nd-PK stress tensor
- Finite difference method
- SOECs and TOECs

DFT Parameters

- DFT Software: Quantum ESPRESSO
- Pseudopotentials: Norm-conserving
- GGA functional: PBE
- Dispersion Correction: N/A
- k-points: Dense uniform mesh
- SCF Convergence: 10^{-6}a.u.
- Smearing Energy: 0.02 Ry

P. Giannozzi et al., J. Phys. Condens. Matter **21**, 395502 (2009).
N. Troullier and J. L. Martins, Phys. Rev. B **43**, 1993 (1991).
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Energy Density & Convergence Testing

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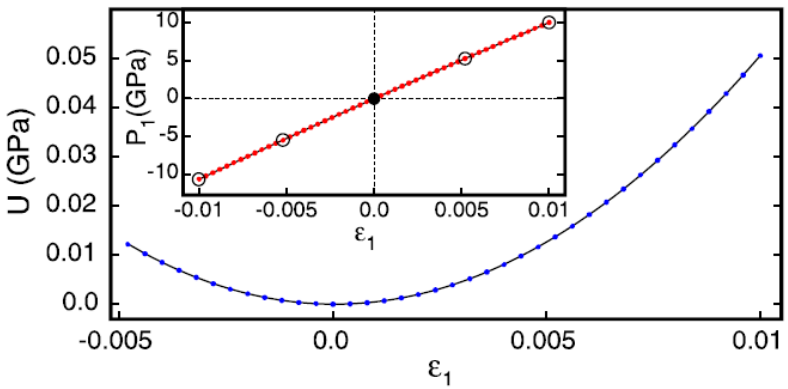

FIG. 1. Energy density U [Eq. (3)] of diamond versus normal uniaxial (Lagrangian) strain ε_1. Inset: Component P_1 of the 2nd-PK stress tensor versus ε_1. Colored disks show the results obtained from DFT calculations [19] using an energy cutoff of 300 Ry. Solid lines are guides to the eye. To calculate $C_{11}^{(2)}$ and $C_{111}^{(3)}$, we use the value of P_1 at the unstressed state (large black disk) and those obtained at either $\varepsilon_1 = \pm 0.005$ or $\varepsilon_1 = \pm 0.010$ (circles).

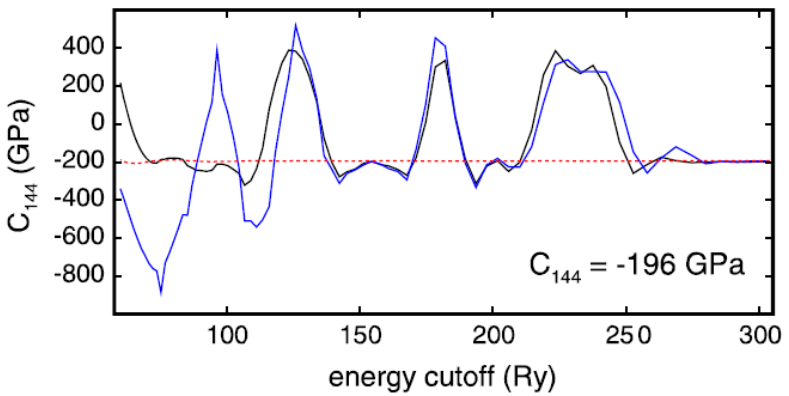

FIG. 2. $C_{144}^{(3)}$ of diamond obtained from Eq. (7) by using values of P_1 calculated by DFT at increasing energy cutoffs. $C_{144}^{(3)}$ is calculated by using the value of P_1 at an unstressed state and values of P_1 of crystals accommodating a shear strain of $\varepsilon_4 = \pm 0.005$. The blue (black) solid line shows the results obtained by (not) including in the Cauchy stress the Pulay corrective terms of Eq. (9). The red dashed line shows the results obtained by replacing P_1 at the unstressed state in Eq. (7) with the value obtained by extrapolation from the values of P_1 at $\varepsilon_4 = \pm 0.005$ and ± 0.010.

The Pulay Correction Term: $\sigma_{ij}^{p} = -\frac{2}{3}\frac{\partial E}{\partial \log E_c}\delta_{ij}$

SOECs and TOECs for 3D Materials

TABLE I. Independent SOECs and TOECs (in GPa) of diamond, silicon, aluminum, and magnesium obtained by using Eqs. (6)–(8) and the numerical solutions described in the text. Experimental data are also shown for comparison. DFT calculations are carried out by using energy cutoffs of 100 (diamond and silicon), 50 (aluminum), and 30 Ry (magnesium). All calculations are carried out by using stringent convergence thresholds, and in the case of the metals, we use fractional occupations and a smearing energy of 0.02 Ry.

	$C^{(2)}_{11}$	$C^{(2)}_{33}$	$C^{(2)}_{66}$	$C^{(2)}_{44}$	$C^{(2)}_{13}$	$C^{(2)}_{12}$	$C^{(3)}_{111}$	$C^{(3)}_{112}$	$C^{(3)}_{113}$	$C^{(3)}_{222}$	$C^{(3)}_{123}$	$C^{(3)}_{133}$	$C^{(3)}_{333}$	$C^{(3)}_{144}$	$C^{(3)}_{155}$	$C^{(3)}_{344}$	$C^{(3)}_{456}$
Diamond	1037	···	···	552	···	120	−5876	−1593	···	···	618	···	···	−197	−2739	···	−1111
Exp. Ref. [10]	1082	···	···	579	···	125	−7750	−2220	···	···	604	···	···	−1780	−2800	···	−30
Exp. Ref. [6]	···	···	···	···	···	···	−7603	−1909	···	···	835	···	···	1438	−3938	···	−2316
Silicon	142	···	···	72	···	51	−744	−393	···	···	−59	···	···	4	−297	···	−59
Exp. Ref. [27]	166	···	···	80	···	64	−795	−445	···	···	−75	···	···	15	−310	···	−86
Aluminum	108	···	···	33	···	59	−1100	−371	···	···	104	···	···	39	−421	···	−22
Exp. Ref. [7]	107	···	···	28	···	60	−1076	−315	···	···	36	···	···	−23	−340	···	−30
Magnesium	58	62	17	16	19	24	−602	−190	4	−762	−55	−107	−657	−60	−50	−163	···
Exp. Ref. [8]	59	62	17	16	···	26	−663	−178	30	−864	−76	−86	−726	−30	−58	−193	···

SOECs and TOECs for 2D Materials

PHYSICAL REVIEW LETTERS **121,** 216001 (2018)

TABLE II. SOECs and TOECs (in N m^{-1}) of monolayer graphene (G) and washboard-graphane (W) calculated by using Eqs. (6)–(8). DFT calculations are carried out by using energy cutoffs of 100 Ry and a vacuum region of 12 Å.

	$C^{(2)}_{11}$	$C^{(2)}_{22}$	$C^{(2)}_{12}$	$C^{(2)}_{44}$	$C^{(3)}_{111}$	$C^{(3)}_{222}$	$C^{(3)}_{112}$	$C^{(3)}_{122}$	$C^{(3)}_{144}$	$C^{(3)}_{244}$
G	348	348	59	144	−2920	−2873	−448	−515	−569	−639
W	276	162	21	80	−2580	−1211	−92	−295	−291	−405

We can confirm this using symmetry:

$$C^{(3)}_{244} = \frac{2C^{(3)}_{111} - C^{(3)}_{222} - C^{(3)}_{112}}{4} = -629 \text{ Nm}^{-1}$$

This check implies that there is only a $\pm 2\%$ error with this method.

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Applications:

- Alloys
- Defected Crystals
- 2D Films
- Nanomechanics
- Nonlinear acoustics
- Mechanical engineering

Praise:

- Great implementation of finite difference method
- Fantastic results on tested materials (2D & 3D)
- Good accuracy ($\pm 2\%$ vs. $\pm 50\%$)
- Decent DFT techniques

Critiques:

- Limited detail on DFT methods
- Questionable energy cutoffs
- Right for the wrong reasons?

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Acknowledgements

Questions?

Want My Slides?

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2nd-PK Stress Tensor Components vs. Shear Strain

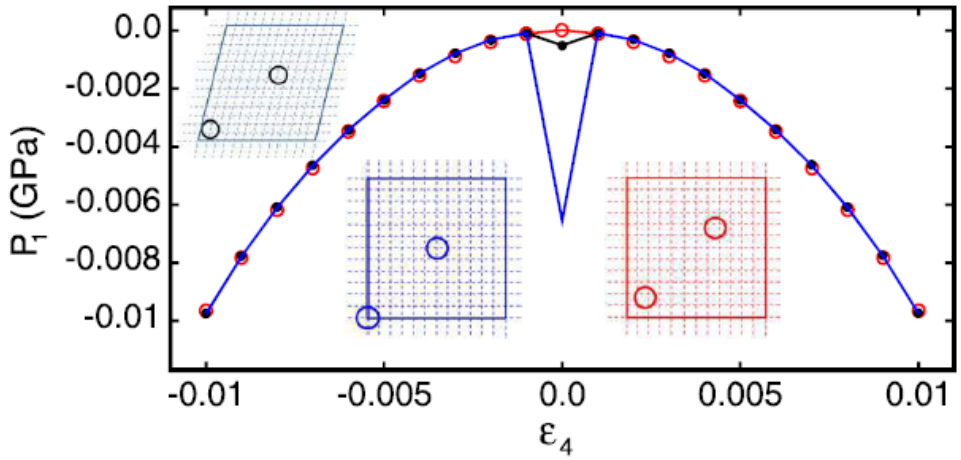

FIG. 3. Component P_1 of the 2nd-PK stress tensor of a diamond crystal accommodating a shear strain ε_4. Disks show results obtained from DFT calculations carried out using energy cutoffs of 100 (blue and black) and 200 Ry (red), with atoms in the unstressed primitive unit cell having fractional coordinates (0,0,0) and (0.25,0.25,0.25) (blue) and (x, y, z) and $(0.25 + x, 0.25 + y, 0.25 + z)$ (black and red), where x, y, z are random numbers in the interval (0,1). Insets: Schematic representations of unstressed (blue and black) and shear strained (red) unit cells, with lattice coordinates that are (blue) or are not (black and red) aligned with the real-space grid of points used to represent wave functions in plane-wave-based DFT calculations.