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Title: Application of Strain Functionals for Physics Informed Machine Learning

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Application of Strain Functionals for Physics Informed Machine Learning

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Introduction

- Quantify MD simulations of dislocation-GB interactions
  - Stukowski approaches (OVITO): *ad hoc* and incomplete
  - SOAP more complete (& redundant): no direct physical interpretation
- Development of quantifiable metrics
  - Strain Functional Descriptors (initial development XWG6)
  - Mathematically complete and unique (non-redundant)
- Basis for Physics Informed Machine Learning analysis
  - Leading to physically justifiable models
  - Also maps onto diffraction analysis cleanly

N. Mathew, J.P. Tavenner, C.M. Adams and E.M. Kober, *Development of Strain Functionals to Characterize Atomistic Geometries,* in preparation.

Strain Functional Derivation:
Map atomic quantities to continuum field

Map atomic quantities g_j to continuum field G using a Gaussian kernel

$$G(\boldsymbol{r}) = \sum_j g_j W_j = \sum_j \frac{g_j}{V_0} exp\left(-\frac{|\boldsymbol{r}-\boldsymbol{r_j}|^2}{2\sigma^2}\right)$$

N = number density	$g_j = 1$
ρ = number density	g_j = atomic mass
U = velocity field	g_j = atomic velocity

Define local number density (N) as a Taylor series expansion about $\mathbf{r_i}$: $\mathbf{r} = \mathbf{r_i} + \Delta\mathbf{r}$

$$N(\boldsymbol{r}) \approx N(\boldsymbol{r_i}) + \Delta\boldsymbol{r} \odot \left.\frac{\partial N}{\partial r}\right|_{\boldsymbol{r_i}} + \frac{\Delta\boldsymbol{r}\otimes\Delta\boldsymbol{r}}{2} \odot \left.\frac{\partial^2 N}{\partial r^2}\right|_{\boldsymbol{r_i}} + \frac{\Delta\boldsymbol{r}\otimes\Delta\boldsymbol{r}\otimes\Delta\boldsymbol{r}}{6} \odot \left.\frac{\partial^3 N}{\partial r^3}\right|_{\boldsymbol{r_i}} + \cdots$$

$$\left.\frac{\partial N}{\partial r}\right|_{\boldsymbol{r_i}} = \sum_j \left.\frac{\partial W_j}{\partial r}\right|_{\boldsymbol{r_i}} = -\sum_j \frac{\boldsymbol{r_{ij}}}{\sigma^2}\frac{1}{V_0} exp\left(-\frac{|\boldsymbol{r_{ij}}|^2}{2\sigma^2}\right) = -\sum_j \frac{\boldsymbol{r_{ij}}}{\sigma^2} w_{ij}$$

Weighted sum of neighbor distances

$$\left.\frac{\partial^2 N}{\partial r^2}\right|_{\boldsymbol{r_i}} = \frac{1}{\sigma^2}\sum_j \left[\frac{\boldsymbol{r_{ij}}\otimes\boldsymbol{r_{ij}}}{\sigma^2} - \boldsymbol{I_2}\right] w_{ij}$$

~ conventional strain: deviatoric and total (trace) (Han, Zimmerman)

$$\left.\frac{\partial^4 N}{\partial r^4}\right|_{\boldsymbol{r_i}} = \frac{1}{\sigma^4}\sum_j \left[\frac{\boldsymbol{r_{ij}}\otimes\boldsymbol{r_{ij}}\otimes\boldsymbol{r_{ij}}\otimes\boldsymbol{r_{ij}}}{\sigma^4} - 6\frac{\boldsymbol{r_{ij}}\otimes\boldsymbol{r_{ij}}}{\sigma^2}\otimes\boldsymbol{I_2} + \boldsymbol{I_4}\right] w_{ij}$$

Tensor Hermite polynomials

Strain Functional Derivation:
Taylor Series Expansion & Atomic Orbital Analogy

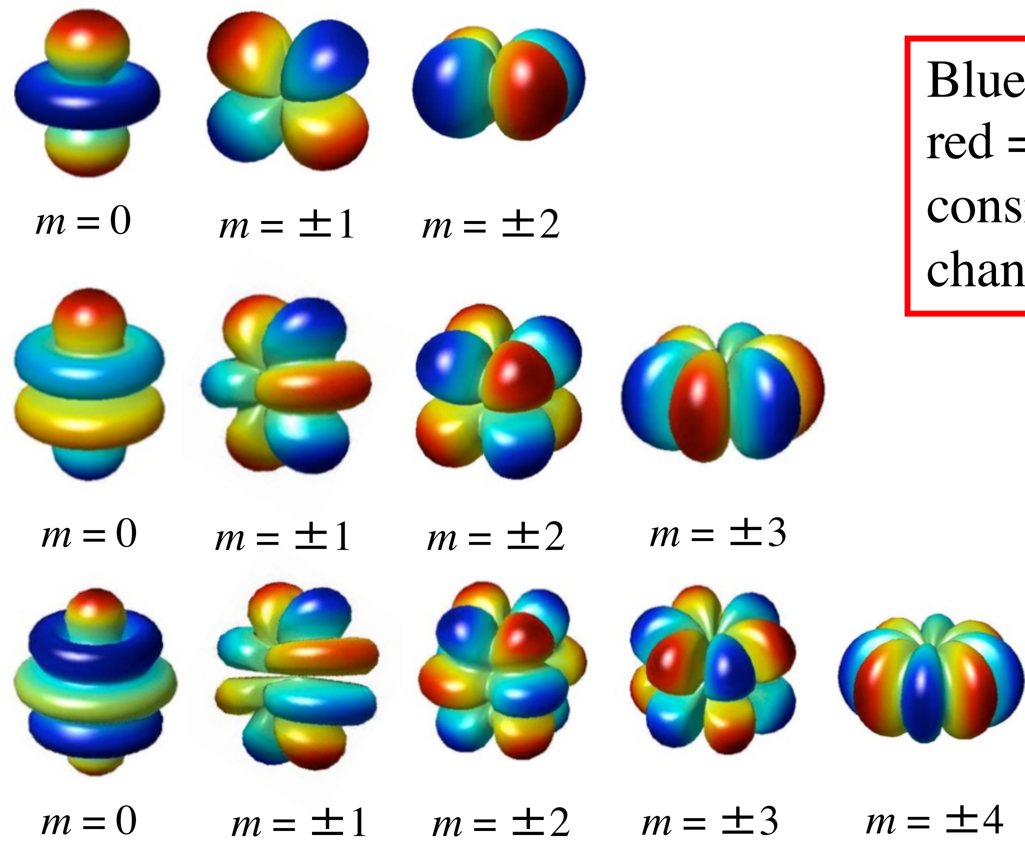
- Standard *nth* order convergence in accuracy of describing the neighborhood
- Local *nth* order derivatives ⇔ local *nth* order moments (shapes)
- Atomic volume V_0 defines σ (~1.2 Å for Cu)
  - 50-80 neighbors for numerical precision
  - Shapes are strongly dominated by the 1^{st} nearest neighbors
- Hermite polynomials readily map onto Harmonic polynomials
  - Solid spherical harmonics with pure Gaussian weighting
  - That transformation generates radial nodes for subspaces (e.g. 1s vs 2s orbital)
  - Retain Principal Quantum Number (PQN) notation vs bispectrum approach
  - Readily partitioned onto rotation sub-spaces of the SO(3) 3D rotation space

Strain Functional Derivation:
Solid Harmonic Polynomials: $r^l\ Y_{lm}(\theta,\phi)\ \exp(-br^2)$

$l = 2$
d orbital
tension, shear

$l = 3$
f orbital
Tetrahedral, **3-fold symmetry, strain gradients**

$l = 4$
g orbital
Octahedral, **4-fold, Cubic crystal habit**



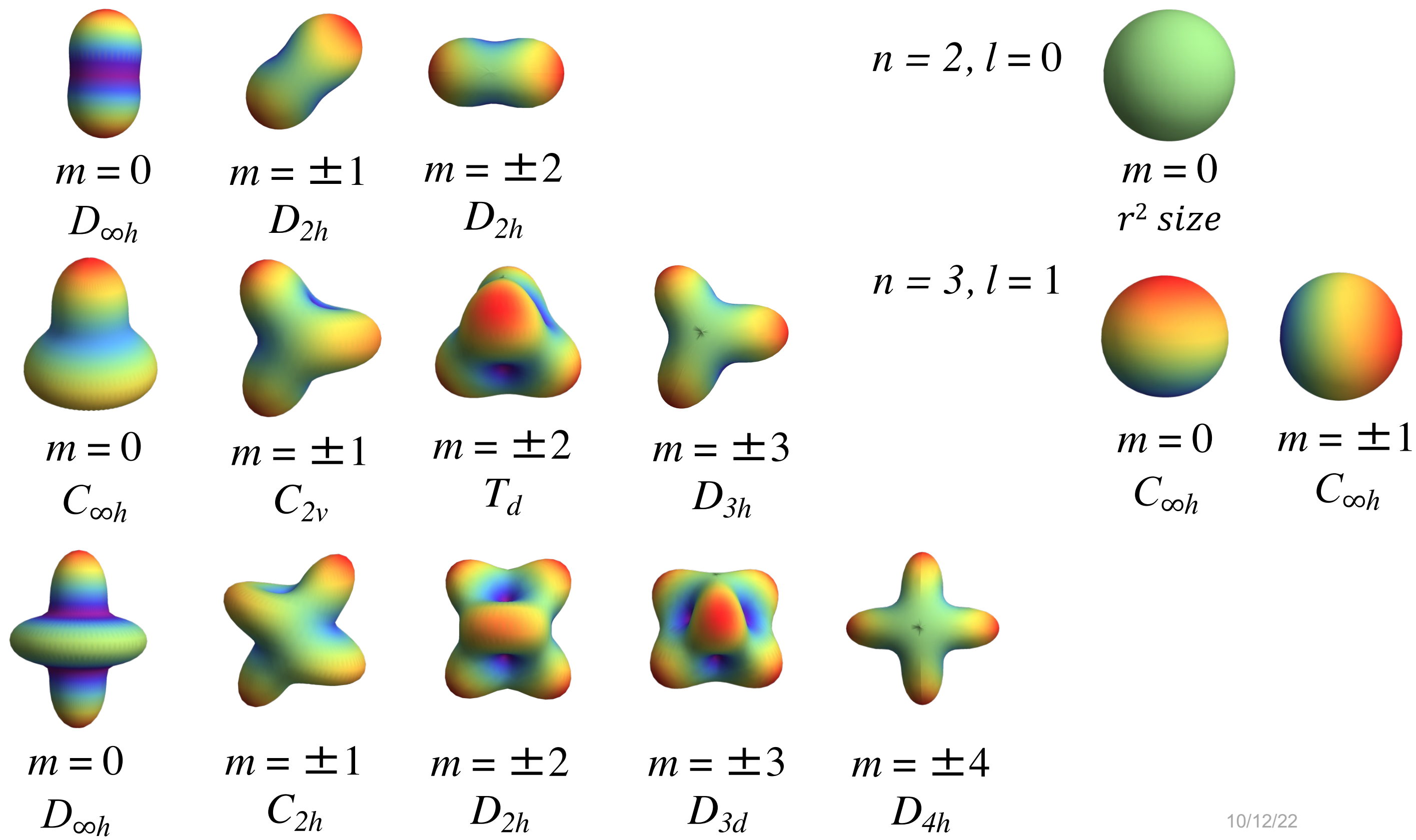
Blue = positive phase, red = negative phase; consider as density changes to a sphere…

Strain Functional Derivation:
Solid Harmonic Polynomials: $R_{nlm} \sim r^n Y_{lm}(\theta,\phi) \exp(-br^2)$

$n = 2, l = 2$
d orbital
tension, shear

$n = 3, l = 3$
f orbital
Tetrahedral, **3-fold symmetry, strain gradients**

$n = 4, l = 4$
g orbital
Octahedral, **4-fold, Cubic crystal habit**



Strain Functional Derivation: Contrasts with SOAP (GAP), SNAP

- Use of pure Gaussian weights
  - Transformation generates radial nodes defined by σ
  - Analogous to hydrogen-like orbitals with Principal Quantum Numbers: *n, l, m*
  - The *nth* shell tracks the *nth* order of the Taylor series expansion
- Use of non-Gaussian weights loses this
  - Requires the bispectrum approach which mixes terms between orders: convergence?
  - SOAP, GAP (Csanyi group): truncated Gaussian, Bessel Functions
  - SNAP (Thompson): stronger cut-off function: completeness
  - General spherical harmonic properties retained: Y_{lm}, *but not* R_{nlm}
- SFDs and PQN labels map directly onto Spherical Tensors
  - Spherical Tensor ⇔ Angular Momentum Vector ⇔ $\mathbf{Y_{lm}}$ ⇔ $\{Y_{l\text{-}l}, \ldots, Y_{ll}\}$
  - These map onto different subspaces of SO(3) 3D rotation space
  - General rank *n* tensor can be expressed in terms of irreducible spherical tensors

Strain Functionals: Irreducible Spherical Tensors

"The description of the physical properties of condensed matter using irreducible tensors"
J. Jerphagnon, D. Chemla, R. Bonneville
Advances in Physics **27**, 609 (1978)

Identifies number of independent components and subspaces for various physical properties

Stress: 6 = 1x5 + 1x1
Strain Gradient: 10 = 1x7 + 1x3
Cauchy: 15 = 1x9 + 1x5 + 1x1
Elasticity: 21 = 1x9 + 2x5 + 2x1

Each subspace should be expressible as rotational invariants…

Table 1. Reduction spectrum of tensors up to rank 4.

Rank	Indices partition	Example	Number of components		Reduction spectrum				
				J :	0	1	2	3	4
				$2J+1$:	1	3	5	7	9
				Name :	scalar	vector	deviator	septor	nonor
0		Pressure	1		1				
1	r	Spontaneous polarization	3			1			
2	rs	Optical activity	9		1	1	1		
	(rs)	Stress and strain	6		1		1		
3	rst	Optical mixing	27		1	3	2	1	
	$(rs)t$	Piezo-electric effect	18			2	1	1	
	(rst)	Kleinman symmetry in SHG	10			1		1	
4	$rstu$	Optical mixing	81		3	6	6	3	1
	$(rs)tu$	Photo-elastic effect	54		2	3	4	2	1
	$(rs)(tu)$	Kerr effect	36		2	1	3	1	1
	$(rst)u$	Third harmonic generation	30		1	1	2	1	1
	$((rs)(tu))$	Elasticity	21		2		2		1
	$(rstu)$	Cauchy relations	15		1		1		1

Construction of Rotational Invariants

- Addition of angular momentum vectors: $v_{l(n)}{}^{m} \sim r^{n}\ Y_{l}^{m}\ exp(-br^{2})$
  - $\boldsymbol{v_l} = \{v_l^{-l}, v_l^{-l+1}, \ldots, v_l^{l-1}, v_l^{l}\}$: $2l+1$ terms (DOF)
  - Addition using Clebsch-Gordan coupling coefficients (Lo & Don, Edmonds)
  - *Analogous to tensor inner & outer products, contractions*
  - Can then add in a third, fourth, … vector (infinite…)

$$v(l,l')_j^k = \sum_{m=-l}^{l} \langle l, m, l', k-m | l, l', j, k \rangle\, v_l^m v_{l'}^{k-m}$$

- For $j=0$, the result is a rotationally invariant scalar
  - For $l=l'$, $j=0$ this is the norm of the vector $\boldsymbol{v_l}$
  - For two different vectors $\boldsymbol{v_l} \neq \boldsymbol{v_l}'$, $j=0$ ➔ dot product defining relative orientation
  - $2l+1$ contractions define the $2l+1$ DOF: no more, no less
  - But an infinite number of possible contractions…

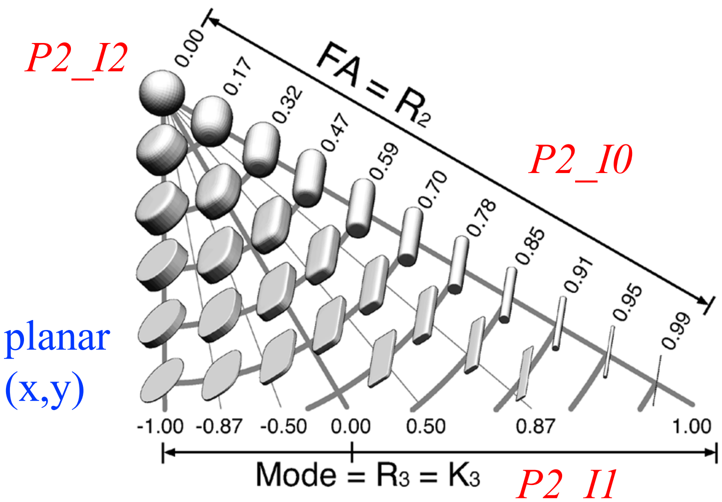
"3-D Moment Forms: Their Construction and Application to Object Identification and Positioning" C.-H. Lo, H. S. Don *IEEE Trans. Patt. Analysis Mach. Intel.* **11**, 1053 (1989)
"Angular Momentum and Quantum Mechanics" A. R. Edmonds, Princeton, 1974

Rank 2 Invariants: Shear & Size

- Rank 2 moment tensors have 6 independent factors
  - Traceless rank 2 tensor & scalar trace: 1x5 + 1x1
  - Scalar is the mean of the eigenvalues (EV): $P2\_I2 = \nu_{0(2)}{}^{0}$
  - Traceless rank 2 tensor (spherical tensor) has two invariants
    - Net 2-fold distortion: rms EV: $P2\_I0 = \nu(2,2)_0{}^0$
    - Skewness EV: $P2\_I1 = \nu((2,2)_2,2)_0{}^0$
  - 3 degrees of freedom define orientation wrt arbitrary axis
    - $O2\_I0 = \nu(2,Z^2)_0{}^0$
    - $O2\_I1 = \nu((2,2)_2, Z^2)_0{}^0$
    - $O2\_I2 = \nu((2,2)_2, X^2\text{-}Y^2)_0{}^0$

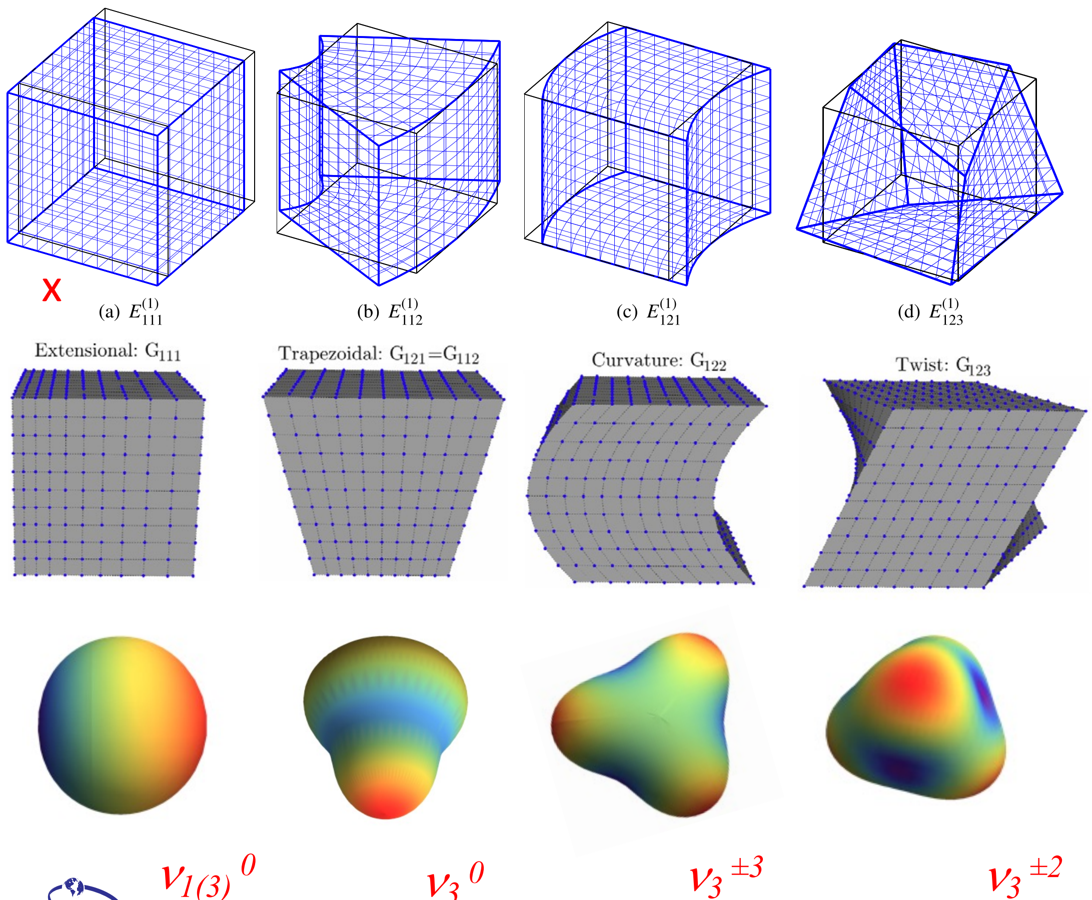
$$M = \begin{bmatrix} XX & XY & XZ \\ XY & YY & YZ \\ XZ & YZ & ZZ \end{bmatrix}$$

$$\boldsymbol{Z^2} = \frac{1}{\sqrt{6}}\begin{bmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 2 \end{bmatrix} \quad \boldsymbol{X^2}-\boldsymbol{Y^2} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & 0 \end{bmatrix}$$



MRI Analysis: Water diffusion tensor
G. Kindlmann *IEEE Trans. Med. Imag.* 2007, **26**, 1483

Rank 3 Tensors = Strain Gradients



Admal, N.C., J. Marian, and G. Po, *The atomistic representation of first strain-gradient elastic tensors.* Journal of the Mechanics and Physics of Solids, 2017. **99**: p. 93-115.

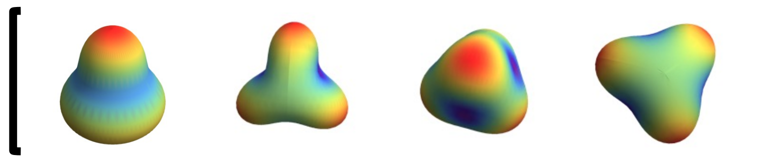
Luscher, D.J., D.L. McDowell, and C.A. Bronkhorst, *A second gradient theoretical framework for hierarchical multiscale modeling of materials.* International Journal of Plasticity, 2010. **26**(8): p. 1248-1275.

Rank 3 Invariants = Strain Gradients

$\nu(3,3)_0^0 = |\nu_3^0, \nu_3^{\pm1}, \nu_3^{\pm2}, \nu_3^{\pm3}|$

Net 3rd order distortions

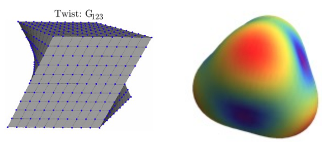
P3_I0



$\nu_3^0\,(C_{\infty h})$ $\nu_3^1\,(C_{2v})$ $\nu_3^2\,(T_d)$ $\nu_3^3\,(D_{3h})$

$\nu((3,3)_3,3)_0^0 = 0$

$\nu((3,3)_3,(3,3)_3)_0^0 = k\,[\nu(3,3)_0^0]^2$



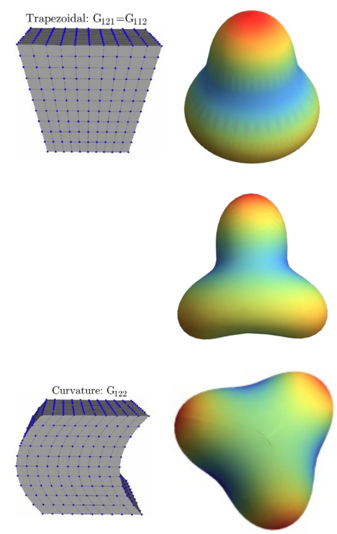
Tetrahedron
Most symmetric
3rd order distortion

0 →

P3_I1

$\nu((3,3)_2,(3,3)_2)_0^0$

Non-tetrahedral



axial (z)

0

P3_I2

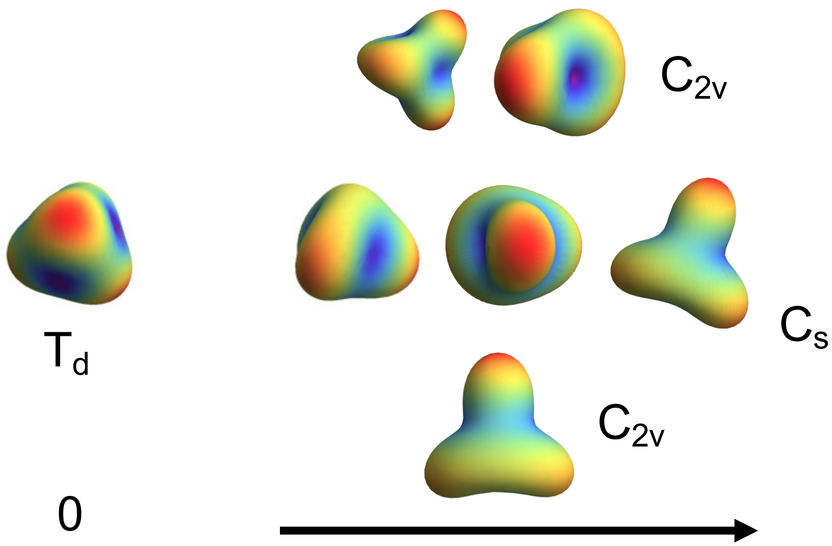
$\nu(((3,3)_2,(3,3)_2)_2,(3,3)_2)_0^0$

skewness

planar (xy)

P3_I2 defines internal axes

Rank 3 Invariants = Strain Gradients



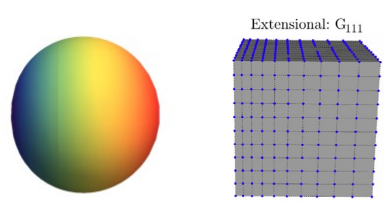
Angle between
~C_2 and ~C_3 axes

0 P3_I3
$\nu(((3,3)_4,(3,3)_4)_4,(3,3)_4)_0^0$
2^{nd} skewness

P3_I1 $\nu((3,3)_2,(3,3)_2)_0^0$

$A\ \nu((3,3)_2,(3,3)_2)_0^0 + B\ \nu((3,3)_4,(3,3)_4)_0^0 = [\nu(3,3)_0^0]^2$
$C\ \nu((3,3)_2,(3,3)_2)_0^0 + D\ \nu((3,3)_6,(3,3)_6)_0^0 = [\nu(3,3)_0^0]^2$
$E\ \nu((3,3)_4,(3,3)_4)_0^0 + F\ \nu((3,3)_6,(3,3)_6)_0^0 = [\nu(3,3)_0^0]^2$

P3_I4 $\nu(1_3,1_3)_0^0$



$\partial ZZ/\partial z$
Separate
subspace

Rank 3 Invariants (Strain Gradients 3x3x3): 10 DOF

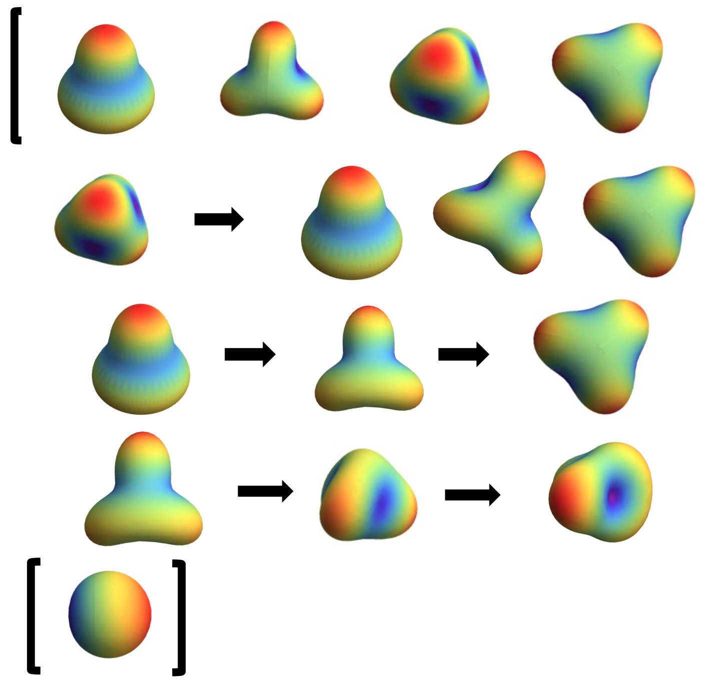
$P3\_I0 = v(3,3)_0^0$ $= |\nu_3^0, \nu_3^{\pm1}, \nu_3^{\pm2}, \nu_3^{\pm3}|$
General 3rd order deviatoric

$P3\_I1 = v((3,3)_2,(3,3)_2)_0^0$
Non-tetrahedral

$P3\_I2 = v(((3,3)_2,(3,3)_2)_2,(3,3)_2)_0^0$
Axial skewness, axes

$P3\_I3 = v(((3,3)_4,(3,3)_4)_4,(3,3)_4)_0^0$
2nd skewness, low symmetry

$P3\_I4 = v(1_3,1_3)_0^0$
Extensional gradient



External orientation

$O3\_I0 = v((3,3)_2,Z^2)_0^0$
$O3\_I1 = v(((3,3)_2,(3,3)_2)_2,Z^2)_0^0$
$O3\_I2 = v(((3,3)_2,(3,3)_2)_2,X^2\text{-}Y^2)_0^0$

Internal orientation

$P3\_I5 = v((3,3)_2,(1,1)_2)_0^0$
$P3\_I6 = v(((3,3)_2,(3,3)_2)_2,(1,1)_2)_0^0$

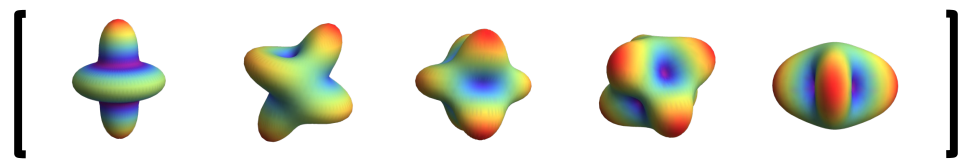
10 DOF: complete and non-redundant

Rank 4 Invariants = Cubic deformations

$\nu(4,4)_0^0 = |\nu_4^0, \nu_4^{\pm1}, \nu_4^{\pm2}, \nu_4^{\pm3}, \nu_4^{\pm4}|$

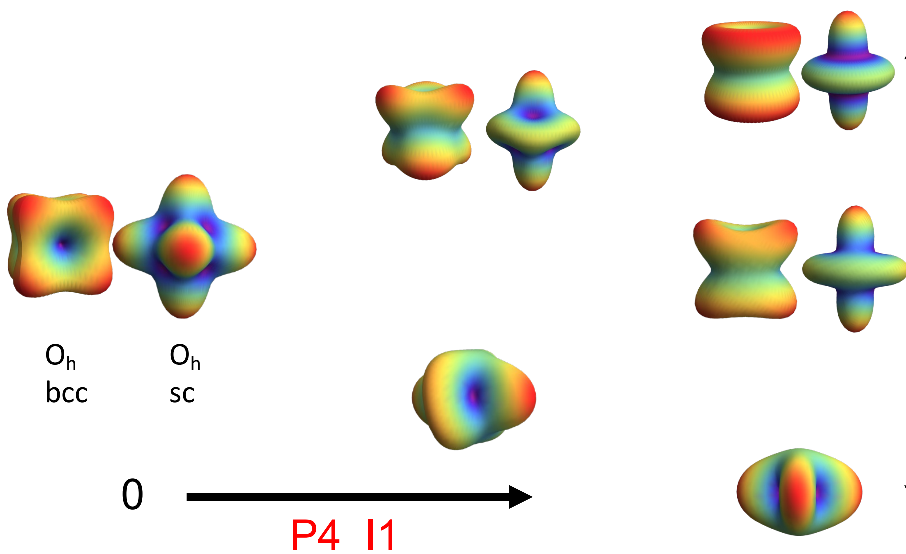
Net 4th order distortions

P4_I0



$\nu_4^0\,(D_{\infty h})$ $\nu_4^1\,(C_{2h})$ $\nu_4^2\,(D_{2h})$ $\nu_4^3\,(D_{3d})$ $\nu_4^4\,(D_{4h})$

Octahedron
Most symmetric
4th order distortion



P4_I1

$\nu((4,4)_2,(4,4)_2)_0^0$

Non-octahedral

axial (z)
Tetragonal a > b = c

P4_I2

$\nu(((4,4)_2,(4,4)_2)_2,(4,4)_2)_0^0$

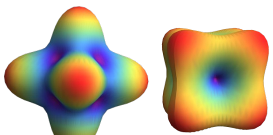
rhombohedral

planar (xy)
Tetragonal a < b = c

P4_I2 defines internal axes

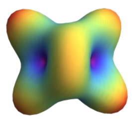
Rank 4 Invariants = Cubic deformations

Cubic
4 C_3 & 6 C_2
O_h



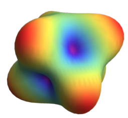
O_h O_h

Monoclinic
1 C_2
C_{2h}



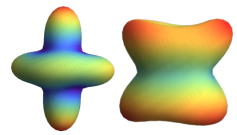
$\upsilon_4^1 + \upsilon_4^4$
C_{2h}

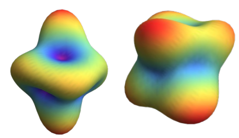
Trigonal
1 C_3 & 3 C_2
D_{3d}



υ_4^3
D_{3d}

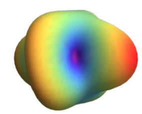
0





$\nu((4,4)_4,(4,4)_4)_0^0$

P4_I1 $\nu((4,4)_2,(4,4)_2)_0^0$



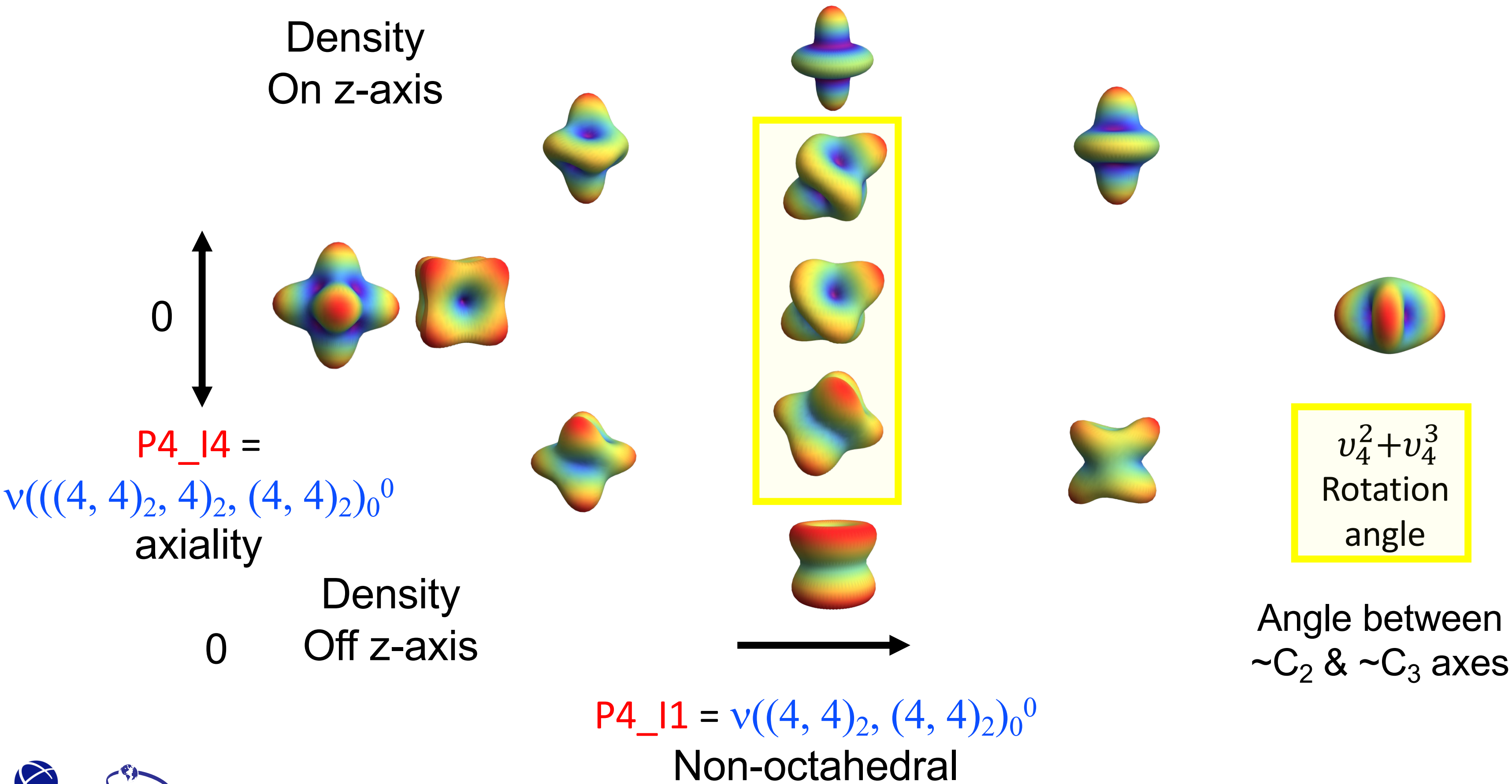
Monoclinic
C_{2h}

0 P4_I3

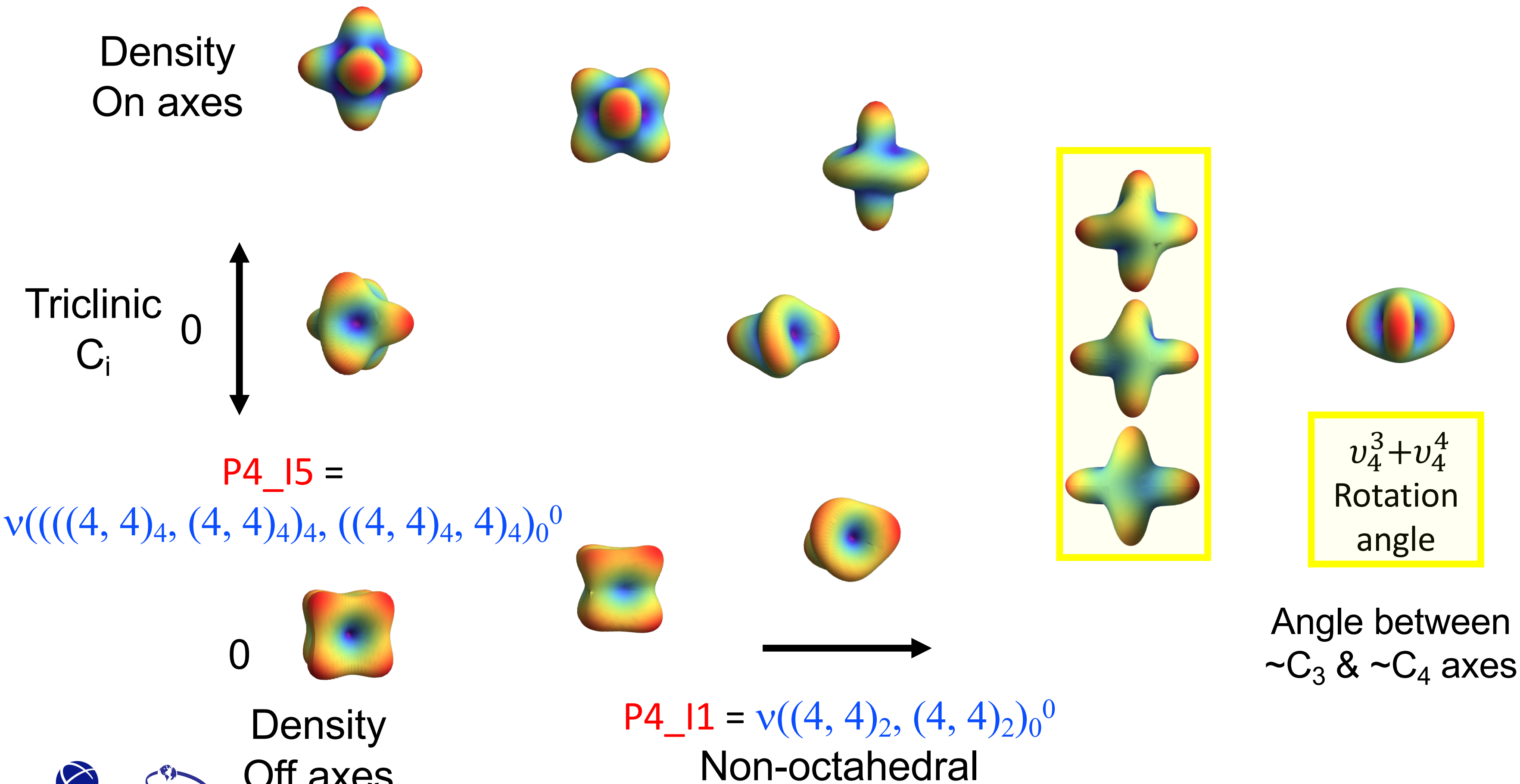
$\nu(((4,4)_4,(4,4)_4)_4,(4,4)_4)_0^0$

Trigonal metric
Quality & number
of ~C_3 axis

Rank 4 Invariants = Cubic deformations

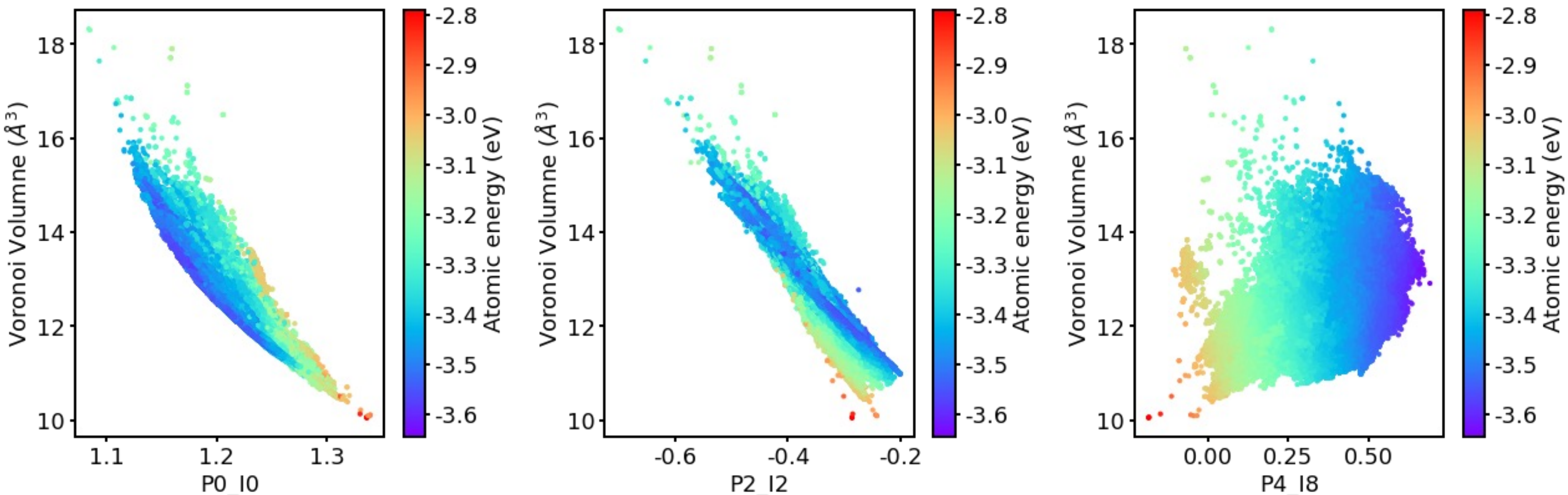


Rank 4 Invariants = Cubic deformations



Voronoi volume and SFDs

- Combined dataset shows also a correlation of 0.94 is observed between Voronoi volume and P0_I0



Rank 4 Invariants: 15 for Cauchy ($\partial^4/\partial r^4$) unique & complete

	Harmonic Polynomials	Rotational Invariants	
R_{44m} (5g)	ν_4^{4}	$\nu(4, 4)_0^0$	4^{th} order shapes
	ν_4^{3}	$\nu((4, 4)_2, (4, 4)_2)_0^0$	
	ν_4^{2}	$\nu(((4, 4)_2, (4, 4)_2)_2, (4, 4)_2)_0^0$	
	ν_4^{1}	$\nu(((4, 4)_4, (4, 4)_4)_4, (4, 4)_4)_0^0$	
	ν_4^{0}	$\nu(((4, 4)_2, 4)_2, (4, 4)_2)_0^0$	
	ν_4^{-1}	$\nu((((4, 4)_4, (4, 4)_4)_4, ((4, 4)_4, 4)_4)_0^0$	
	ν_4^{-2}	$\nu((4, 4)_2, Z^2)_0^0$	Orientations with respect to external frame
	ν_4^{-3}	$\nu(((4, 4)_2, (4, 4)_2)_2, Z^2)_0^0$	
	ν_4^{-4}	$\nu(((4, 4)_2, (4, 4)_2)_2, X^2\text{-}Y^2)_0^0$	
R_{42m} (4d)	$\nu_2^{2} \bullet (r^2\text{-}a)$	$\nu(2_4, 2_4)_0^0$	2nd order shapes (with 1 radial node)
	$\nu_2^{1} \bullet (r^2\text{-}a)$	$\nu((2_4, 2_4)_2, 2_4)_0^0$	
	$\nu_2^{0} \bullet (r^2\text{-}a)$	$\nu((4, 4)_2, 2_4)_0^0$	Orientation 2^{nd} order wrt 4^{th} order shapes
	$\nu_2^{-1} \bullet (r^2\text{-}a)$	$\nu((2_4, 2_4)_2, (4, 4)_2)_0^0$	
	$\nu_2^{-2} \bullet (r^2\text{-}a)$	$\nu(((4, 4)_2, (4, 4)_2)_2, 2_4)_0^0$	
R_{400} (3s)	$\nu_0^{0} \bullet (r^4\text{-}br^2\text{-}c)$	$\nu(0_4, 0_4)_0^0$	r^4 radial extent (with 2 radial nodes)

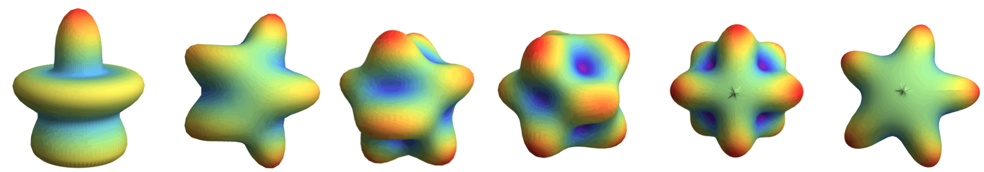
Elasticity (compliance) tensor has 21 elements with additional 4d' & 3s' terms arising from inequivalence of XYXY and XXYY type terms

Rank 5 Invariants

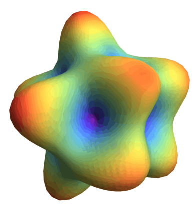
$\nu(5,5)_0^0 = |\nu_5^0, \nu_5^{\pm1}, \nu_5^{\pm2}, \nu_5^{\pm3}, \nu_5^{\pm4}, \nu_5^{\pm5}|$

Net 5th order distortions

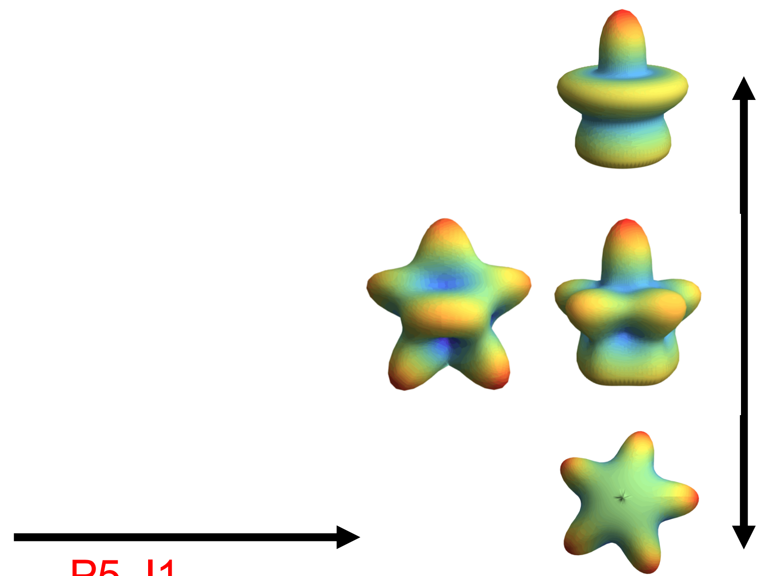
P5_I0



$\nu_5^0\,(C_{\infty h})$ $\nu_5^1\,(C_{2v})$ $\nu_5^2\,(D_{2d})$ $\nu_5^3\,(D_{3h})$ $\nu_5^4\,(D_{4d})$ $\nu_5^5\,(D_{5h})$



“The Blob” C_s
No symmetric
5th order structure



axial (z)

0

P5_I2

$N[[[5,5]_2,[5,5]_2]_2,[5,5]_2]_0^0$

skewness

planar (xy)

0

P5_I1

$N[[5,5]_2,[5,5]_2]_0^0$

5-fold character

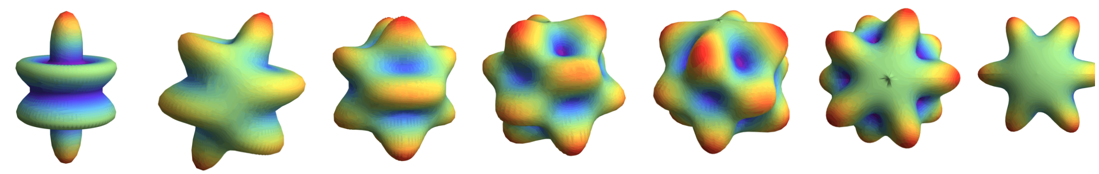
P5_I2 defines
internal axes

Rank 6 Invariants

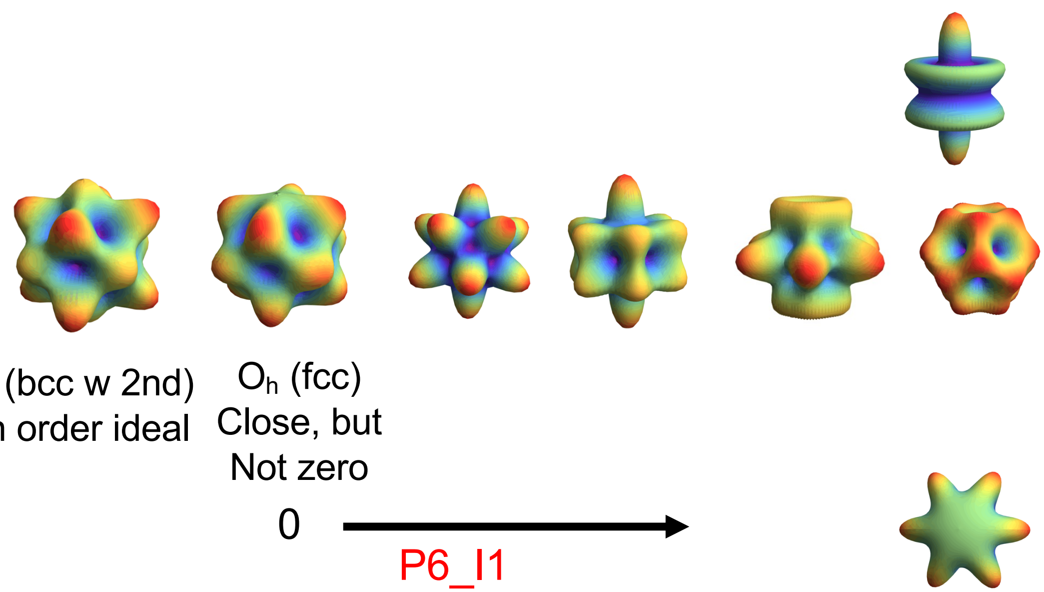
$\nu(6,6)_0^0 = |\nu_6^0, \nu_6^{\pm1}, \nu_6^{\pm2}, \nu_6^{\pm3}, \nu_6^{\pm4}, \nu_6^{\pm5}, \nu_6^{\pm6}|$

Net 6th order distortions

P6_I0



$\nu_6^0\,(D_{\infty h})$ $\nu_6^1\,(C_{2h})$ $\nu_6^2\,(D_{2h})$ $\nu_6^3\,(D_{3d})$ $\nu_6^4\,(O_h)$ $\nu_6^5\,(D_{5d})$ $\nu_6^6\,(D_{6h})$



O_h (bcc w 2nd)
6th order ideal

O_h (fcc)
Close, but
Not zero

0

P6_I1

$N[[6,6]_2,[6,6]_2]_0^0$

5-fold character

axial (z)

0

P6_I2

$N[[[6,6]_2,[6,6]_2]_2,[6,6]_2]_0^0$

skewness

planar (xy)

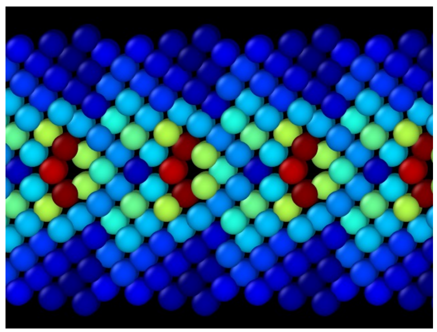
P6_I2 defines
internal axes

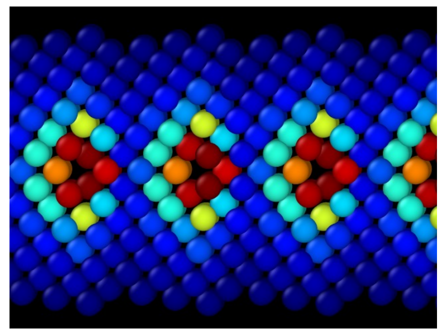
Characterizing Simulations

- SFDs provide numerical measures of different geometric distortions
- Single snapshots can be noisy: time-average or minimize
- Physically complete and interpretable basis for classification

{100} symmetric tilt
Misorientation = 74°

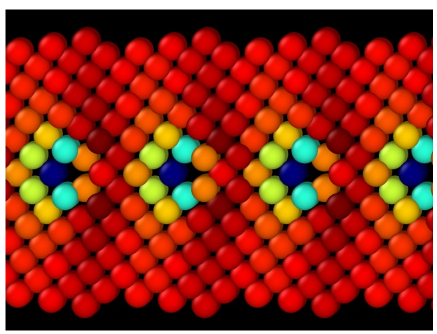
P4_I1
Non-fcc (O_h) metric

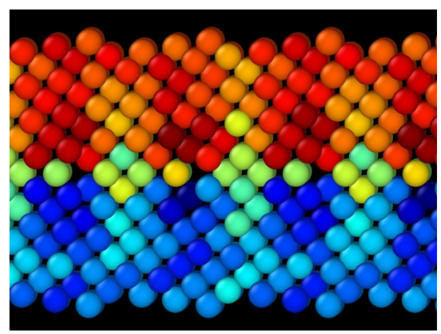




P3_I0
net strain gradient

P2_I2
average r^2





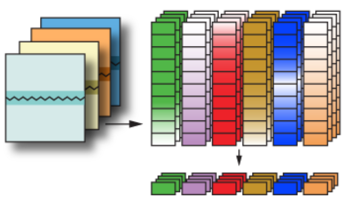
O4_I2
rotation angle

GBE prediction using GMM classes

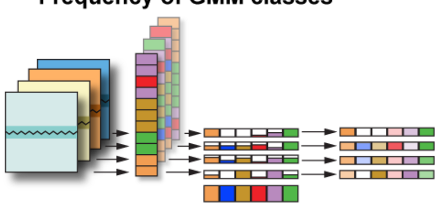
- Regression models are developed using **GMM class probability** and **frequency**

Six-class GMM

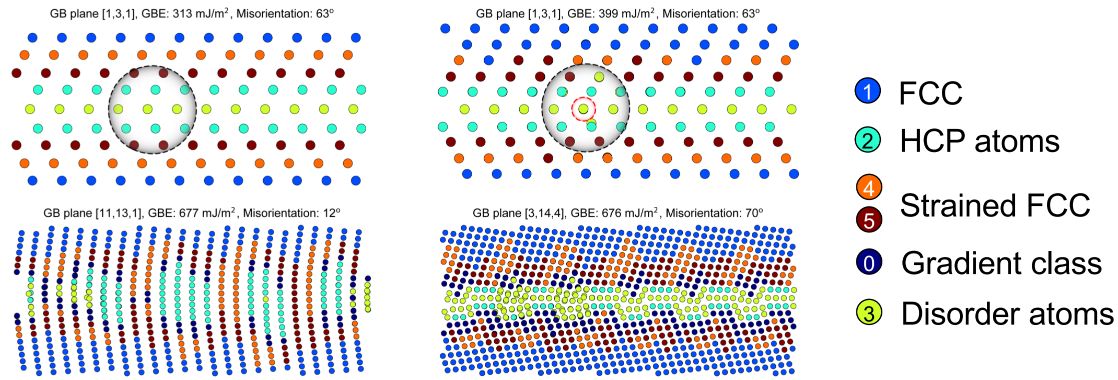
GMM class probability



Frequency of GMM classes



<112> symmetric tilt

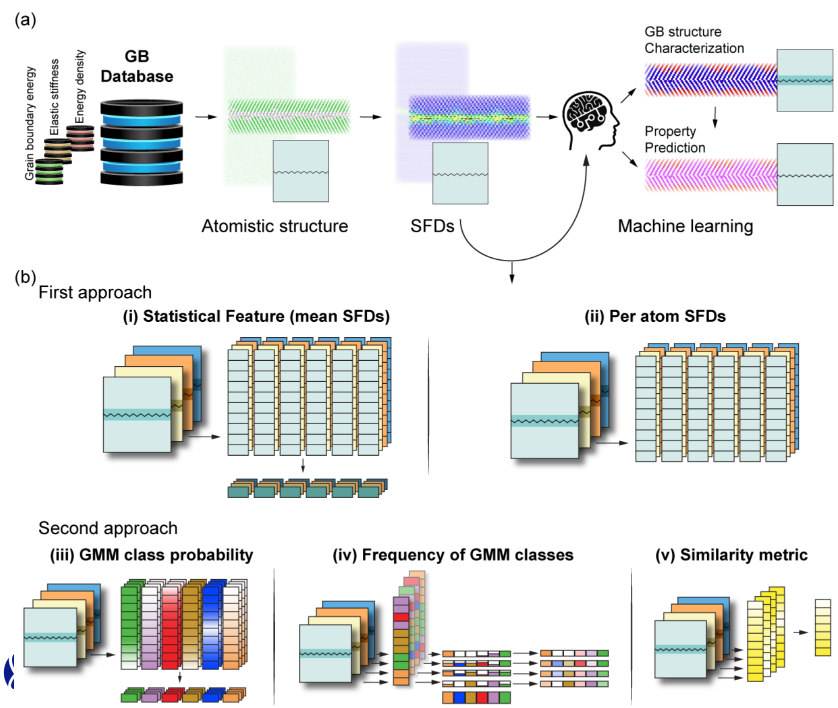


GMClass	P0_I0	P1_I0	P2_I0	P2_I1	P2_I2	P3_I0	P3_I1	P3_I2	P3_I3	P3_I4	P4_I0	P4_I1	P4_I2	P4_I3	P4_I4	P4_I5	P4_I6	P4_I7	P4_I8
0	1.232	0.000	0.051	0.011	-0.288	0.089	0.052	0.023	0.022	0.034	0.506	0.287	-0.035	0.006	-0.090	-0.203	0.098	0.027	0.485
1	1.234	0.000	0.008	0.000	-0.276	0.010	0.007	0.004	0.001	0.003	0.481	0.172	0.104	0.113	-0.143	-0.327	0.011	0.000	0.519
2	1.227	0.000	0.059	0.010	-0.306	0.137	0.081	0.044	0.036	0.041	0.522	0.369	-0.162	-0.048	0.010	-0.058	0.111	0.006	0.461
3	1.222	0.001	0.093	0.005	-0.332	0.196	0.104	0.053	0.068	0.081	0.502	0.335	-0.111	-0.057	-0.025	-0.093	0.217	0.049	0.396
4	1.238	0.000	0.021	0.004	-0.270	0.031	0.019	0.007	0.003	0.009	0.479	0.151	0.001	0.084	-0.138	-0.130	0.032	0.010	0.509
5	1.230	0.000	0.022	0.001	-0.283	0.032	0.021	0.011	0.005	0.011	0.495	0.244	0.060	0.078	-0.122	-0.330	0.034	0.000	0.518

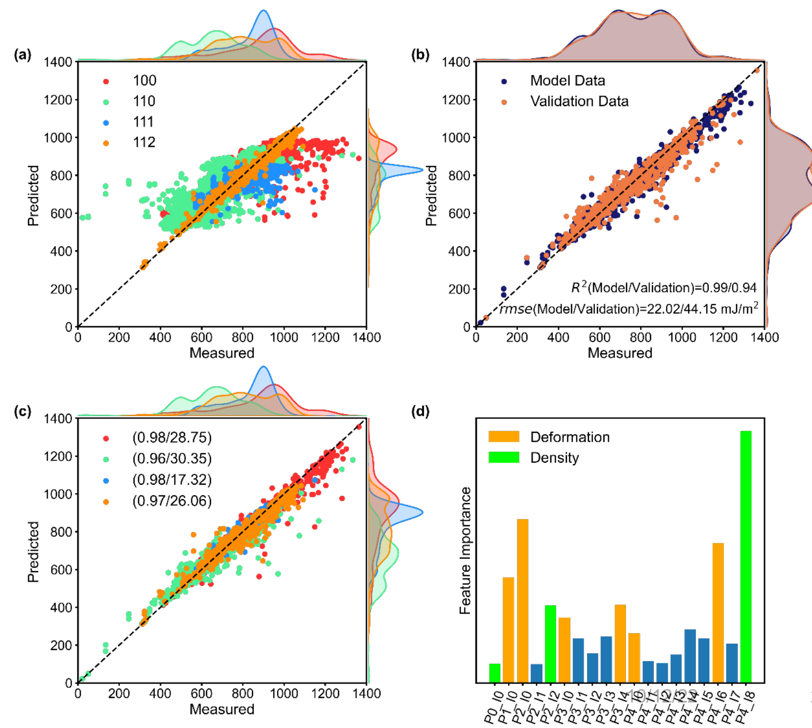
Grain boundary database and strain field descriptor

- Symmetric tilt grain boundary database of Cu (>5000) and grain boundary energy (GBE) prediction using ML

Database and workflow



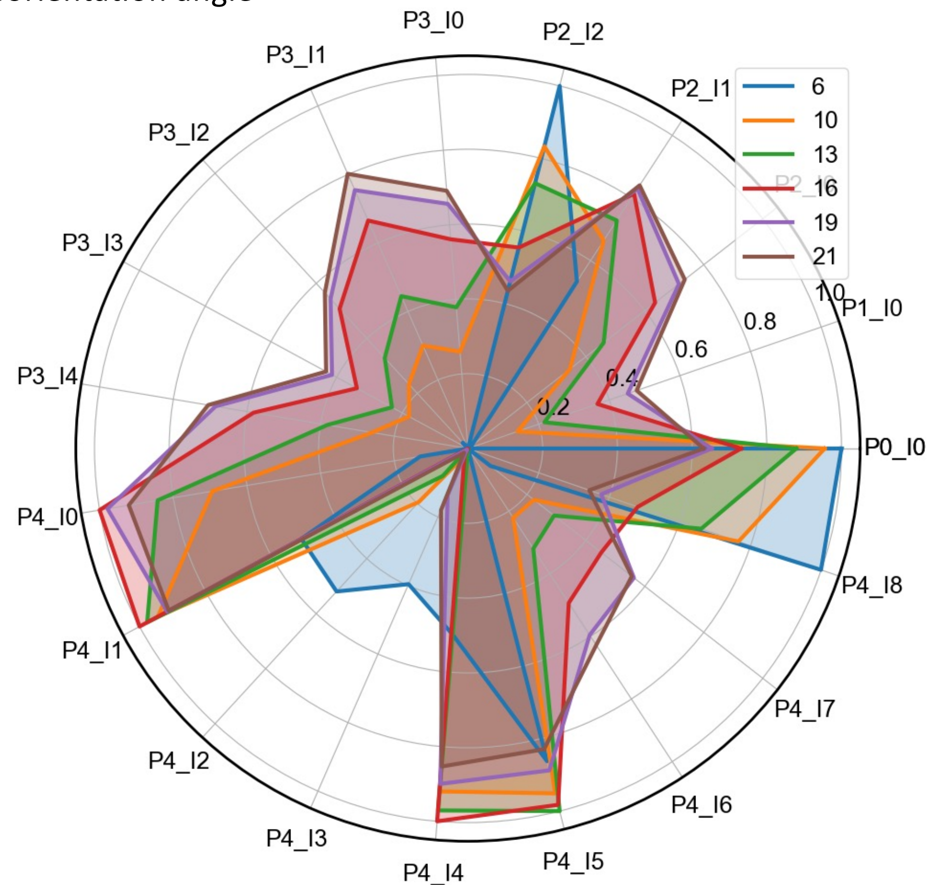
GBE prediction using ML



(100) Symmetric tilt

Label are misorientation angle

	c11	c22	c33	c44	c55	c66	GBE	mis
3	170.40	169.78	168.73	75.91	74.19	75.61	485.00	6.00
0	170.03	170.68	165.46	75.95	72.22	75.51	656.00	10.00
18	170.23	170.01	165.67	76.27	72.10	74.32	720.00	13.00
14	169.34	172.34	162.97	66.72	71.68	29.57	796.00	16.00
13	170.43	174.46	161.12	79.32	70.76	76.18	838.00	19.00
1	170.57	177.14	159.89	72.73	71.06	15.27	865.00	21.00
9	168.46	175.85	158.93	75.14	71.00	28.78	878.00	23.00
7	170.28	177.19	159.53	81.92	70.44	69.35	915.00	28.00
15	169.06	174.87	160.61	79.18	71.78	32.41	939.00	32.00
6	167.31	180.24	161.46	82.21	73.04	61.70	905.00	37.00
10	173.80	183.34	162.44	81.48	72.69	56.92	983.00	44.00
16	176.36	186.27	162.77	79.30	73.90	37.92	988.00	46.00
4	178.68	195.10	159.14	86.15	74.38	13.32	951.00	53.00
2	189.12	194.70	163.25	77.23	74.48	16.49	941.00	56.00
19	190.52	198.42	162.92	78.48	74.32	28.48	917.00	58.00
11	193.30	200.42	163.50	78.11	74.38	34.32	856.00	62.00
5	202.32	204.96	164.57	77.38	74.44	30.09	790.00	67.00
17	204.86	210.69	165.41	77.20	74.89	28.26	732.00	71.00
8	209.36	213.41	166.08	77.66	75.18	27.26	677.00	74.00
12	213.14	218.77	166.92	78.15	75.68	26.09	595.00	77.00
20	218.82	221.86	168.69	76.73	76.09	24.20	411.00	83.00



Summary

- Demonstrated SFDs as a rigorous approach to describing atomic environments
  - Minimal, complete and non-redundant for *nth* order expansion
  - Physical basis for classification, machine learning
- SFD further development
  - Extension to sixth order (full characterization of hexagonal space groups)
  - Application to diffraction analysis, neutron scattering of defects
  - Extension to vector (displacement) & tensors (compliance)
- Application future
  - Characterize general GBs (twist & tilt): 2D patterns
  - Characterize GB changes with transmission, absorption
  - Strong basis for general ML: GBs, dislocations, diffraction

Funding LDRD-DR “Investigating How Material’s Interfaces and Dislocations Affect Strength (iMIDAS)” (XX9A, Abby Hunter, PI)