Least-Square Atomic Strain

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Since strain is by definition a relative measure[1], usually one needs two atomistic configurations, the reference and the current, in order to compute the local strain. A specialized trick could work if the reference configuration is known to be of high symmetry, and that only provides the shear invariant[2, 3]. To compute the full transformation matrix $\mathbf{J}$ and strain tensor $\boldsymbol{\eta}$, one needs two configurations.

Define integer N_i to be the number of neighbors of atom i in the present configuration. For each neighbor j of atom i, their present separation is

$$\mathbf{d}_{ji} \;\equiv\; \mathbf{x}_j - \mathbf{x}_i, \tag{1}$$

and their old separation was

$$\mathbf{d}^0_{ji} \;\equiv\; \mathbf{x}^0_j - \mathbf{x}^0_i. \tag{2}$$

Note that in our present programs[4, 5, 6], $\mathbf{d}_{ji}$ and $\mathbf{d}^0_{ji}$ etc. are all considered to be row vectors.

We seek a locally affine transformation matrix $\mathbf{J}_i$, that best maps

$$\{\mathbf{d}^0_{ji}\} \;\rightarrow\; \{\mathbf{d}_{ji}\}, \quad \forall j \in N_i \tag{3}$$

in other words, we seek $\mathbf{J}_i$ that minimizes:

$$\begin{aligned}
\sum_{j\in N_i} |\mathbf{d}^0_{ji}\mathbf{J}_i - \mathbf{d}_{ji}|^2 &= \sum_{j\in N_i} (\mathbf{d}^0_{ji}\mathbf{J}_i - \mathbf{d}_{ji})(\mathbf{d}^0_{ji}\mathbf{J}_i - \mathbf{d}_{ji})^T \\
&= \sum_{j\in N_i} \mathrm{Tr}((\mathbf{d}^0_{ji}\mathbf{J}_i - \mathbf{d}_{ji})^T(\mathbf{d}^0_{ji}\mathbf{J}_i - \mathbf{d}_{ji})) \\
&= \mathrm{Tr}\sum_{j\in N_i} (\mathbf{J}_i^T\mathbf{d}^{0T}_{ji} - \mathbf{d}^T_{ji})(\mathbf{d}^0_{ji}\mathbf{J}_i - \mathbf{d}_{ji}).
\end{aligned} \tag{4}$$

Performing arbitrary matrix variation $\delta \mathbf{J}_i^T$ in above, we get

$$\begin{aligned} 0 &= \mathrm{Tr} \sum_{j \in N_i} \delta \mathbf{J}_i^T \mathbf{d}_{ji}^{0T} (\mathbf{d}_{ji}^0 \mathbf{J}_i - \mathbf{d}_{ji}) \\ &= \mathrm{Tr} \delta \mathbf{J}_i^T \sum_{j \in N_i} \mathbf{d}_{ji}^{0T} (\mathbf{d}_{ji}^0 \mathbf{J}_i - \mathbf{d}_{ji}). \end{aligned} \tag{5}$$

For the above to be true for any $\delta \mathbf{J}_i^T$, the matrix

$$\sum_{j \in N_i} \mathbf{d}_{ji}^{0T} (\mathbf{d}_{ji}^0 \mathbf{J}_i - \mathbf{d}_{ji}) \tag{6}$$

has to be zero. In other words, there must be:

$$\left(\sum_{j \in N_i} \mathbf{d}_{ji}^{0T} \mathbf{d}_{ji}^0 \right) \mathbf{J}_i = \sum_{j \in N_i} \mathbf{d}_{ji}^{0T} \mathbf{d}_{ji}. \tag{7}$$

If we define

$$\mathbf{V}_i \equiv \sum_{j \in N_i} \mathbf{d}_{ji}^{0T} \mathbf{d}_{ji}^0, \quad \mathbf{W}_i \equiv \sum_{j \in N_i} \mathbf{d}_{ji}^{0T} \mathbf{d}_{ji}, \tag{8}$$

then there is simply

$$\mathbf{J}_i = \mathbf{V}_i^{-1} \mathbf{W}_i \tag{9}$$

The Lagrangian strain matrix is then calculated as

$$\boldsymbol{\eta}_i = \frac{1}{2} \left(\mathbf{J}_i \mathbf{J}_i^T - \mathbf{I} \right). \tag{10}$$

And we can then compute its hydrostatic invariant

$$\eta_i^{\mathrm{hydro}} = \frac{1}{3} \mathrm{Tr} \boldsymbol{\eta}_i, \tag{11}$$

calibrated to $\eta_{xx} = \eta_{yy} = \eta_{zz} = a$, and the local shear invariant,

$$\begin{aligned} \eta_i^{\mathrm{Mises}} &= \sqrt{\frac{1}{2} \mathrm{Tr} (\eta - \eta_m \mathbf{I})^2} \\ &= \sqrt{\eta_{yz}^2 + \eta_{xz}^2 + \eta_{xy}^2 + \frac{(\eta_{yy} - \eta_{zz})^2 + (\eta_{xx} - \eta_{zz})^2 + (\eta_{xx} - \eta_{yy})^2}{6}}. \end{aligned} \tag{12}$$

calibrated to $\eta_{xy} = \eta_{yx} = b$, and all others zero.

Note that

1. The order of $\mathbf{J}_i$ and $\mathbf{J}_i^T$ in (10) matrix product is important. The wrong product order would also give you a symmetric matrix, but that symmetric matrix has nothing to do with the strain.

2. The product order of (10) *appears* to be the reverse of that of [1], because we adopt row-based vector scheme now [4, 5, 6], while column-based scheme was adopted in [1].

References

[1] J. H. Wang, J. Li, S. Yip, S. Phillpot, and D. Wolf. Mechanical instabilities of homogeneous crystals. *Phys. Rev. B*, 52:12627–12635, 1995.

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