Central Symmetry Parameter

Ju Li

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The central symmetry parameter $\{c_i\}$, $i = 1..N$ is used to characterize the degree of inversion symmetry breaking in each atom's local environment. Especially, it is useful for visualizing planar faults in FCC and BCC crystals[1]. This write-up is to standardize the notation.

Define integer constant M to be the maximum number of neighbors for the computation of $\{c_i\}$. For FCC lattice, we may want to use $M = 12$. For BCC lattice, we may want to use $M = 8$. The computer of course does not know whether the configuration is FCC- or BCC-based, so by default it is going to use,

$$M_{\text{default}} \equiv \left\lfloor \frac{N_{\text{most}}}{2} \right\rfloor \times 2, \tag{1}$$

where N_{most} is the most popular coordination number in the set $\{N_i\}$, $i = 1..N$ of the configuration. The user is able to override the default. But in any case, M must be even as we will be counting *pairs* of atoms.

Now for each atom $i \in 1..N$, define,

$$\tilde{m}_i \equiv \min(M, N_i). \tag{2}$$

If $\tilde{m}_i = 0$, $c_i \equiv 0$ because an isolated atom should have perfect inversion symmetry. If $\tilde{m}_i = 1$, $c_i \equiv 1$, because a coordination-1 atom has no inversion image to compare with, so

in a sense its inversion symmetry is the most broken. For $\tilde{m}_i \geq 2$, define,

$$m_i \equiv \left\lfloor \frac{\tilde{m}_i}{2} \right\rfloor \times 2, \tag{3}$$

and we use the following procedure to determine c_i.

1. Sort the $j = 1..N_i$ neighbors of atom i according to their distances $|\mathbf{d}_j|$ to atom i in ascending order. Pick the smallest m_i-set.

2. Take the closest neighbor $\mathbf{d}_1$. Search, among the other $m_i - 1$ neighbors, the one that minimizes,

$$\tilde{D}_j \equiv |\mathbf{d}_1 + \mathbf{d}_j|^2, \tag{4}$$

   and let us define,

$$j' \equiv \arg\min_{j=2..m_i} \tilde{D}_j, \quad D_1 \equiv \tilde{D}_{j'}. \tag{5}$$

3. Throw atoms 1 and j' out of the set, and look for the closest neighbor in the remaining set. Then repeat step 2 until the set is empty. We then have obtained $D_1, D_2, .., D_{m_i/2}$. Define,

$$c_i \equiv \frac{\sum_{k=1}^{m_i/2} D_k}{2\sum_{j=1}^{m_i} |\mathbf{d}_j|^2}. \tag{6}$$

(6) is dimensionless. In the case of $m_i = 2$, suppose the two neighbors are independently randomly oriented, it is easy to show that,

$$E[c_i] = \frac{1}{2}. \tag{7}$$

On the other hand, we can prove that,

$$\max_{\{\mathbf{d}_j\}} c_i = 1, \tag{8}$$

so this matches with the definition of $c_i \equiv 1$ at $\tilde{m}_i = 1$. But when $m_i \gg 2$,

$$E[c_i] < \frac{1}{2}, \tag{9}$$

because of the minimization process. For instance, at the intrinsic stacking fault in FCC lattice ABC|BCA, there is a loss of inversion symmetry in the two layers C|B, and c_i is,

$$c_i = \frac{3 \times 0 + 3 \times (d\sqrt{3}/2 \times 1/3 \times 2)^2}{2 \times 12d^2} = \frac{1}{24} \approx 0.0416, \tag{10}$$

assuming perfect stacking.

The good thing about (6) is that according to the Lindemann/Gilvarry rule[2], a crystal melts when the atomic vibrational amplitudes reach about $\sim 12\%$ of the nearest neighbor distance, therefore c_i for perfect crystal should be < 0.01 even at finite temperature, and so is easy to threshold out versus a true stacking fault (10) despite of (9).

References

[1] C.L. Kelchner, S.J. Plimpton, J.C. Hamilton, "Dislocation nucleation and defect structure during surface indentation," *Physical Review* B **58** (1998) 11085-8.

[2] J.J. Gilvarry, "The Lindemann and Gruneisen Laws", *Phys. Rev.* **102**, 308 (1956).