Machine-learned embedded atom method

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APPENDIX

A. The stress equation

Assume we have:

$$\mathbf{h} = \begin{pmatrix} h_{xx} & h_{xy} & h_{xz} \\ h_{yx} & h_{yy} & h_{yz} \\ h_{zx} & h_{zy} & h_{zz} \end{pmatrix} \tag{1}$$

$$\mathbf{n} = \begin{pmatrix} n_x \\ n_y \\ n_z \end{pmatrix} \tag{2}$$

where $\mathbf{h}$ is the 3×3 cell tensor and $\mathbf{n}$ represents the periodic boundary shift vector. Then we can get:

$$\frac{\partial r_{ij\mathbf{n}}}{\partial h_{\alpha\beta}} = \frac{1}{r_{ij\mathbf{n}}} \cdot \Delta_{ij\mathbf{n}\beta} \cdot n_\alpha \tag{3}$$

$$\Delta_{ij\mathbf{n}\beta} = r^{(0)}_{j,\beta} - r^{(0)}_{i,\beta} + \sum_\alpha n_\alpha h_{\alpha\beta} \tag{4}$$

So we can compute the derivative of E^{total} with respect to $h_{\alpha\beta}$:

$$\begin{aligned}
\frac{\partial E^{total}}{\partial h_{\alpha\beta}} &= \sum_i^N \frac{\partial E_i}{\partial h_{\alpha\beta}} = \sum_i^N \frac{\partial \left(\sum_j \sum_\mathbf{n} \phi_{ij}(r_{ij\mathbf{n}}) + F_i \left(\sum_j \sum_\mathbf{n} \rho_{ij}(r_{ij\mathbf{n}}) \right) \right)}{\partial h_{\alpha\beta}} \\
&= \sum_i^N \left(\sum_j \sum_\mathbf{n} \frac{\partial \phi_{ij}(r_{ij\mathbf{n}})}{\partial h_{\alpha\beta}} + \frac{\partial F_i(\rho_i)}{\partial \rho_i} \cdot \sum_j \sum_\mathbf{n} \frac{\partial \rho_{ij}(r_{ij\mathbf{n}})}{\partial h_{\alpha\beta}} \right) \\
&= \sum_i^N \sum_j \sum_\mathbf{n} \left(\frac{\partial \phi_{ij}(r_{ij\mathbf{n}})}{\partial h_{\alpha\beta}} + \frac{\partial F_i(\rho_i)}{\partial \rho_i} \cdot \frac{\partial \rho_{ij}(r_{ij\mathbf{n}})}{\partial h_{\alpha\beta}} \right) \\
&= \sum_i^N \sum_j \sum_\mathbf{n} \left(\frac{\partial \phi_{ij}(r_{ij\mathbf{n}})}{\partial r_{ij\mathbf{n}}} + \frac{\partial F_i(\rho_i)}{\partial \rho_i} \cdot \frac{\partial \rho_{ij}(r_{ij\mathbf{n}})}{\partial r_{ij\mathbf{n}}} \right) \cdot \frac{\partial r_{ij\mathbf{n}}}{\partial h_{\alpha\beta}} \\
&= \sum_i^N \sum_j \sum_\mathbf{n} \left(\frac{\partial \phi_{ij}(r_{ij\mathbf{n}})}{\partial r_{ij\mathbf{n}}} + \frac{\partial F_i(\rho_i)}{\partial \rho_i} \cdot \frac{\partial \rho_{ij}(r_{ij\mathbf{n}})}{\partial r_{ij\mathbf{n}}} \right) \cdot \frac{1}{r_{ij\mathbf{n}}} \cdot \Delta_{ij\mathbf{n}\beta} \cdot n_\alpha \\
&= -\sum_i^N \sum_j \sum_\mathbf{n} f_{ij\mathbf{n}\beta} \cdot n_\alpha
\end{aligned} \tag{5}$$

where $f_{ij\mathrm{n}\beta}$ is the partial force:

$$f_{ij\mathrm{n}\beta} = \left(\frac{\partial \phi_{ij}(r_{ij\mathbf{n}})}{\partial r_{ij\mathbf{n}}} + \frac{\partial F_i(\rho_i)}{\partial \rho_i} \cdot \frac{\partial \rho_{ij}(r_{ij\mathbf{n}})}{\partial r_{ij\mathbf{n}}} \right) \cdot \frac{1}{r_{ij\mathbf{n}}} \cdot \Delta_{ij\mathbf{n}\beta} \tag{6}$$

Then, we can have:

$$\begin{aligned}
\left(\left(\frac{\partial E^{total}}{\partial \mathbf{h}}\right)^T \mathbf{h}\right)_{\alpha\beta} &= \sum_{\gamma} \frac{\partial E^{total}}{\partial h_{\gamma\alpha}} h_{\gamma\beta} \\
&= -\sum_{\gamma} \sum_{i}^{N} \sum_{j} \sum_{\mathbf{n}} f_{ij\mathbf{n}\alpha} \cdot n_{\gamma} \cdot h_{\gamma\beta} \\
&= -\sum_{i}^{N} \sum_{j} \sum_{\mathbf{n}} f_{ij\mathbf{n}\alpha} \cdot \sum_{\gamma} n_{\gamma} h_{\gamma\beta} \qquad (7)
\end{aligned}$$

Thus, the virial stress tensor ϵ can be expressed with a simpler form:

$$\epsilon = -F^T R + \left(\frac{\partial E^{total}}{\partial \mathbf{h}}\right)^T \mathbf{h} \qquad (8)$$

where F is the $N \times 3$ total forces matrix and R is the $N \times 3$ positions matrix.

B. The elastic constant tensor

The elastic constant tensor $C^{\alpha\beta\gamma\delta}$ can be computed with the following equation:

$$C^{\alpha\beta\gamma\delta} = \frac{1}{V} \cdot \left(\frac{\partial \epsilon}{\partial \mathbf{h}}\right)^{\alpha\beta\gamma\eta} \mathbf{h}^{\eta\delta} \qquad (9)$$

where $\alpha, \beta, \gamma, \eta, \delta = x, y, z$, ϵ is the stress tensor, $\mathbf{h}$ is the lattice tensor and V is the volume.