

The form of the Lennard-Jones potential in lammmps adopted as:

$$V_{ij}(r) = \begin{cases} 4\varepsilon_{ij} \left[\left(\frac{\sigma_{ij}}{r_{ij}} \right)^{12} - \left(\frac{\sigma_{ij}}{r_{ij}} \right)^6 \right] & (R_{ij} \leq r_c) \\ 0 & (R_{ij} > r_c) \end{cases}$$

where r_{ij} is the distance between two atoms; ε_{ij} and σ_{ij} are the energy and distance constants, respectively.

According to the Lorentz-Berthelot mixing rules, the energy and distance constants can be obtained in the following way:

$$\sigma_{ij} = \frac{1}{2}(\sigma_i + \sigma_j)$$

$$\varepsilon_{ij} = \sqrt{\varepsilon_i \varepsilon_j}$$

Of course, the last parameter that applies to lammmps needs to be converted by unit.