

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

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

where  $r_{ij}$  is the distance between two atoms;  $\varepsilon_{ij}$  and  $\sigma_{ij}$  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.