The Vashishta potential

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Brief descriptions

- This is the Vashishta potential corresponding to [Vashishta 2007].
- It only applies to systems with two atom types.

Potential form

- The Vashishta potential is essentially a pairwise potential plus a modified form of the three-body part of the Stillinger-Weber potential. Therefore, the site potential can be written in the same form as the Stillinger-Weber potential:

$$U_i = \frac{1}{2} V_2(r_{ij}) + \frac{1}{2} \sum_{j \neq i} \sum_{k \neq i,j} h_{ijk}.$$

- The two-body part reads

$$V_2(r_{ij}) = \frac{H}{r_{ij}^{\eta}} + \frac{1}{4\pi\epsilon_0} \frac{q_i q_j}{r_{ij}} e^{-r_{ij}/\lambda} - \frac{1}{4\pi\epsilon_0} \frac{D}{2r_{ij}^4} e^{-r_{ij}/\xi} - \frac{W}{r_{ij}^6}.$$

The four terms on the right hand side of the above equation correspond to steric size effects, charge-charge interactions, charge-dipole interactions, and dipole-dipole interactions, respectively. The original paper has used Gauss units for the middle two terms and we have used the SI units.

- The two-body part is shifted in terms of both potential and force:

$$V_2^{\text{shifted}}(r_{ij}) = V_2(r_{ij}) - V_2(r_c) - (r - r_c) \frac{dV_2(r_{ij})}{dr_{ij}}\Big|_{r=r_c}.$$

Therefore, both the potential and the force for the two-body part are continuous at the cutoff distance r_c.

- The three-body part is

$$h_{ijk} = B \exp\left[\frac{\gamma}{r_{ij} - r_0} + \frac{\gamma}{r_{ik} - r_0}\right] \frac{(\cos\theta_{ijk} - h)^2}{1 + C(\cos\theta_{ijk} - h)^2}.$$

The parameter γ is always 1 A and is thus redundant.

Parameters

Parameter	Units
B	eV
h	dimensionless
C	dimensionless
r_0	A
r_c	A
H	eV A^{η}
η	dimensionless
q	e
λ	A
D	e^2 A^3
ξ	A
W	eV A^6

Potential file format

- The potential file for this potential model reads

```
vashishta 2
B_0   B_1     h_0     h_1        C     r0     rc
H_00  eta_00  q0*q0   lambda_00  D_00  xi_00  W_00
H_01  eta_01  q0*q1   lambda_01  D_01  xi_01  W_01
H_11  eta_11  q1*q1   lambda_11  D_11  xi_11  W_11
```

- The parameter η should be entered as an integer in the potential file.

References

- [1] Priya Vashishta, Rajiv K. Kalia, and Aiichiro Nakano, *Interaction potential for silicon carbide: A molecular dynamics study of elastic constants and vibrational density of states for crystalline and amorphous silicon carbide* (https://doi.org/10.1063/1.2724570), J. Appl. Phys. **101**, 103515 (2007).