LAMMPS Polymorphic version of Noritake's potential

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1 The potential

Noritake's potential [1] is composed of a sum of two and three body contributions. The pair part is given by

$$U_{\text{duet}} = \frac{1}{4\pi\varepsilon_0}\frac{Z_i Z_j e^2}{r} + f_0 b_{ij} \exp\left(\frac{a_{ij} - r_{ij}}{b_{ij}}\right) + \frac{c_{ij}}{r_{ij}^6} + D_{ij} \exp\left(-\beta_{ij} r_{ij}\right) + D'_{ij} \exp\left(-\beta'_{ij} r_{ij}\right),$$

whereas the three body part reads

$$U_{\text{triplet}} = -f\left\{\cos\left[2\left(\theta_{ijk} - \theta_0\right)\right] - 1\right\}\sqrt{k_{ij} k_{ik}},$$

with

$$k_{ij} = \frac{1}{\exp\left[g_r\left(r_{ij} - r_m\right)\right] - 1}.$$

2 LAMMPS polymorphic

Apart from the Coulombic contribution (which can be added later through the LAMMPS hybrid pair_style), Noritake's potential can be mapped into LAMMPS polymorphic pair_style [2, 3] through the following relations:

$$\eta_{ij} = \delta_{ij}(\eta = 0),\ \ \xi_{ij} = 0$$

$$U_{IJ} = f_0 b_{ij} \exp\left(\frac{a_{ij} - r_{ij}}{b_{ij}}\right) + \frac{c_{ij}}{r_{ij}^6} + D_{ij}\exp\left(-\beta_{ij} r_{ij}\right) + D'_{ij}\exp\left(-\beta'_{ij} r_{ij}\right)$$

$$V_{IJ} = 1$$

$$F_{IJ} = X$$

$$P_{JIK}\left(\Delta r\right) = P_{IK}\left(\Delta r\right) = \left\{\frac{1}{\exp\left[g_r\left(r - r_m\right)\right] - 1}\right\}^{1/2}$$

$$W_{IJ} = \left\{\frac{1}{\exp\left[g_r\left(r - r_m\right)\right] - 1}\right\}^{1/2}$$

$$G_{JIK} = f\left[\left(2\cos^2\theta - 1\right)\cos 2\theta_0 - 2\sqrt{1-\cos^2\theta}\cos\theta\sin 2\theta_0 - 1\right],\ \ (-\pi \leq \theta \leq 0).$$

Note: In private communication with one of the authors I was told that the function k_{ij} has a cutoff $r_c = r_m$ making this function purely negative. Thus it is necessary to take its absolute value when calculating P_{JIK} and W_{IJ}.

References

[1] F. Noritake, K. Kawamura, T. Yoshino, E. Takahashi, J. Non Cryst. Solids **358,** 3109 (2012).

[2] X. W. Zhou, M. E. Foster, R. E. Jones, P. Yang, H. Fan, and F. P. Doty, J. Mater. Sci. Res. **4**, 15 (2015).

[3] https://docs.lammps.org/pair_polymorphic.html.