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# 1 Tersoff potential

$$U = \frac{1}{2} \sum_{i,j} f_C(r_{ij}) [a_{ij} f_R(r_{ij}) + b_{ij} f_A(r_{ij})] \quad (1)$$

$$f_R(r) = A e^{-\lambda_1 r} \quad (2)$$

$$f_A(r) = -B e^{-\lambda_2 r} \quad (3)$$

$$f_C(r) = \begin{cases} 1, & r < R - D \\ \frac{1}{2} - \frac{1}{2} \sin \left[ \frac{\pi}{2} (r - R) / D \right], & R - D < r < R + D \\ 0, & r > R + D. \end{cases} \quad (4)$$

$$b_{ij} = (1 + \beta^n \zeta_{ij}^n)^{-1/2n}, \quad (5)$$

$$\zeta_{ij} = \sum_{k \neq i,j} f_C(r_{ik}) g_{ik}(\theta_{ijk}) e^{\lambda_3^m (r_{ij} - r_{ik})^m} \quad (6)$$

$$g_{ik}(\theta_{ijk}) = \gamma_{ik} \left[ 1 + \frac{c_{ik}^2}{d_{ik}^2} - \frac{c_{ik}^2}{d_{ik}^2 + (h_{ik} - \cos \theta_{ijk})^2} \right] \quad (7)$$

$$a_{ij} = (1 + \alpha^n \eta_{ij}^n)^{-1/2n} \quad (8)$$

$$\eta_{ij} = \sum_{k \neq i,j} f_C(r_{ik}) e^{\lambda_3^m (r_{ij} - r_{ik})^m} \quad (9)$$

## Notes

- For details, see original paper [1]
- Typically,  $m = 3$
- In all published potentials (to my knowledge),  $\alpha = 0 \Rightarrow a_{ij} = 1$
- In original Tersoff potentials,  $\gamma = 1$ .
- $\gamma$  can also be used as a three-body parameter,  $\gamma_{ik} \Rightarrow \gamma_{ijk}$ .
- In LAMMPS,  $h$  is called  $\cos \theta_0$

## 2 Brenner hydrocarbon potential (1990)

$$U = \sum_i \sum_{j>i} f_C(r_{ij}) [V_R(r_{ij}) - \bar{b}_{ij} V_A] \quad (10)$$

$$V_R(r_{ij}) = \frac{D}{S-1} e^{-\beta\sqrt{2S}(r_{ij}-r_0)} \quad (11)$$

$$V_A(r_{ij}) = \frac{SD}{S-1} e^{-\beta\sqrt{2/S}(r_{ij}-r_0)} \quad (12)$$

$$\bar{b}_{ij} = \frac{b_{ij} + b_{ji}}{2} + F_{ij}(N_i, N_j, N_{ij}^{\text{conj}}) \quad (13)$$

$$b_{ij} = \left[ 1 + \sum_{k(\neq i,j)} f_C(r_{ij}) g(\theta_{ijk}) e^{\alpha_{ijk}[(r_{ij}-r_{0,ij})-(r_{ik}-r_{0,ik})]} + H_{ij}(N_i^H, N_i^C) \right]^{-\delta} \quad (14)$$

$$g(\theta) = a_0 \left[ 1 + \frac{c^2}{d^2} - \frac{c^2}{d^2 + (1 + \cos \theta)^2} \right] \quad (15)$$

$$N_{ij}^{\text{conj}} = 1 + \sum_{k(\neq i,j)} f_C(r_{ik}) P(x_{ik}) + \sum_{l(\neq i,j)} f_C(r_{jl}) P(x_{jl}), \quad (16)$$

where the sums go over carbon atoms only.

$$P(x_{ik}) = \begin{cases} 1 & x_{ik} \leq 2 \\ \frac{1}{2} + \frac{1}{2} \cos[\pi(x_{ik} - 2)] & 2 < x_{ik} < 3 \\ 0 & x_{ik} \geq 3 \end{cases} \quad (17)$$

and  $x_{ik} = N_k - f_C(r_{ik})$ , where  $N_k$  is the number of neighbours of atom  $k$ .

### Notes

- For details, see original paper [2].
- Sum is written over  $j > i$  only using symmetric bond order  $\bar{b}_{ij}$  function.
- Pair potentials rewritten for closer resemblance to the Morse potential [3] and to make more physical sense (i.e.  $D_0$  is now the dimer bond energy, Tersoff's  $A$  and  $B$  mean nothing).
- Correction functions  $F, H$  introduced to account for conjugated bonds in C-H systems.
- The  $h$  parameter is here fixed to 1 (note also sign difference compared to Tersoff's form).

### 3 Analytical bond order potential (ABOP)

$$U = \sum_i \sum_{j>i} f_C(r_{ij}) [V_R(r_{ij}) - \bar{b}_{ij} V_A] \quad (18)$$

$$V_R(r_{ij}) = \frac{D_0}{S-1} e^{-\beta\sqrt{2S}(r_{ij}-r_0)} \quad (19)$$

$$V_A(r_{ij}) = \frac{SD_0}{S-1} e^{-\beta\sqrt{2/S}(r_{ij}-r_0)} \quad (20)$$

$$f_C(r) = \begin{cases} 1, & r \leq R - D \\ \frac{1}{2} - \frac{1}{2} \sin \left[ \frac{\pi}{2}(r - R)/D \right], & R - D < r < R + D \\ 0, & r \geq R + D \end{cases} \quad (21)$$

$$\bar{b}_{ij} = \frac{b_{ij} + b_{ji}}{2} \quad (22)$$

$$b_{ij} = (1 + \chi_{ij})^{-p} \quad (23)$$

$$\chi_{ij} = \sum_{k(\neq i,j)} f_C(r_{ik}) g_{ik}(\theta_{ijk}) \omega_{ijk} e^{\alpha_{ijk}(r_{ij}-r_{ik})} \quad (24)$$

$$g_{ik}(\theta_{ijk}) = \gamma_{ik} \left[ 1 + \frac{c_{ik}^2}{d_{ik}^2} - \frac{c_{ik}^2}{d_{ik}^2 + (h_{ik} + \cos \theta_{ijk})^2} \right] \quad (25)$$

#### Notes

- For details, see e.g. [4]
- Essentially the Brenner potential without the hydrocarbon-specific correction functions.
- $p = 1/2$  by default in all published potentials.
- The  $\alpha_{ijk}$  parameter(s) is in some versions replaced by the two-body parameter  $2\mu$ , and is often set to zero. If  $\alpha > 0$ , the  $r$ -dependence of the bond order function is switched on, and the contribution by the atom  $k$  to the bond order of the bond  $ij$  will be dependent on the bond lengths  $r_{ij}$  and  $r_{ik}$ . If atom  $k$  is closer than atom  $j$  ( $r_{ij} > r_{ik}$ ), the contribution to  $b_{ij}$  by the bond  $ik$  is enhanced, i.e. the weakening of bond  $ij$  is stronger. Vice versa, if atom  $k$  is further away than atom  $j$  ( $r_{ij} < r_{ik}$ ), the contribution to  $b_{ij}$  by the bond  $ik$  is reduced, i.e. the weakening of bond  $ij$  is reduced. This dependence can sometimes be useful.
- The three-body  $\omega_{ijk}$  parameter(s) in Equation 24 is new compared to the Tersoff and Brenner potentials. If  $\omega_{ijk} = 1$  for all  $ijk$  triplets, the bond order function reduces to a form similar to the Tersoff form. If  $\omega_{ijk} = e^{-\alpha_{ijk}(r_{0,ij}-r_{0,ik})}$ , the bond order function is similar to the Brenner version in Equation 14.  $\omega_{ijk} = 1$  is the standard choice, but they can also be fitted individually for all  $ijk$  triplets in case of tricky compounds. This essentially transforms  $\gamma$  into a three-body parameter and can be done to avoid or favour specific three-body interactions by scaling the contribution to the bond order value.
- Note the sign in Equation 25,  $h + \cos \theta$  here, but  $h - \cos \theta$  in Tersoff's version.

### 3.1 Description of ABOP parameters

$D_0$	(eV)	Dimer bond energy.
$r_0$	(Å)	Dimer bond length.
$\beta$	(Å <sup>-1</sup> )	Modifies the curvature of the potential energy minimum and thus the ground-state frequency of the dimer (see e.g. [4]) and the bulk moduli of crystals.
$S$		Can be obtained from the slope of a 'Pauling plot' or fit to dimer curve.
$\gamma$		Scales coordination dependence and defines minimum of angular function.
$c$		Controls the strength of the angular dependence (together with $d$ ).
$d$		Controls the 'sharpness' of the angular dependence (together with $c$ ).
$h$		Defines the optimal angle $\theta_{ijk}$ .
$\alpha$	(Å <sup>-1</sup> )	Often = 0. If > 0, it enables the $r$ -dependence of the bond order function.
$\omega$		Often = 1. "Three-body- $\gamma$ ", can scale $\gamma$ for specific three-body interactions.
$R$	(Å)	Defines cutoff distance (mid-point of cutoff region).
$D$	(Å)	Defines width of cutoff region.

## 4 Converting ABOP parameters to Tersoff

When generating LAMMPS potential files, for example, it is necessary to convert ABOP parameters to the original Tersoff parameters. The Tersoff parameters can be calculated as follows:

$R, D, c, d$  are the same

$$m = 1$$

$$n = 1$$

$$\beta = 1 \text{ (note: not the same } \beta \text{ as in the ABOP)}$$

$\gamma_{ik}$  is the same if  $\omega_{ijk} = 1.0 \forall ijk$ . Otherwise  $\gamma_{ijk} = \gamma_{ik}\omega_{ijk}$

$$\lambda_1 = \beta\sqrt{2S}$$

$$\lambda_2 = \beta\sqrt{2/S}$$

$$\lambda_3 = \alpha_{ijk} \text{ (or } 2\mu)$$

$$h = -h$$

$$A = D_0 \exp(\lambda_1 r_0) / (S - 1)$$

$$B = SD_0 \exp(\lambda_2 r_0) / (S - 1)$$

## 5 ZBL-stiffening of Tersoff-type potentials

Tersoff-type potentials reach a finite value as  $r_{ij} \rightarrow 0$ , making an unmodified Tersoff potential unusable for simulations involving high kinetic energies. A simple stiffening is achieved by scaling the original potential energy function  $U_{\text{orig.}}$  by the Ziegler-Biersack-Littmarck (ZBL) universal screening potential [5] according to

$$U_{\text{mod.}}(r) = [1 - F(r)]U_{\text{ZBL}}(r) + F(r)U_{\text{orig.}}(r). \quad (26)$$

The ZBL potential is given by

$$U_{\text{ZBL}}(r) = \frac{1}{4\pi\epsilon_0} \frac{Z_1 Z_2 e^2}{r} \phi(r/a) \quad (27)$$

$$a = \frac{0.8854a_0}{Z_1^{0.23} + Z_2^{0.23}} \quad (28)$$

$$\phi(x) = 0.1818e^{-3.2x} + 0.5099e^{-0.9423x} + 0.2802e^{-0.4029x} + 0.02817e^{-0.2016x}. \quad (29)$$

$F(r)$  is the Fermi function

$$F(r) = \frac{1}{1 + e^{-b_f(r-r_f)}}. \quad (30)$$

The use of the Fermi function results in a smooth transition to the ZBL at short interatomic distances.  $b_f$  and  $r_f$  are chosen to keep the potential around the equilibrium distances essentially unmodified.  $b_f$  controls the width of the transition region (higher  $b_f \Rightarrow$  sharper transition, typically  $b_f \approx 10$ ), and  $r_f$  the mid-point of the transition region (typically  $r_f \approx 1.0$ ).

## References

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