The Tersoff-mini potential

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Brief descriptions

- This is the Tersoff-mini potential corresponding to [Fan 2020].
- It currently only applies to systems with a single atom type.
- One can use the GPUGA package (https://github.com/brucefan1983/GPUGA) to fit this potential for new systems.

Potential form

- The **site potential** can be written as

$$U_i = \frac{1}{2} \sum_{j \neq i} f_{\mathrm{C}}(r_{ij}) \left[f_{\mathrm{R}}(r_{ij}) - b_{ij} f_{\mathrm{A}}(r_{ij}) \right].$$

- The function f_{C} is a **cutoff function**, which is 1 when $r_{ij} < R_{IJ}$ and 0 when $r_{ij} > S_{IJ}$ and takes the following form in the intermediate region:

$$f_{\mathrm{C}}(r_{ij}) = \frac{1}{2} \left[1 + \cos\left(\pi \frac{r_{ij} - R}{S - R} \right) \right].$$

- The **repulsive function** f_{R} and the **attractive function** f_{A} take the following forms:

$$f_{\mathrm{R}}(r_{ij}) = \frac{D_0}{S-1} \exp\left(\alpha r_0 \sqrt{2S}\right) e^{-\alpha \sqrt{2S} r_{ij}};$$

$$f_{\mathrm{A}}(r_{ij}) = \frac{D_0 S}{S-1} \exp\left(\alpha r_0 \sqrt{2/S}\right) e^{-\alpha \sqrt{2/S} r_{ij}}.$$

- The **bond-order function** is

$$b_{ij} = \left(1 + \zeta_{ij}^n\right)^{-\frac{1}{2n}},$$

where

$$\zeta_{ij} = \sum_{k \neq i,j} f_C(r_{ik}) g_{ijk};$$

$$g_{ijk} = \beta(h - \cos\theta_{ijk})^2.$$

Parameters

Parameter	Units
D_0	eV
α	A^{-1}
r_0	A
S	dimensionless
n	dimensionless
β	dimensionless
h	dimensionless
R	A
S	A

Potential file format

Single-element systems

- The potential file reads

```
tersoff_mini 1
D alpha r0 S beta n h R S
```

References

- [Fan 2020] Zheyong Fan, Yanzhou Wang, Xiaokun Gu, Ping Qian, Yanjing Su, and Tapio Ala-Nissila, *A minimal Tersoff potential for diamond silicon with improved descriptions of elastic and phonon transport properties* (https://doi.org/10.1088/1361-648X/ab5c5f), J. Phys.: Condens. Matter **32**, 135901 (2020).

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