SAND2012-2032P

pair_style bop command

Syntax:

```
pair_style style
```

- style = *bop*

Examples:

```
pair_style     bop
pair_coeff     * * ../potentials/CdTe.bop 4.90 off Cd Te
communicate    single cutoff 14.70

pair_style     bop
pair_coeff     * * ../potentials/CdTe.bop.table 4.90 on Cd Te table no_a
communicate    single cutoff 14.70
```

Description:

The *bop* pair style computes Bond-Order Potentials (BOP) based upon quantum mechanical theory incorporating both σ and π bondings. By analytically deriving the BOP from quantum mechanical theory its transferability to different phases can approach that of quantum mechanical methods. This potential is extremely effective at modeling III-V and II-VI compounds such as GaAs and CdTe. This potential is similar to the original BOP developed by Pettifor[1-4] and later updated by Murdock et al and Ward et al [5,6].

The BOP potential consists of four terms:

$$E=\frac{1}{2}\sum_{i=1}^{N}\sum_{j=i_1}^{i_N}\phi_{ij}\left(r_{ij}\right)-\sum_{i=1}^{N}\sum_{j=i_1}^{i_N}\beta_{\sigma,ij}\left(r_{ij}\right)\cdot\Theta_{\sigma,ij}-\sum_{i=1}^{N}\sum_{j=i_1}^{i_N}\beta_{\pi,ij}\left(r_{ij}\right)\cdot\Theta_{\pi,ij}+U_{prom} \qquad (1)$$

where $\phi_{ij}(r_{ij})$ is a short-range two-body function representing the repulsion between a pair of ion cores, $\beta_{\sigma,ij}(r_{ij})$ and $\beta_{\pi,ij}(r_{ij})$ are respectively σ and π bond integrals, $\Theta_{\sigma,ij}$ and $\Theta_{\pi,ij}$ are σ and π bond-orders, and U_{prom} is the promotion energy for sp-valent systems.

Only a single pair_coeff command is used with the *bop* style which specifies a BOP potential file, a cutoff radius, on-the-fly option, atom types, and optional table file feature.

- filename
- maximum cutoff radius
- on-the-fly option (“on” use on-the-fly; “off” do not use on-the-fly)
- *N* element names = mapping of BOP elements to atom types
- table file option (include “table” if pair functions are pre-tabulated; omit if function file does not include pre-tabulated pair functions)
- a_σ =0 option (if no_a is selected then a second level series expansion is used for the σ bond-order, rather than the full fourth level expansion, as described below)

The 1st 2 arguments must be * * so as to span all LAMMPS atom types. Two types of potential files can be used; first a potential file containing all of the parameters necessary for the pair functions as well as the bond order formulation, or secondly, a file containing pre-tabulated pair functions for $\phi_{ij}(r_{ij})$, $\beta_{\sigma,ij}(r_{ij})$, and $\beta_{\pi,ij}(r_{ij})$ (as described below). These are mapped to LAMMPS atom types by specifying *N* additional arguments after the filename, cutoff radius, and on-the-fly option in the pair_coeff command, where *N* is the number of LAMMPS atom types. The cutoff radius is the maximum cutoff radius for all interaction types. The on-the-fly option gives the user the option to either calculate the distances, angles, and derivatives of angles as the potential calculates the bond orders, which can take longer but save memory, or in advance, which can be faster but requires more memory. In many cases having the on-the-fly option is faster than having it off, it is best to test this option to optimize the speed of BOP for your particular system configuration. The *table* option gives the user the choice of which type of potential input file LAMMPS will ready. If the input file contains pre-tabulated pair functions this option must be included at the end of the pair_coeff command. The *no_a* modifies the BOP formulation from the full four-level approximation from Drautz [7] Eq. 23 and reduces it to Eq. 8 of Murdick [5]. This is accomplished by introducing a new constant a_σ into Drautz Eq. 23 [7] as shown below:

$$\Theta^{(1/2)}_{\sigma,ij} = \frac{1}{\sqrt{1 + c_{\sigma,ij} \cdot \frac{2 \cdot \Phi_{2\sigma} + a_{\sigma,ij} \cdot R_{4\sigma,ij} + a_{\sigma,ij} \cdot \tilde{\Phi}^{i}_{2\sigma} \tilde{\Phi}^{j}_{2\sigma} \cdot \left(2 + \Delta\tilde{\Phi}_{4\sigma}\right)}{\left(1 + a_{\sigma,ij} \cdot \Delta\tilde{\Phi}_{4\sigma}\right)^2}}} \qquad (2)$$

This option should not be used for potentials parameterized for a four moment σ bond-order. BOP potentials given in Murdick [5] and Ward [6] are derived for a_σ=0

As an example, if your LAMMPS simulation has 4 atom types and you want the 1st 3 to be Cd, and the 4th to be Te, with a maximum cutoff of 4.90 Å, using on-the-fly options, without pre-tabulated options you would use the following pair_coeff command:

```
pair_coeff * * CdTe.bop 4.90 on Cd Cd Cd Te
```

The first three Cd arguments map LAMMPS atom types 1,2,3 to the Cd element in the BOP file. The final Te argument maps LAMMPS atom type 4 to the Te element in the BOP file.

The parameters/coefficients format for the BOP potentials input file is given below with variables matching the formulation of Ward [6]. Each header line containing a ":" is preceded by a blank line.

- Line 1: elements: (header)
- Line 2: # elements *N*

The first two lines are followed by *N* lines containing the atomic number and mass of each element.

NON-TABULATED INPUT FILE FORMAT

Following the definition of the elements is the block of global variables for spline and quadratic fits of $\Theta_{S,ij}$ and its components Θ_0, Θ_1, and S.

- Line 1: global: (header)
- Line 2: ς_1-ς_7 (if all are not used in the particular formulation, set unused values to 0.0)
- Line 3: ncutoff, r_{big}, r_{small} (r_{big} and r_{small} are parameters for pairwise parameter γ typically set to 0.99 and 0.01, respectively. See Ward et al [6] Eq. A-2)
- Line 4: *which*, α, *nfunc* (These are options for the spline *which*=1.0 (means using a smooth function, Eqs. 13-16 from Murdick [5]); which=2.0 (spline, Eqs. (A-7)-(A-8) from Ward [6]), α is a limit parameter for the spline (the 5/8 from Eqs. 15-16 in Murdick [5]), *nfunc* is the type of GSP function (f_{ij}) (*nfunc*=1 is Eq. 5 from Ward [6]; *nfunc*=2 $f_{ij}(r_{ij}) = \exp(n_{ij} \cdot r_{ij})$; *nfunc*=3 $f_{ij}(r_{ij}) = 1/r_{ij}^{n_{ij}}$).
- Line 5: α_1, β_1, γ_1 (α_1=first coefficient for Θ_0; β_1=first exponent for Θ_0; γ_1=second exponent for Θ_0. In the case of Eq. A-8 Ward [6]; α_1=15.737980, β_1=1.137622, γ_1=2.087779)
- Line 6: α_2, β_2 (α_2=second coefficient for S; β_2= first exponent for S. In the case of Eq. A-8 Ward [6]; α_2=22.180680, β_2=2.689731)
- Line 7: α_3, β_3 (α_3=first coefficient for Θ_1; β_3= second coefficient for Θ_1. In the case of Eq. A-8 Ward [6]; α_3=2.0, β_3=1.0)

The next block contains constants for the environment depend promotional energy for sp-valent systems, each of which are species dependent. As well as one species dependent parameter p_π.

- Line 1: ptrs: (header)

Following the ptrs header there are N lines for e_1-e_N containing $A_{ij}^{\mu\nu}$, δ^{u}, p_π. ($A_{ij}^{\mu\nu}$ and δ^{u} in Eq. 49-50 from Pettifor [4], p_π in Eq. A-9 in Ward [6]).

- Line 2: $A_{ij}^{\mu\nu}$, δ^{u}, p_π (for e_1)
- Line 3: $A_{ij}^{\mu\nu}$, δ^{u}, p_π (for e_2 and continues to e_N)

The next block contains constants for the pair interactions.

- Line 1: pairs:

Following the header the block contains a series of constants for the number of pair interaction types, the block will be broken up into parameters for e_i- e_j, with i=0->N, j=i->N. Each single interaction section for this block will contain (see Ward [6] for parameter definitions):

- Line 2: r_0, r_c, r_1, r_{cut} (for e_1- e_1 interactions, Eq. 5 and Eqs. (A-1)-(A-3) from Ward [6])
- Line 3: m, n, n_c (Eqs. 2-5 from Ward [6])
- Line 4: ϕ_0, $\beta_{\sigma,0}$, $\beta_{\pi,0}$ (Eqs. 2-4 from Ward [6])

- Line 5: a_σ, c_σ, δ_σ (a_σ and c_σ described above in Eq. 2, δ_σ is a redundant small number and should be set to zero)
- Line 6: a_π, c_π, δ_π (a_π controls the magnitude of the π bond-order similar to a_σ, c_π from Eqs.24 in Drautz [7], δ_π is a redundant small number and should be set to zero)
- Line 7: f_σ, k_σ, ς_3 (f_σ, k_σ from Eq. 7 in Ward [6], ς_3 a atom type dependent small number from Eq. 8 in Ward [6])
- Line 8: r_0, r_c, r_1, r_{cut} (for e_1-e_2 interactions and repeats as above)

The next block contains three-body coefficients $g_{\sigma 0}$, $g_{\sigma 1}$, $g_{\sigma 2}$. These are the coefficients for Eq. A-5 from Ward [6]. Where:

$$g_{\sigma 0} = \frac{\left(b_{\sigma,jik} - g_{0,jik}\right)\cdot u_{\sigma,jik}^2 - \left(g_{0,jik} + b_{\sigma,jik}\right)\cdot u_{\sigma,jik}}{2\cdot\left(1-u_{\sigma,jik}^2\right)},$$

$$g_{\sigma 1} = \frac{g_{0,jik} + b_{\sigma,jik}}{2}, \text{ and} \tag{3}$$

$$g_{\sigma 2} = \frac{g_{0,jik} - b_{\sigma,jik} + \left(g_{0,jik} + b_{\sigma,jik}\right)\cdot u_{\sigma,jik}}{2\cdot\left(1-u_{\sigma,jik}^2\right)}$$

- Line 1: tris: (header)

Following the header there is a line for each three body interaction types as e_j-e_i-e_k with i->N, j->N, k=j->N

- Line 2: $g_{\sigma 0}$, $g_{\sigma 1}$, $g_{\sigma 2}$ (for e_1-e_1-e_1)
- Line 3: $g_{\sigma 0}$, $g_{\sigma 1}$, $g_{\sigma 2}$ (for e_1-e_1-e_2)

This would be the end of the potential parameter file ***without*** pre-tabulated

TABULATED INPUT FILE FORMAT

The parameters/coefficients format for the BOP potentials input file containing pre-tabulated functions of is given below with variables matching the formulation of Ward [6].

- Line 1: # elements N)

Line 1 is followed by N lines containing the atomic number and mass of each element.

Following the definition of the elements several global variables for the tabulated functions are given.

- Line 1: *nr*, *nBOt* (*nr* is the number of divisions the radius is broken into for function tables and MUST be a factor of 5; *nBOt* is the number of divisions for the tabulated values of $\Theta_{S,ij}$, Eq. A-7 from Ward [6], also must be a factor of 5)
- Line 2: δ_1-δ_7 (see above)

Following this N lines for e_1-e_N containing p_π (see above for the definition).

- Line 3: p_π (for e_1)
- Line 4: p_π (for e_2 and continues to e_N)

The next section contains several pair constants for the number of interaction types e_i-e_j, with i=1->N, j=i->N (see above for the definitions).

- Line 1: r_{cut} (for e_1-e_1 interactions)
- Line 2: c_σ, a_σ, c_π, a_π
- Line 3: δ_σ, δ_π
- Line 4: f_σ, k_σ, δ_3
- Line 5: r_{cut} (for e_1-e_2 interactions and continues to e_N-e_N)

The next section contains there is a line for each three body interaction types as e_j–e_i–e_k with i=0->N, j=0->N, k=j->N(see above for the defintions).

- Line1: $g_{\sigma 0}$, $g_{\sigma 1}$, $g_{\sigma 2}$ (for e_1–e_1–e_1)
- Line 2: $g_{\sigma 0}$, $g_{\sigma 1}$, $g_{\sigma 2}$ (for e_1–e_1–e_2 and continues to to e_N-e_N-e_N)

The next section contains a block for each interaction type for the $\phi_{ij}(r_{ij})$ (see Eq. 2 from Ward [6]). Each block has *nr* entries with 5 entries per line.

- Line 1: $\phi(r1)$, $\phi(r2)$, $\phi(r3)$, $\phi(r4)$, $\phi(r5)$ (for the e_1-$e_1$interaction type)
- Line 2: $\phi(r6)$, $\phi(r7)$, $\phi(r8)$, $\phi(r9)$, $\phi(r10)$ (this continues until *nr*)

  .

  .

  .

- Line *nr*/5+1: $\phi(r1)$, $\phi(r2)$, $\phi(r3)$, $\phi(r4)$, $\phi(r5)$ (for the e_1-e_1 interaction type)

The next section contains a block for each interaction type for the $\beta_{\sigma,ij}(r_{ij})$ (see Eq. 3 Ward [6]). Each block has *nr* entries with 5 entries per line.

- Line 1: $\beta_\sigma(r1)$, $\beta_\sigma(r2)$, $\beta_\sigma(r3)$, $\beta_\sigma(r4)$, $\beta_\sigma(r5)$ (for the e_1-e_1 interaction type)
- Line 2: $\beta_\sigma(r6)$, $\beta_\sigma(r7)$, $\beta_\sigma(r8)$, $\beta_\sigma(r9)$, $\beta_\sigma(r10)$ (this continues until *nr*)

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  .

- Line *nr*/5+1: $\beta_\sigma(r1)$, $\beta_\sigma(r2)$, $\beta_\sigma(r3)$, $\beta_\sigma(r4)$, $\beta_\sigma(r5)$ (for the e_1-e_2 interaction type)

The next section contains a block for each interaction type for $\beta_{\pi,ij}(r_{ij})$ (see Eq. 4 from Ward [6]). Each block has *nr* entries with 5 entries per line.

- Line 1: $\beta_\pi(r1)$, $\beta_\pi(r2)$, $\beta_\pi(r3)$, $\beta_\pi(r4)$, $\beta_\pi(r5)$ (for the e_1-e_1 interaction type)
- Line 2: $\beta_\pi(r6)$, $\beta_\pi(r7)$, $\beta_\pi(r8)$, $\beta_\pi(r9)$, $\beta_\pi(r10)$ (this continues until *nr*)

  .

  .

  .
- Line *nr*/5+1: $\beta_\pi(r1)$, $\beta_\pi(r2)$, $\beta_\pi(r3)$, $\beta_\pi(r4)$, $\beta_\pi(r5)$ (for the e_1-e_2 interaction type)

The next section contains a block for each interaction type for the $\Theta_{S,ij}(\Theta^{1/2}_{\sigma,ij}, f_{\sigma,ij})$ (see Eq. A-7 from Ward [6]). Each block has *nBOt* entries with 5 entries per line.

- Line 1: $\Theta_{S,ij}(r1)$, $\Theta_{S,ij}(r2)$, $\Theta_{S,ij}(r3)$, $\Theta_{S,ij}(r4)$, $\Theta_{S,ij}(r5)$ (for the e_1-e_2 interaction type)
- Line 2: $\Theta_{S,ij}(r6)$, $\Theta_{S,ij}(r7)$, $\Theta_{S,ij}(r8)$, $\Theta_{S,ij}(r9)$, $\Theta_{S,ij}(r10)$ (this continues until *nBOt*)

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  .
- Line *nBOt*/5+1: $\Theta_{S,ij}(r1)$, $\Theta_{S,ij}(r2)$, $\Theta_{S,ij}(r3)$, $\Theta_{S,ij}(r4)$, $\Theta_{S,ij}(r5)$ (for the e_1-e_2 interaction type)

The next section contains a block of *N* lines for e_1-e_N (see above for definition).

- Line 1: δ^μ (for e_1)
- Line 2: δ^μ (for e_2 and repeats to e_N)
- …

The next section contains more constants for e_1-e_N (see above for definition).

- Line 1: $A^{\mu\nu}_{ij}$ (for e_1)
- Line 2: $A^{\mu\nu}_{ij}$ (for e_2 and repeats to e_N)
- …

This would be the end of the potential parameter file ***without*** pre-tabulated

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Mixing, shift, table, tail correction, and restart:

These pair styles do not support the pair_modify mix, shift, table, and tail options.

These pair styles do not write their information to binary restart files, since it is stored in potential files. Thus, you need to re-specify the pair_style and pair_coeff commands in an input script that reads a restart file.

Restrictions:

If using create_atoms command atomic masses MUST be defined in the input script. If using read_data atomic masses MUST be defined in the atomic structure data file.

These pair styles are part of the MANYBODY package. They are only enabled if LAMMPS was built with that package (which it is by default). See the Making LAMMPS section for more info.

These pair potentials require the newton setting to be "on" for pair interactions.

The CdTe.bop and GaAs.bop potential files provided with LAMMPS (see the potentials directory) are parameterized for metal units. You can use the BOP potential with any LAMMPS units, but you would need to create your own BOP potential file with coefficients listed in the appropriate units if your simulation doesn't use "metal" units.

Related commands:

pair_coeff

Default: non-tabulated potential file, $a_\sigma \neq 0$

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[1] D.G. Pettifor, and I.I. Oleinik, *Phys. Rev. B*, **59**, 8487 (1999).

[2] D.G. Pettifor, and I.I. Oleinik, *Phys. Rev. Lett.*, **84**, 4124 (2000).

[3] D.G. Pettifor, and I.I. Oleinik, *Phys. Rev. B*, **65**, 172103 (2002).

[4] D.G. Pettifor, M.W. Finnis, D. Nguyen-Manh, D.A. Murdick, X.W. Zhou, H.N.G. Wadley, *Mat. Sci. Eng*, **A365**, 2 (2004)

[5] D.A. Murdick, X.W. Zhou, H.N.G. Wadley, D. Nguyen-Manh, R. Drautz, and D.G. Pettifor, *Phys. Rev. B*, **73**, 45206 (2006).

[6] D.K. Ward, X.W. Zhou, B.M. Wang, R.P. Doty, *Phys. Rev. B* (2012)

[7] R. Drautz, D.A. Murdick, D. Nguyen-Manh, X.W. Zhou, H.N.G. Wadley, D.G. Pettifor, *Phys. Rev. B*, **72**, 144105 (2005)