The embedded atom method (EAM) potential

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Contents

Brief descriptions

- This is the EAM potential in some **analytical** forms as in [Zhou 2004] and [Dai 2006].
- It currently only applies to systems with a **single atom type**.

Potential form

General form

- The site potential energy is

$$U_i = \frac{1}{2} \sum_{j \neq i} \phi(r_{ij}) + F(\rho_i).$$

- Here, the part with $\phi(r_{ij})$ is a pairwise potential and $F(\rho_i)$ is the embedding potential, which depends on the electron density ρ_i at site i. The many-body part of the EAM potential comes from the embedding potential.

- The density $F(\rho_i)$ is contributed by the neighbors of i:

$$\rho_i = \sum_{j \neq i} f(r_{ij}).$$

- Therefore, the form of an EAM potential is completely determined by the three functions: ϕ, f, and F.

The version by [Zhou 2004]

- The pair potential between two atoms of the same type a is

$$\phi^{aa}(r) = \frac{A^a \exp[-\alpha(r/r_e^a - 1)]}{1 + (r/r_e^a - \kappa^a)^{20}} - \frac{B^a \exp[-\beta(r/r_e^a - 1)]}{1 + (r/r_e^a - \lambda^a)^{20}}.$$

- The contribution of the electron density from an atom of type a is

$$f^a(r) = \frac{f_e^a \exp[-\beta(r/r_e^a - 1)]}{1 + (r/r_e^a - \lambda^a)^{20}}.$$

- The pair potential between two atoms of different types a and b is then constructed as

$$\phi^{ab}(r) = \frac{1}{2}\left[\frac{f^b(r)}{f^a(r)}\phi^{aa}(r) + \frac{f^a(r)}{f^b(r)}\phi^{bb}(r)\right].$$

- The embedding energy function is piecewise:

$$F(\rho) = \sum_{i=0}^{3} F_{ni}\left(\frac{\rho}{\rho_n} - 1\right)^i, \quad (\rho < 0.85\rho_e)$$

$$F(\rho) = \sum_{i=0}^{3} F_i\left(\frac{\rho}{\rho_e} - 1\right)^i, \quad (0.85\rho_e \le \rho < 1.15\rho_e)$$

$$F(\rho) = F_e\left[1 - \ln\left(\frac{\rho}{\rho_s}\right)^\eta\right]\left(\frac{\rho}{\rho_s}\right)^\eta, \quad (\rho \ge 1.15\rho_e)$$

The version by [Dai 2006]

This is a very simple EAM-type potential which is an extension of the Finnis-Sinclair potential. The function for the pair potential is

$$\phi(r) = \begin{cases} (r-c)^2 \sum_{n=0}^{4} c_n r^n & r \le c \\ 0 & r > c \end{cases}$$

The function for the density is

$$f(r) = \begin{cases} (r-d)^2 + B^2(r-d)^4 & r \le d \\ 0 & r > d \end{cases}$$

The function for the embedding energy is

$$F(\rho) = -A\rho^{1/2}.$$

Parameters

See [Zhou 2004] and [Dai 2006].

Potential file format

- The potential file for the version in [Zhou 2004] reads

```
eam_zhou_2004 1
r_e
f_e
rho_e
rho_s
alpha
beta
A
B
kappa
lambda
F_n0
F_n1
F_n2
F_n3
F_0
F_1
F_2
F_3
eta
F_e
cutoff
```

- The last parameter $cutoff$ is the cutoff distance which is not intrinsic to the model. The order of the parameters is the same as in Table III of the paper by Zhou *et al.*.
- The potential file for the version in [Dai 2006] reads

```
eam_dai_2006 1
A
d
c
c_0
c_1
c_2
c_3
c_4
B
```

References

- [Zhou 2004] X. W. Zhou, R. A. Johnson, and H. N. G. Wadley, *Misfit-energy-increasing dislocations in vapor-deposited CoFe/NiFe multilayers* (https://doi.org/10.1103/PhysRevB.69.144113), Phys. Rev. B **69**, 144113 (2004).
- [Dai 2006] X D Dai, Y Kong, J H Li and B X Liu, *Extended Finnis–Sinclair potential for bcc and fcc metals and alloys* (https://doi.org/10.1088/0953-8984/18/19/008), J. Phys.: Condens. Matter **18**, 4527 (2006).

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