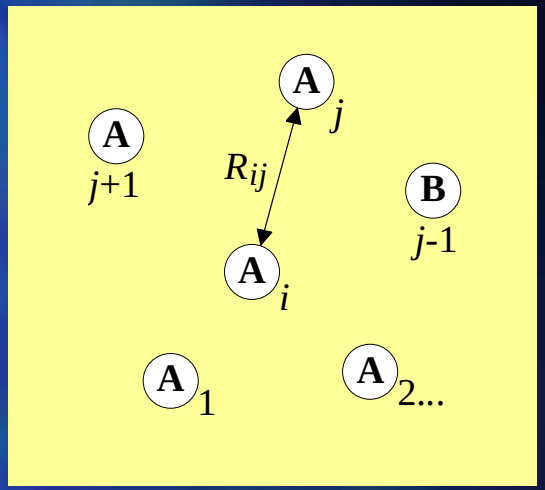
Let's program an original EAM !

Dimer Reference EAM (DR-EAM)



- EAM hypothesis

$$E_{\mathrm{tot}} = \sum_i E_i \qquad E_i = F_i(\bar{\rho}_i) + \frac{1}{2}\sum_{j(i\neq j)} \phi_{ij}(R_{ij})$$

- Embedding function (Baskes type)

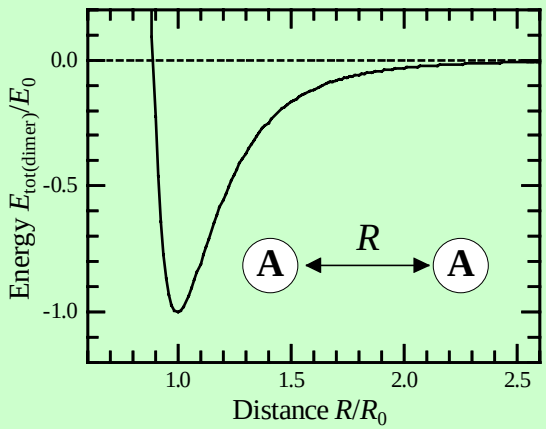
$$F_i(\bar{\rho}_i) = A_i E_0 \frac{\bar{\rho}_i}{\bar{\rho}_i^{\,0}} \ln\left(\frac{\bar{\rho}_i}{\bar{\rho}_i^{\,0}}\right)$$

- Electron density (Linear combination of parameterized)

$$\bar{\rho}_i = \sum_{j(j\neq i)} \rho_j(R_{ij}) \qquad \rho_j(R_{ij}) = \exp\left\{-\beta_j\left(\frac{R_{ij}}{R^0} - 1\right)\right\}$$

- Reference structure (= Dimer)

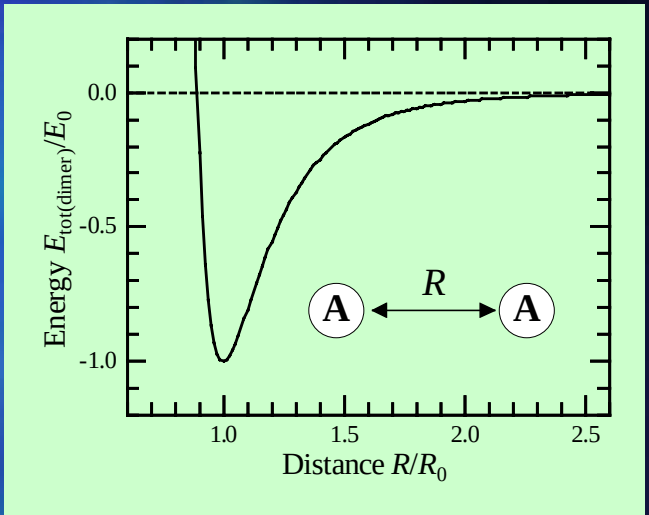
  to determine pair potential term



Any energetics !

Dimer Reference EAM (DR-EAM)

Consider the Reference structure



- **Energetics** (any method is ok.)
  - easy to obtain by precise Quantum calculation, etc...
  - Here, as an example, use LJ potential

$$E_{\mathrm{tot(dimer)}} = E_0 \left\{ \frac{1}{(R/R_0)^{12}} - \frac{2}{(R/R_0)^{6}} \right\}$$

- **Total energy by DR-EAM**

$$E_{\mathrm{tot(dimer)}} = 2\left\{ F_i(\bar{\rho}_i) + \frac{1}{2}\sum_{j(i\neq j)} \phi_{ij}(R_{ij}) \right\} = -2A\beta E_0 \left(\frac{R}{R_0} - 1 \right) \exp\left\{ -\beta \left(\frac{R}{R_0} - 1 \right) \right\} + \phi(R)$$

- **Both of above must be equal.**
  - Pair potential term can be obtained as a function of only distance.
- **DR-EAM parameters for a material**

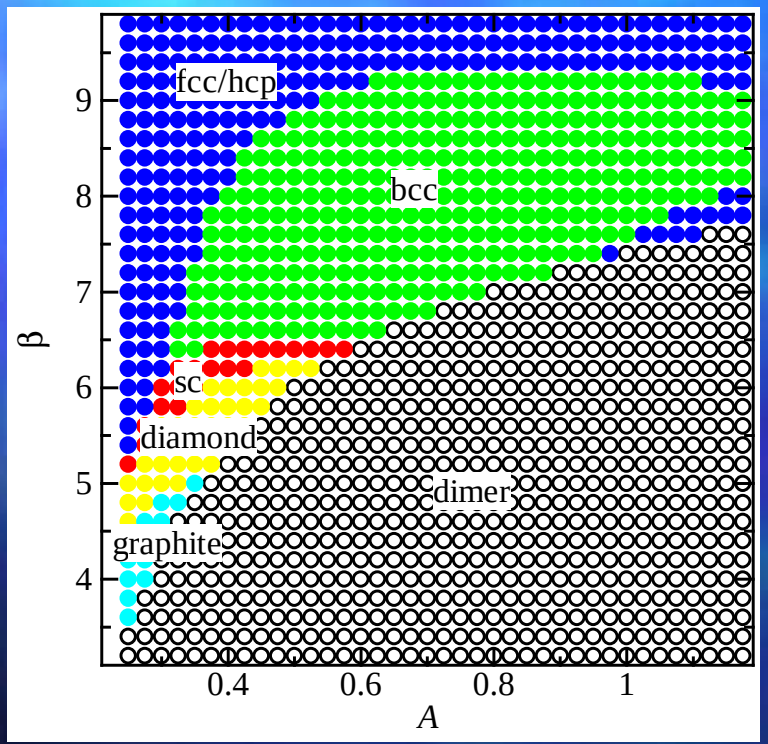
  E_0, R_0, A, β for one material
- **Stable structure is a function of only** A, and β

Dimer Reference EAM (DR-EAM)

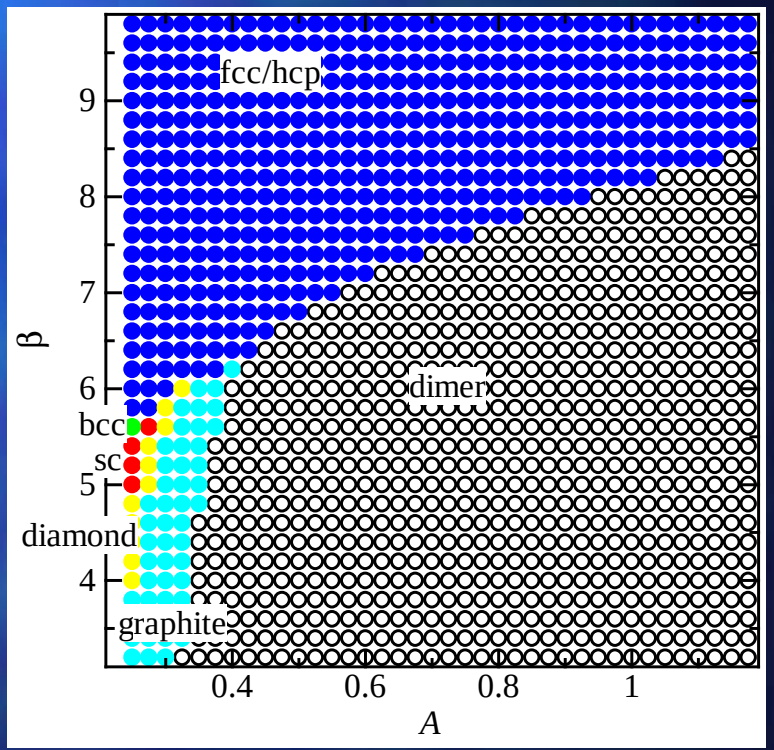
Phase diagram

- comparing total energy by DR-EAM for some structures

with all atoms (without screening)



with only first neighbor atoms



Dimer Reference EAM (DR-EAM)

About DR-EAM; Merit, etc...

- Philosophy of LJ-EAM
  With formalism of EAM (hypothesis of EAM), “dimer reference” is simple !
- Energetics of dimer is easy to obtain.
- DR-EAM parameter is only 4. E_0, R_0, A, β
  With LJ, 2 is determined, 2 should be optimized.
- Compounds just like as MEAM92

Applicability has to be checked.

Farther possibility for extension

- Energetics by precise quantum calculation
  If hypothesis of EAM is correct.
- Difference between FCC and BCC
  with angular dependence term
  number of parameter (for s,p,d,f symmetry)