EAM series and their history

Embedded Atom Method (EAM) and Modified EAM (MEAM)

By

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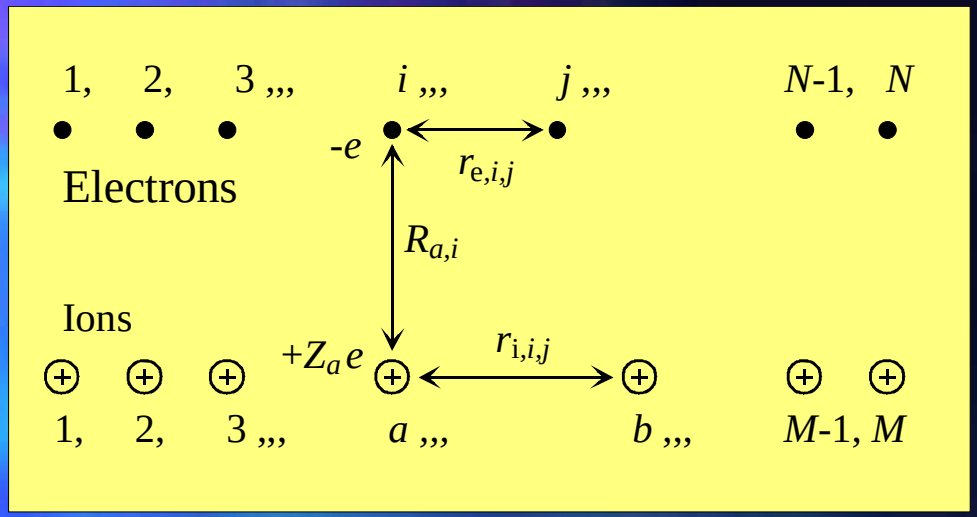
Quantum calculation (1)

with the simplest example



- Schrödinger equation

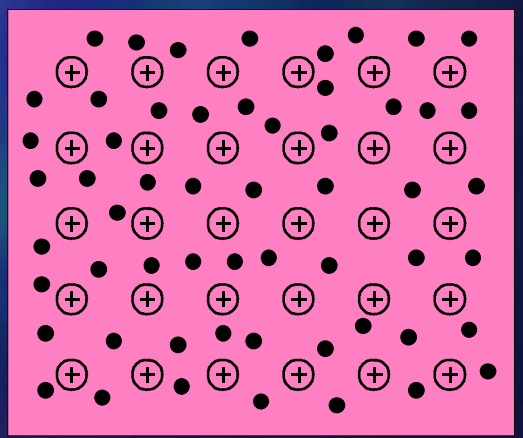
$$H\Psi = \varepsilon\Psi$$

- Hamiltonian
  - even if assuming only Coulomb interaction…

$$H = -\frac{\hbar^2}{2m}\sum_{i=1}^{N}\nabla_i^{\,2} + \frac{1}{4\pi\varepsilon_0}\left(\sum_{\substack{i,j=1\\(i>j)}}^{N}\frac{e^2}{r_{e,i,j}} - \sum_{a=1}^{M}\sum_{i=1}^{N}\frac{Z_a e^2}{R_{a,i}} + \sum_{\substack{a,b=1\\(a>b)}}^{M}\frac{Z_a Z_b e^2}{r_{i,a,b}}\right)$$

- Wave function ; Slater determinant
  - Molecular orbitals must be arbitrary function.

$$\Psi(\mathbf{x}_1,\cdots,\mathbf{x}_N) = \frac{1}{\sqrt{N!}}\begin{vmatrix} \phi_1(\mathbf{x}_1) & \cdots & \phi_1(\mathbf{x}_N) \\ \vdots & & \vdots \\ \phi_N(\mathbf{x}_1) & \cdots & \phi_N(\mathbf{x}_N) \end{vmatrix}$$



- Do you know exact solution ?

Quantum calculation (2)

How shall we approximate ?

$$\Psi(\mathbf{x}_1,\cdots,\mathbf{x}_N)=\frac{1}{\sqrt{N!}}\begin{vmatrix}\phi_1(\mathbf{x}_1) & \cdots & \phi_1(\mathbf{x}_N)\\ \vdots & & \vdots \\ \phi_N(\mathbf{x}_1) & \cdots & \phi_N(\mathbf{x}_N)\end{vmatrix}$$

- Molecular orbitals
  - Linear combination of atomic orbitals ?
    - Gaussian-type or Slater-type ?
      - How many atomic orbitals ?
        - Basis set is always effective for any situation ? ...

Basis sets are optimized to express equilibrium state.

- Interactions in Hamiltonian
  - Density functional ?
    - Which function ?
      - How determine ? ...

Density functionals are optimized to express bulk properties.

- How many electrons ?
  - Eigenvalue problem, the eigenvalue is similar to each other
  - Cut off of Integration ? ...

Accuracy of matrix calculation arises.

Quantum calculation to EAM series

Inter-atomic Potential for Molecular Mechanics (Dynamics)

- Quantum calculation
  - **Theoretical background**
  - **Reliability of approximation**
- non-Quantum method
  - **Two body potential, Three body…, Muti-body…**
  - **Usually, no theoretical background → reliability**

Which will you choose ?

Quantum calculation to EAM series ;
Embedded Atom Method（EAM） and Modified EAM

- **Applicability to Large System** (EAM and MEAM)
  - Expectable rather than quantum calc. (especially for Bulk)
- **Applicability to Surface Problems** (MEAM)
  - Si 7×7 DAS structure

    Calculation of surface energy and simulation of reconstruction for Si (111) 3X3, 5X5, 7X7, and 9X9...
    (Kunio TAKAHASHI, Chikara NARA, Takahiro YAMAGISHI, and Tadao ONZAWA)
    Applied Surface Science, vol.151 ,no.3-4 , pp.299--301 ,(1999)
  - FCC (110) Missing Row structure

    Modified embedded atom method (MEAM) calculations for reconstructed (110) surfaces of face...
    (Takahiro YAMAGISHI, Kunio TAKAHASHI, and Tadao ONZAWA,)
    Surface Science, vol.445, no.1, pp.18--22 ,(2000)

    ↓
  - Expectable !
  - However, problems remain. (ex. Pd (110) surf., clusters,,,)

    problems induced by the method ? or the parameters ?

(Embedded Atom Method)

Quantum calculation to EAM

- EAM hypothesis

$$E_{\mathrm{tot}} = \sum_i E_i$$

Embedding energy term + Two body term

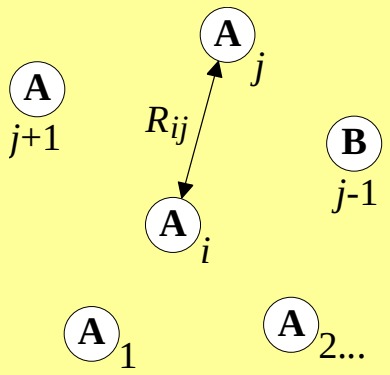
$$E_i = F_i(\bar{\rho}_i) + \frac{1}{2}\sum_{j(i\neq j)} \phi_{ij}(R_{ij})$$

$$\bar{\rho}_i = \sum_{j(j\neq i)} \rho_j(R_{ij})$$

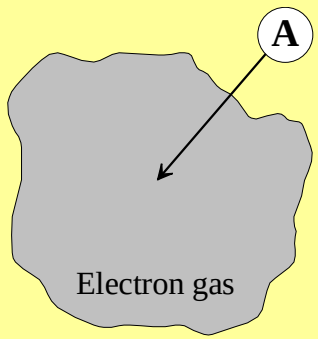
- Difference between EAM and MEAM
  - EAM: spherical symmetry
  - MEAM: includes ***s, p, d, f*** symmetries

$\rho_j(R_{ij})$

- M.W.Finnis and J.E.Sinclair potential
  - FS potential is same as EAM.
  - ... never taking account of ***s,p,d,f*** symmetries
- For non-bulk problems ex. surface, cluster, etc...
  - MEAM rather than EAM or FS potential
- Applicability of MEAM
  - still unknown especially for non-bulk problem



Embedding Energy



History of EAM series

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1999 LJ-MEAM; M.I.Baskes, Phys.Rev.Let. 83, 2592-2595 (1999)

1997 Determination of MEAM parameters for Ni
M.I.Baskes, Mater. Chemist. and Phys., 50, 152-158 (1997)

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M.I.Baskes, J.E.Angelo, and C.L.Bisson,
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M. I. Baskes, Phys. Rev. B, 46, 2727-2742 (1992).

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1986 EAM for fcc metals Cu, Ag, Au, Ni, Pd, Pt and their alloys.
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Phys. Rev. B, 33, 7983-7991 (1986). **EAM**

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Phys. Rev. B, 29, 6443-6453 (1984).

1983 EAM for H in Metals. M. S. Daw and M. I. Baskes,
Phys. Rev. Lett., 50, 1285-1288 (1983).

Theoretical back ground and relation with other theories

...

1987 FS potential for W cluster, L.Marville and W.Andreoni,
J. Phys. Chem., 91, 2645-2649 (1987)

1986 FS potential : Surface energy for bcc metal.
G.J.Ackland and M.W.Finnis,
Philos. Mag. A, 54, 301-315 (1986)

1984 Universal features of the equation of state of metals.
J. H. Rose, J. R. Smith, F. Guinea and J. Ferrante,
Phys. Rev. B, 29, 2963-2969 (1984).

FS potential for transition metal.
M.W.Finnis and J.E.Sinclair, Philos.Mag.A., 50, 45-55(1984),

1982 Effective theory of chemical binding: H in 3d metals.
J. K. Norskov, Phys. Rev. B, 26, 2875-2885 (1982).

1981 Atoms embedded in an electron gas: Immersion energies.
M. J. Puska, R. M. Nieminen and M. Manninen,
Phys. Rev. B, 24, 3037-3047 (1981).

1980 Quasiatoms: atoms in nonuniform electronic systems.
M. J. Stott and E. Zaremba, Phys. Rev. B, 22, 1564-1583 (1980).

1976 Surf.energy.short-range-2body potential
R.A.Johnson and P.J.White,
Phys. Rev.B, 13, 5293-5302 (1976)

Birth of EAM series

EAM84 (Ni, Pd, and H)

- **EAM hypothesis**

  Embedding energy term + Two body term

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

- **Electronic density**

  Superimposition of atomic density

$$\bar{\rho}_i = \sum_{j(j\neq i)} \rho_j(R_{ij})$$

  Atomic density by Roothaan Hartree Fock

  - E.Clementi, C.Roetti, Atomic data and Nuclear data tables, 14, 177-478 (1974)

    (Isolated atom, with ~4 Slater type orbials)

- **Embedding function**
  - J. K. Norskov, Phys. Rev. B, 26, 2875-2885 (1982).
  - M. J. Puska, R. M. Nieminen and M. Manninen, Phys. Rev. B, 24, 3037-3047 (1981).
  - M. J. Stott and E. Zaremba, Phys. Rev. B, 22, 1564-1583 (1980).
- **Pair potential term** $\phi_{ij}(R_{ij}) = Z_i(R_{ij}) Z_j(R_{ij}) / R_{ij}$

  Effective charge distribution function

  determined from Lattice const., Elastic consts., Vacancy formation energy, and heat of sublimation

- **History of EAM series**

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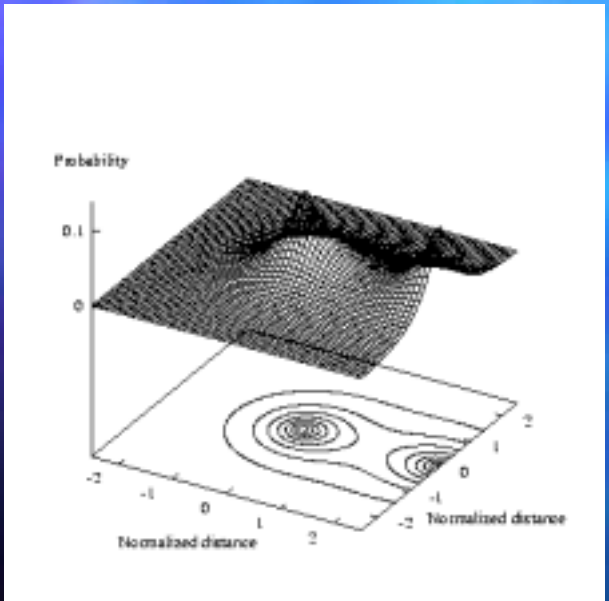
Phys. Rev. Lett., 50, 1285-1288 (1983).

Superimposition of atomic density

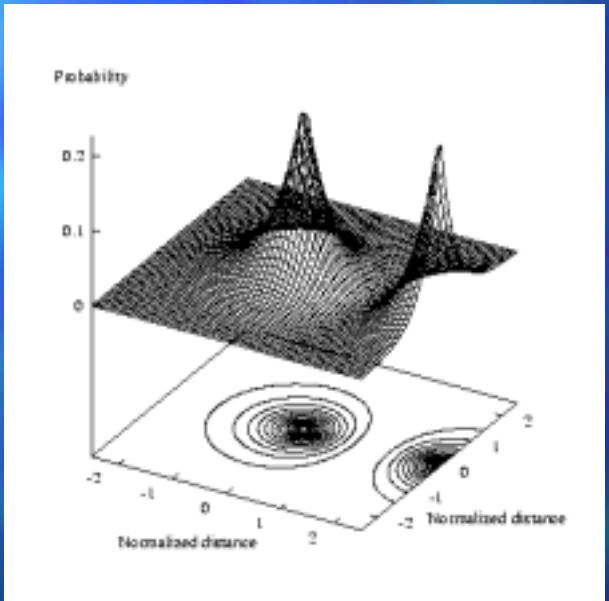
For metals, it must be good approximation.

Example of H_2^+ ion

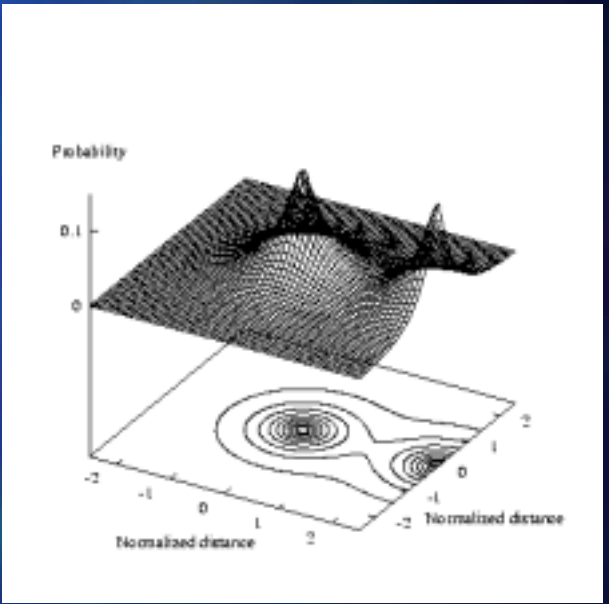
Probability density distribution of electron at equilibrium distance.



Bonding orbital



Anti-bonding orbital



Superimposition of atomic electron distribution

Evolution of EAM series (1)

EAM86 (Cu, Ag, Au, Ni, Pd, Pt, and their alloys)

- **EAM hypothesis**

  Embedding energy term + Two body term

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

- **Electronic density**

  Superimposition of atomic density

  (s and d with contribution ratio n_s and n_d)

  Atomic density of Roothaan Hartree Fock

- **Rose's universal function**

  J. H. Rose, J. R. Smith, F. Guinea and J. Ferrante,
  Phys. Rev. B, 29, 2963-2969 (1984).

  ↓

  Embedding function

  Pair potential term

  Effective charge distribution function

$$\phi_{ij}(R_{ij}) = Z_i(R_{ij}) Z_j(R_{ij}) / R_{ij}$$

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Evolution of EAM series (2)

MEAM92 (Cu, Ag, Au, Ni, Pd, Pt, Al, Pb, Rh, Ir,
Li, Na, K, V, Nb, Ta, Cr, Mo, W, Fe,
C, Si, Ge, H, N, O and their compounds)

- **EAM hypothesis**
  Embedding energy term + Two body term

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

- **Embedding function**
  Fixed

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

- **Electronic density**
  Superimposition of atomic density
  s, p, d, f symmetry
  Parameterized atomic density

$$(\bar{\rho}_i)^2 = \sum_{l=0}^{3} t_i^{(l)} \left(\rho_i^{(l)}\right)^2$$

- **Pair potential term**
  Reference structure

$$\rho_i^{a(l)} = \exp\left\{-\beta_i^{(l)}\left(\frac{R_{ij}}{R_i^0} - 1\right)\right\}$$

- **Rose's universal function**
  J. H. Rose, J. R. Smith, F. Guinea and J. Ferrante,
  Phys. Rev. B, 29, 2963-2969 (1984).
- **Screening function**
  to neglect farther atoms ?

History of EAM series

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Embedding function in MEAM92

- Fixed formalism

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

at equilibrium

$$\frac{\bar{\rho}_i}{\bar{\rho}_i^{\,0}} = 1$$

different from Equilibrium of EAM

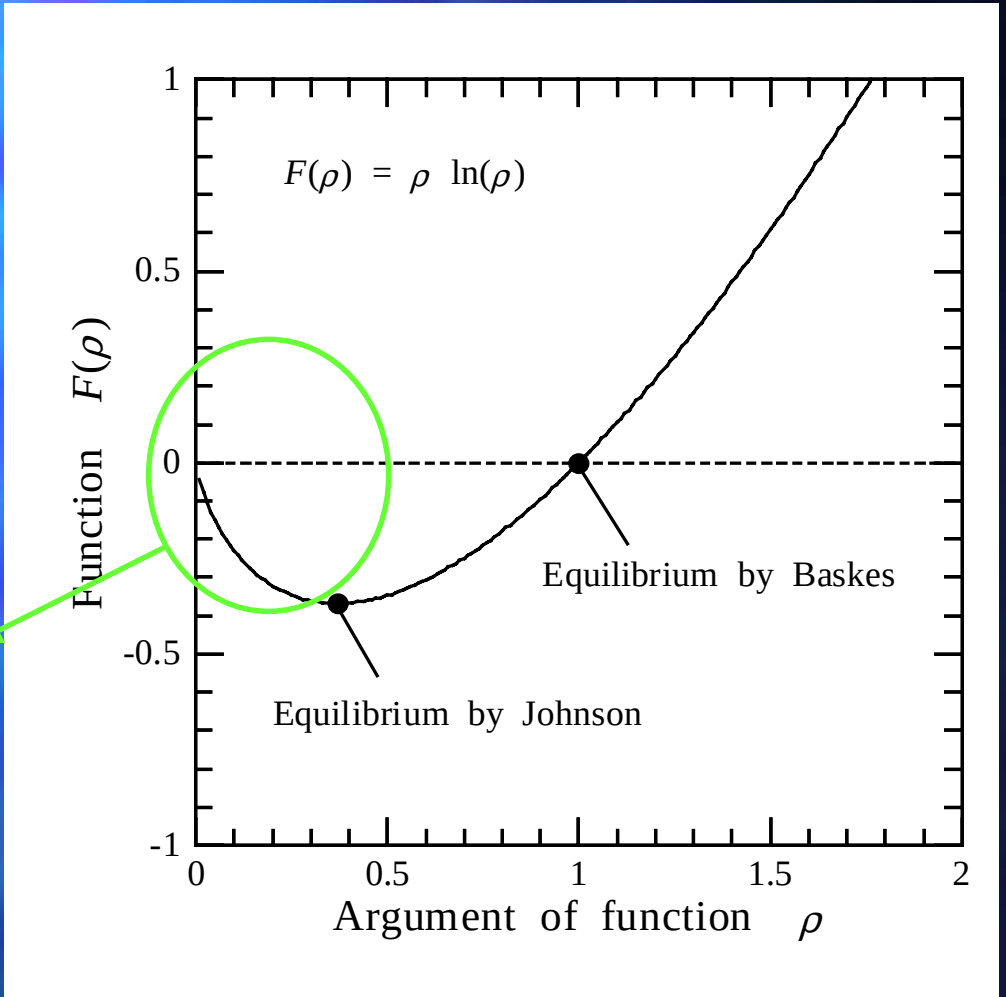
Physical meaning decreased

- Parameterized

Parameter A_i

for stacking fault energy

(FCC, HCP)



"Embedding term can be covered by pair-potential term"

Electronic density in MEAM92

$$E_{tot} = \sum_i E_i$$

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

$$(\bar{\rho}_i)^2 = \sum_{l=0}^{3} t_i^{(l)} \left(\rho_i^{(l)}\right)^2$$

$$\bar{\rho}_i = \rho_i^{(0)} \left\{ 1 + \frac{1}{2}\sum_{l=0}^{3} t_i^{(l)} \left(\rho_i^{(l)} / \rho_i^{(0)}\right)^2 + \ldots \right\}$$

- Superimposition of atomic density
- *s, p, d, f* symmetry

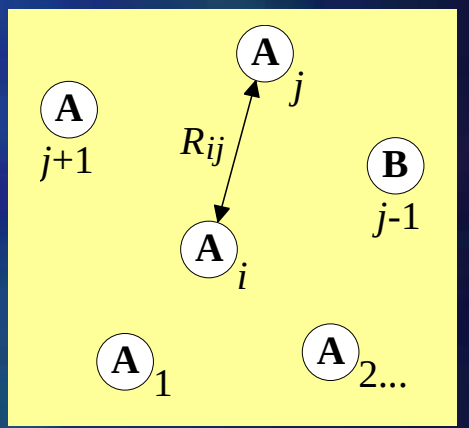
s (*l*=0)
$$\rho_i^{(0)} = \sum_{j(\neq i)} \rho_j^{a(0)}(R_{ij})$$

p (*l*=1)
$$\left(\rho_i^{(1)}\right)^2 = \sum_{\alpha} \left\{ \sum_{j(\neq i)} x_{ij}^{\alpha} \rho_j^{a(1)}(R_{ij}) \right\}^2$$

$$x_{ij}^{\alpha} = R_{ij}{}^{\alpha} / R_{ij}$$

d (*l*=2)
$$\left(\rho_i^{(2)}\right)^2 = \sum_{\alpha,\beta} \left\{ \sum_{j(\neq i)} x_{ij}^{\alpha} x_{ij}^{\beta} \rho_j^{a(2)}(R_{ij}) \right\}^2 - \frac{1}{3}\left\{ \sum_{j(\neq i)} \rho_j^{a(2)}(R_{ij}) \right\}^2$$

f (*l*=3)
$$\left(\rho_i^{(3)}\right)^2 = \sum_{\alpha,\beta,\gamma} \left\{ \sum_{j(\neq i)} x_{ij}^{\alpha} x_{ij}^{\beta} x_{ij}^{\gamma} \rho_j^{a(3)}(R_{ij}) \right\}^2$$



- Parameterized atomic density

$$\rho_i^{a(l)} = \exp\left\{ -\beta_i^{(l)} \left(\frac{R_{ij}}{R_i^0} - 1 \right) \right\}$$

parameters ;

R_i^0 $t_i^{(l)}$ $\beta_i^{(l)}$

About *s, p, d, f* symmetry in MEAM92

- Usual expression (just in case ...)

s

$$\left(\rho_i^{(0)}\right)^2 = \sum_{j,l(\neq i)} \rho_j^{a(0)}(R_{ij})\rho_l^{a(0)}(R_{il})$$

p

$$\left(\rho_i^{(1)}\right)^2 = \sum_{j,l(\neq i)} \rho_j^{a(1)}(R_{ij})\rho_l^{a(1)}(R_{il})\cos\left(\theta_{jil}\right)$$

d

$$\left(\rho_i^{(2)}\right)^2 = \sum_{j,l(\neq i)} \rho_j^{a(2)}(R_{ij})\rho_l^{a(2)}(R_{il})\left\{\cos^2\left(\theta_{jil}\right)-\frac{1}{3}\right\}$$

f

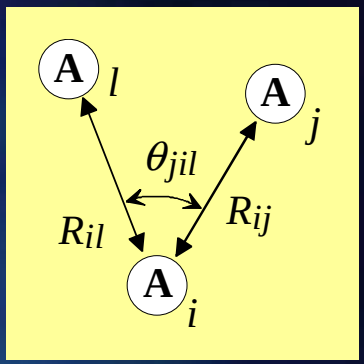
$$\left(\rho_i^{(3)}\right)^2 = \sum_{j,l(\neq i)} \rho_j^{a(3)}(R_{ij})\rho_l^{a(3)}(R_{il})\cos^3\left(\theta_{jil}\right)$$

$$\rho_i^{(0)} = \sum_{j(\neq i)} \rho_j^{a(0)}(R_{ij})$$

$$\left(\rho_i^{(1)}\right)^2 = \sum_{\alpha}\left\{\sum_{j(\neq i)} x_{ij}^{\alpha}\rho_j^{a(1)}(R_{ij})\right\}^2$$

$$\left(\rho_i^{(2)}\right)^2 = \sum_{\alpha,\beta}\left\{\sum_{j(\neq i)} x_{ij}^{\alpha}x_{ij}^{\beta}\rho_j^{a(2)}(R_{ij})\right\}^2 - \frac{1}{3}\left\{\sum_{j(\neq i)}\rho_j^{a(2)}(R_{ij})\right\}^2$$

$$\left(\rho_i^{(3)}\right)^2 = \sum_{\alpha,\beta,\gamma}\left\{\sum_{j(\neq i)} x_{ij}^{\alpha}x_{ij}^{\beta}x_{ij}^{\gamma}\rho_j^{a(3)}(R_{ij})\right\}^2$$



- Superimposition of no wave function but electronic density
  Anti-bonding state would be never expressed.

$$\rho_i^{a(l)} = \exp\left\{-\beta_i^{(l)}\left(\frac{R_{ij}}{R_i^0}-1\right)\right\}$$

Applicability of MEAM92

Still unknown

- Expectable rather than quantum calculation.
  Not only calculation time but also reliability in approcimation
- Accuracy must be examined.
  Accuracy of both Method and Parameters

- Bulk problems
- Surface problems to cluster problems
  - Si 7×7 DAS structure
    Calculation of surface energy and simulation of reconstruction for Si (111) 3X3, 5X5, 7X7, and 9X9...
    (Kunio TAKAHASHI, Chikara NARA, Takahiro YAMAGISHI, and Tadao ONZAWA)
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  - FCC (110) Missing Row structure
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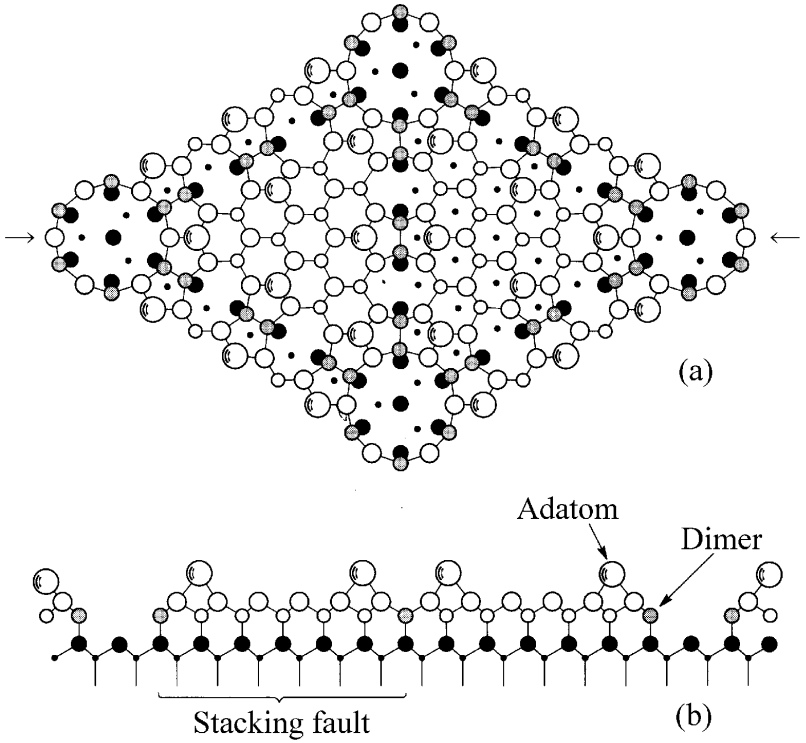
MEAM92 application to Si 7x7 DAS structure (1)

- DAS structure ;

  K.Takayanagi, Y.Tanishiro, M.Takahashi, and S.Takahashi, J. Vac. Sci. Technol. A, 3, 1502 (1985)

- Why 7x7 is observed.

- Sometimes 5x5 is observed rather than 9x9.



	Dimmer	Adatom	Rest atom	Corner home
3×3	3	2	0	1
5×5	6	6	2	1
7×7	9	12	6	1
9×9	12	20	12	1

MEAM92 application to Si 7x7 DAS structure (2)

Kunio TAKAHASHI, Chikara NARA, Takahiro YAMAGISHI, and Tadao ONZAWA, Applied Surface Science, vol.151 ,no.3-4 , pp.299--301 ,(1999)

- 7x7 is stable.
- 5x5 is more stable than 9x9.

First principle calculation :
I.Stich, M.C.Payne, R.D.King-Smith, J-S.Lin, and L.J.Clarke, Phys. Rev. Lett., 68, 1351 (1992).

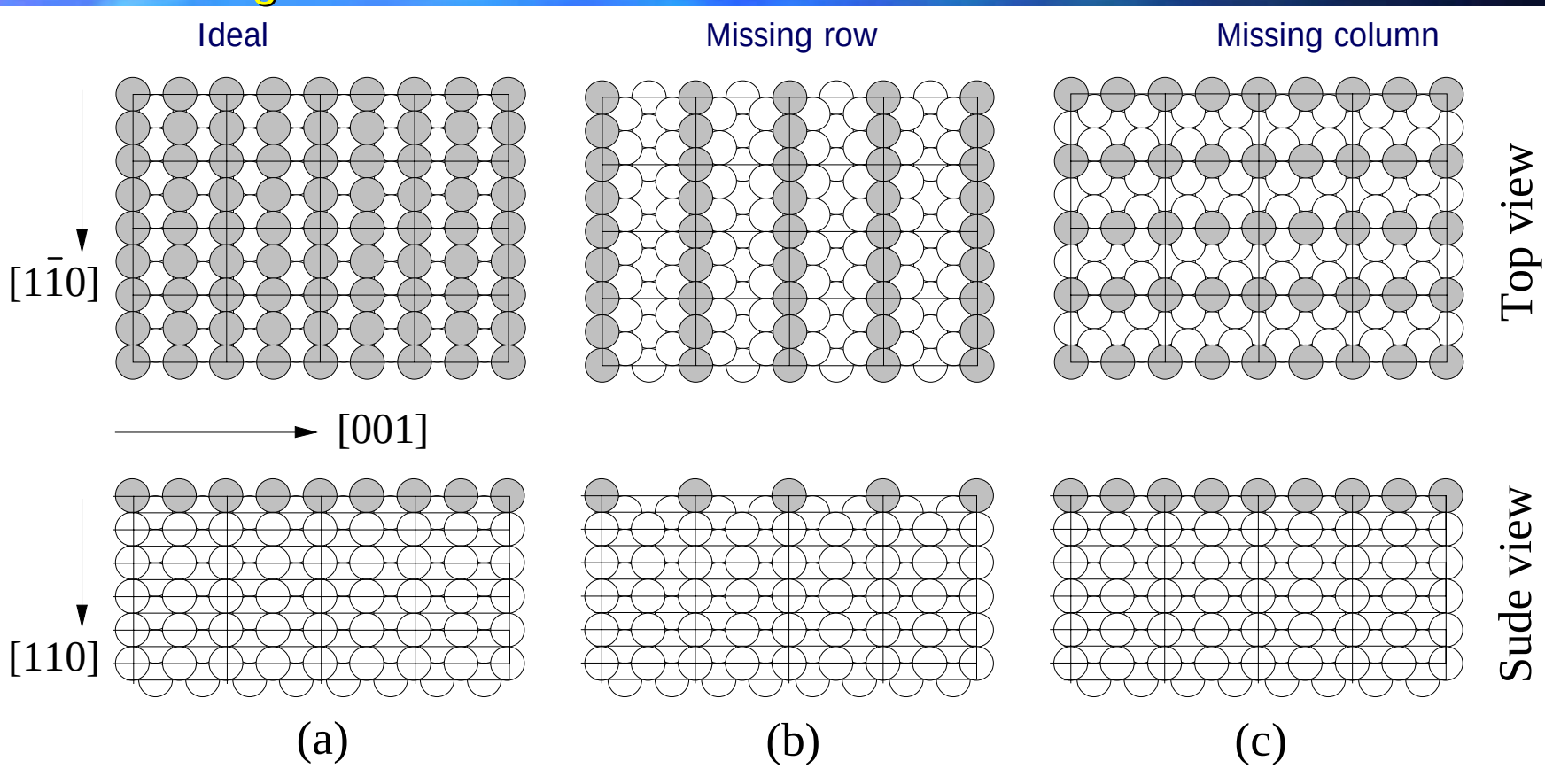
Tight binding estimation :
Y.F.Zhao, H.Q.Yang, J.N.Gao, Z.Q.Xue, and S.J.Pang, Phys. Rev. B, 58, 13824 (1998).

Structure	Surface energy (mJ/m^2)			
	present study		Reference	
	before reconstruction	after reconstruction	Stich	Zhao
3×3	2753	1571	1503	1503
5×5	2533	1530	1468	1468
7×7	2388	1524	1449	1449
9×9	2452	1549	—	1453

MEAM92 application to FCC(110) structure (1)

Takahiro YAMAGISHI, Kunio TAKAHASHI, and Tadao ONZAWA,
Surface Science, vol.445, no.1, pp.18--22 ,(2000)

FCC missing row structure

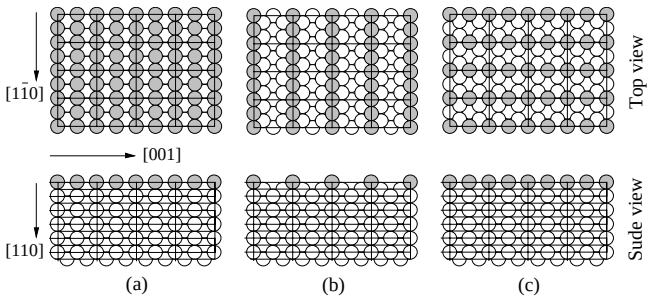


MEAM92 application to FCC(110) structure (2)

Results by MEAM92

- Good agreement
- must be careful
- Problem remains
  method or parameter

Material	Surface Energy (mJ/m^3)			Stable structure (exp.)
	Ideal	M.R.	M.C.	
Au	1081	1035	1152	M.R.
Pt	2252	1723	2077	M.R.
Pb	426	450	481	Ideal
Rh	3488	3526	3695	Ideal
Pd	1830	1642	1829	Ideal
Ni	2813	2372	2821	?



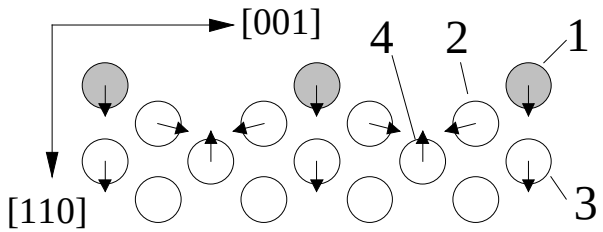
Takahiro YAMAGISHI, Kunio TAKAHASHI, and Tadao ONZAWA,
Surface Science, vol.445, no.1, pp.18--22 ,(2000)

MEAM92 application to FCC(110) structure (3)

Results by MEAM92

- Good agreement
- must be careful
- Problem remains method or parameter

Takahiro YAMAGISHI, Kunio TAKAHASHI, and Tadao ONZAWA, Surface Science, vol.445, no.1, pp.18--22 ,(2000)



Element		1		2		3		4	
Direction		[001]	[110]	[001]	[110]	[001]	[110]	[001]	[110]
Au	MEAM	0	0.31	-0.01	0.07	0	0.09	0	-0.14
	LEED[9]	0	0.23	-0.07	-0.06	0	0.09	0	-0.15
Pt	MEAM	0	0.34	-0.06	0.02	0	0.13	0	-0.16
	LEED[10]	0	0.33	-0.05	0.04	0	0.11	0	-0.06

Applicability of MEAM92

Still unknown

Probably the best method for very large bulk

Maybe useful for large surface problem

Be careful for cluster problem

- Expectable rather than quantum calculation.
  - For large system
  - Not only calculation time but also reliability in calculation
- Accuracy must be examined.
  - Accuracy of Method
    Parameters

Evolution of EAM series (3)

LJ-EAM99

- EAM hypothesis

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

$$F(\bar{\rho}_i) = \frac{A}{2} E_0 \left\{ \frac{\bar{\rho}_i}{\bar{\rho}_i^{\,0}} \ln\left(\frac{\bar{\rho}_i}{\bar{\rho}_i^{\,0}} \right) - 1 \right\}$$

$$\bar{\rho}_i = \sum_{j(j\neq i)} \rho_j(R_{ij}) \qquad \rho_j(R_{ij}) = \exp\left\{ -\beta \left(\frac{R_{ij}}{R_0} - 1 \right) \right\}$$

- No ***s,p,d,f*** symmetry
  no difference between FCC and HCP
- Rose's function -> Lennard Jones (LJ)
  Pair potential term is determined
  so that the results are same as LJ.

Universal feature of material ? A β

- History of EAM series

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1999 LJ-MEAM; M.I.Baskes, Phys.Rev.Let. 83, 2592-2595 (1999)

1997 Determination of MEAM parameters for Ni
M.I.Baskes, Mater. Chemist. and Phys., 50, 152-158 (1997)

1994 Atomistic calculation of composite interface
M.I.Baskes, J.E.Angelo, and C.L.Bisson,
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M. S. Daw, S. M. Foiles and M. I. Baskes,
Mater. Sci. Rep., 9, 251-310 (1993).

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Phys. Rev. B, 40, 6085-6100 (1989).

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M. I. Baskes, Phys. Rev. Lett., 59, 2666-2669 (1987).

1986 EAM for fcc metals Cu, Ag, Au, Ni, Pd, Pt and their alloys.
S. M. Foiles, M. I. Baskes and M. S. Daw,
Phys. Rev. B, 33, 7983-7991 (1986).

1984 EAM for H in Metals. M. S. Daw and M. I. Baskes,
Phys. Rev. B, 29, 6443-6453 (1984).

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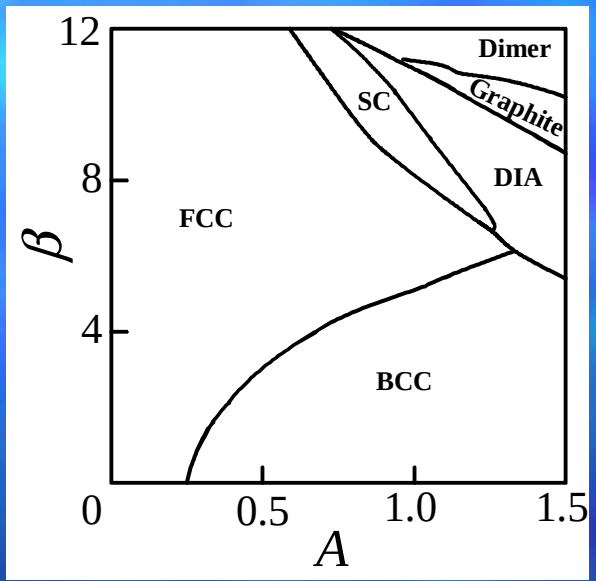
LJ-EAM99

- Universal feature of material ?

A β



- No ***s,p,d,f*** symmetry

  no difference between FCC and HCP

Possibility of extension

- History of EAM series

...

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