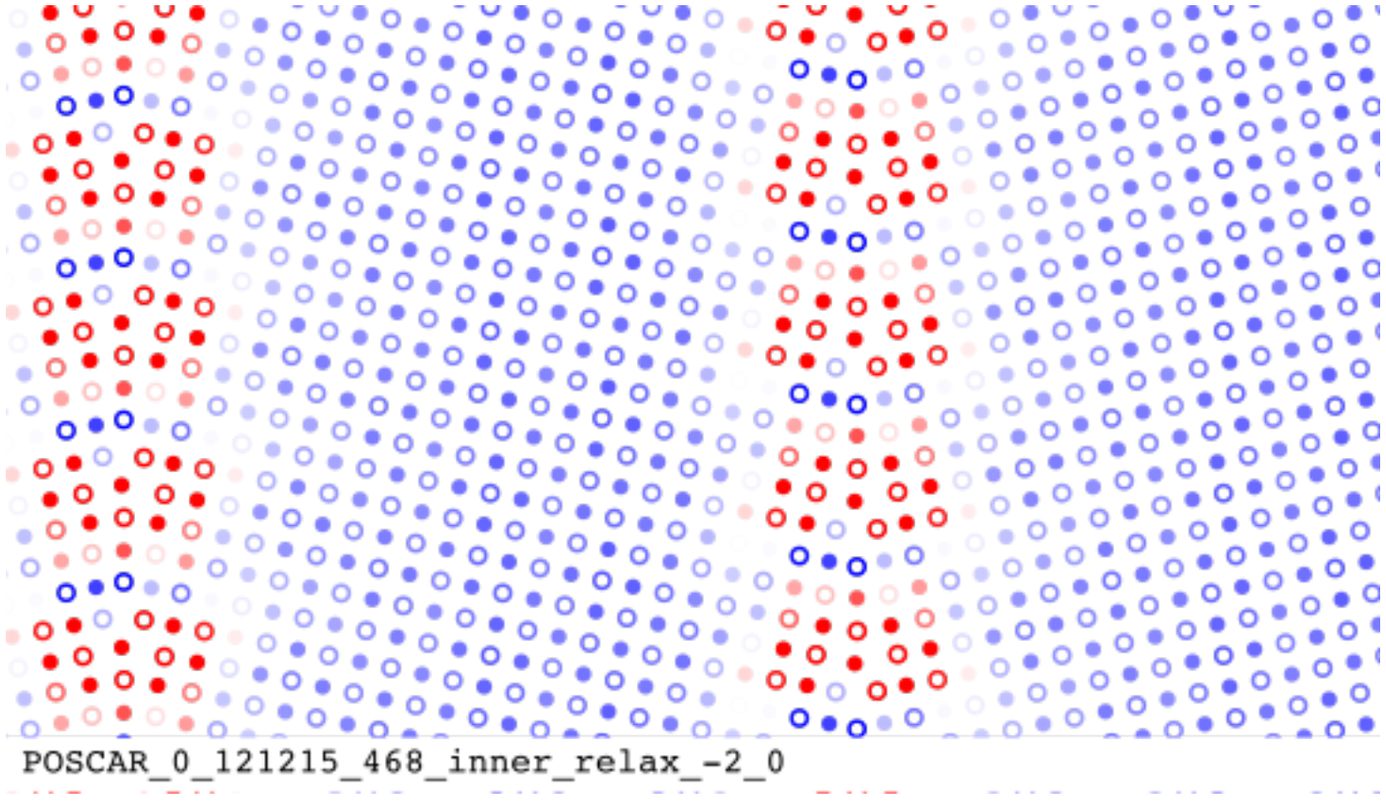
第8回 IFERC-CSC研究会
2018.2.27-3.1
ビジョンセンター日本橋 本館5階501号室

Cuの粒界エネルギーの精密計算



関西学院大学・理工学部・西谷滋人

contents

- Theoretical, experimental and simulated
  - Read and Shockley's theoretical prediction
  - Otsuki's experimental results
  - Others(experimental and calculated)
- First principles(VASP) calculations
  - Al, Cu
- EAM analysis
- Conclusions

Read and Shockley Theoretical Predictions

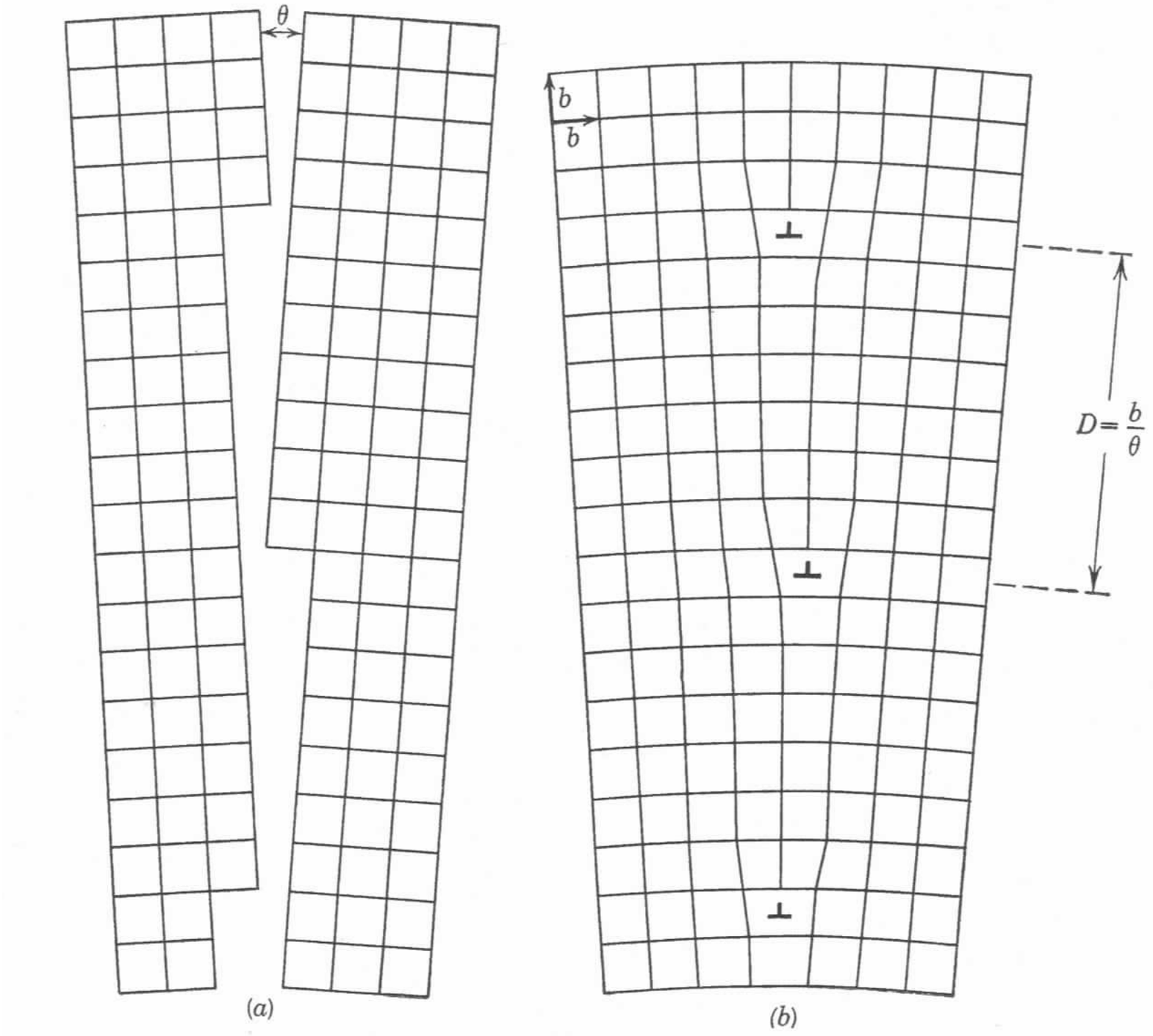
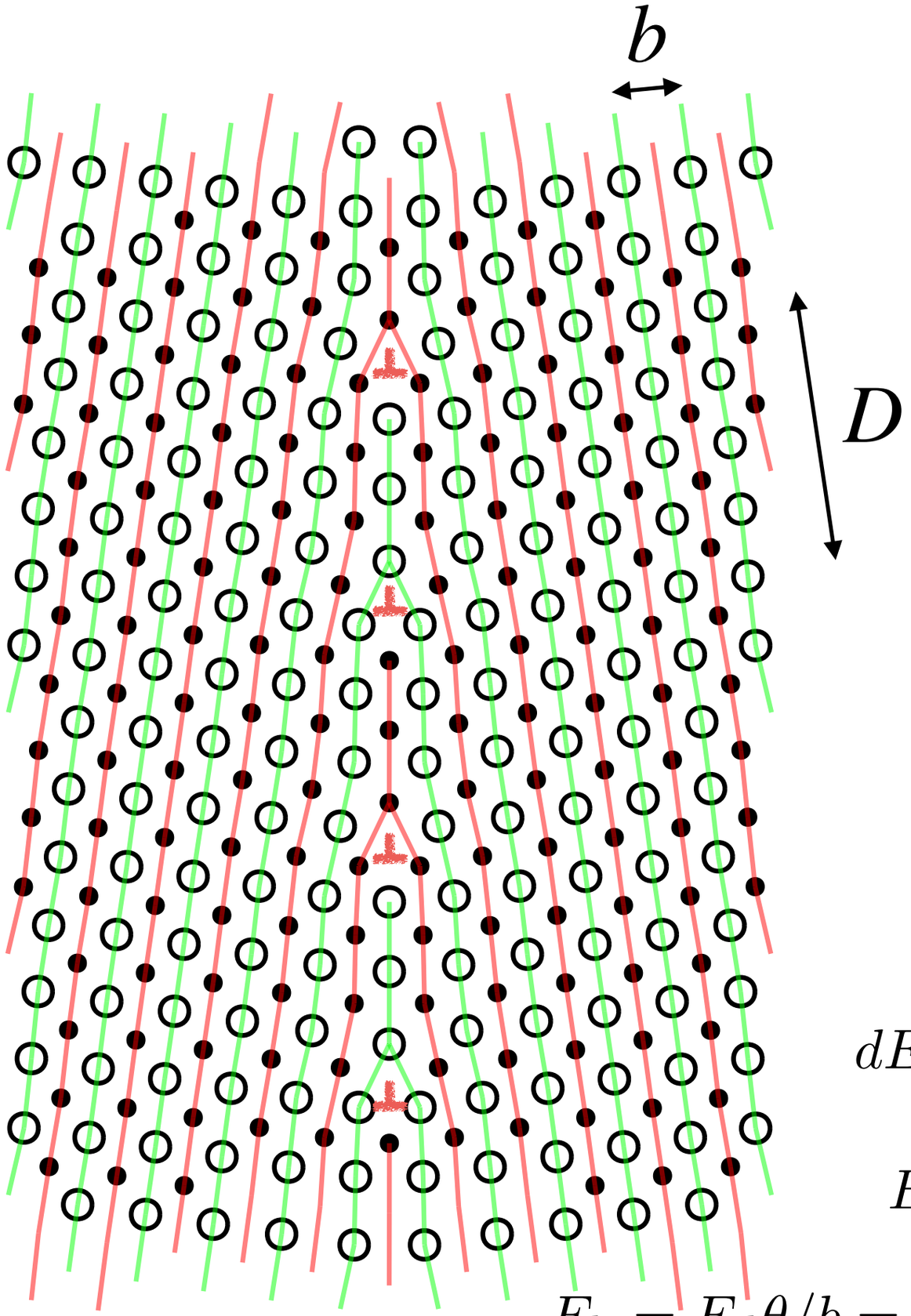
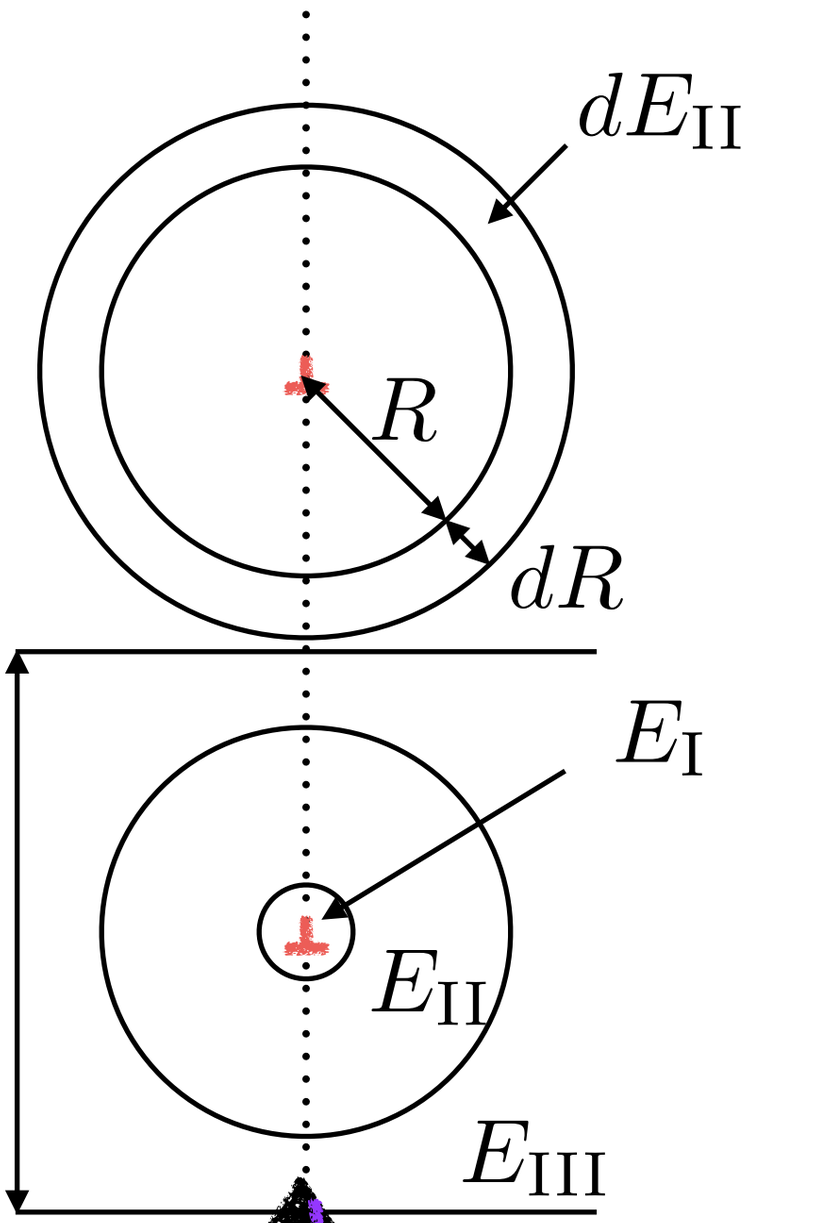


FIG. 1. Simple grain boundary showing (*a*) two grains with common crystal axis and (*b*) method of joining and dislocation model.

"Dislocation Models of Grain Boundaries", W. T. Read Jr., and W. Shockley, "Imperfection in nearly perfect crystals", ed. by W. Shockley, chap.13, (Wiley, New York, 1952) p.352-376.



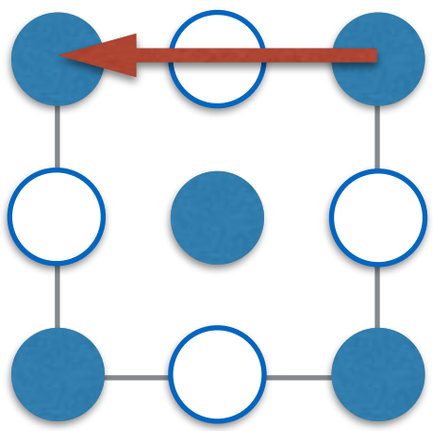


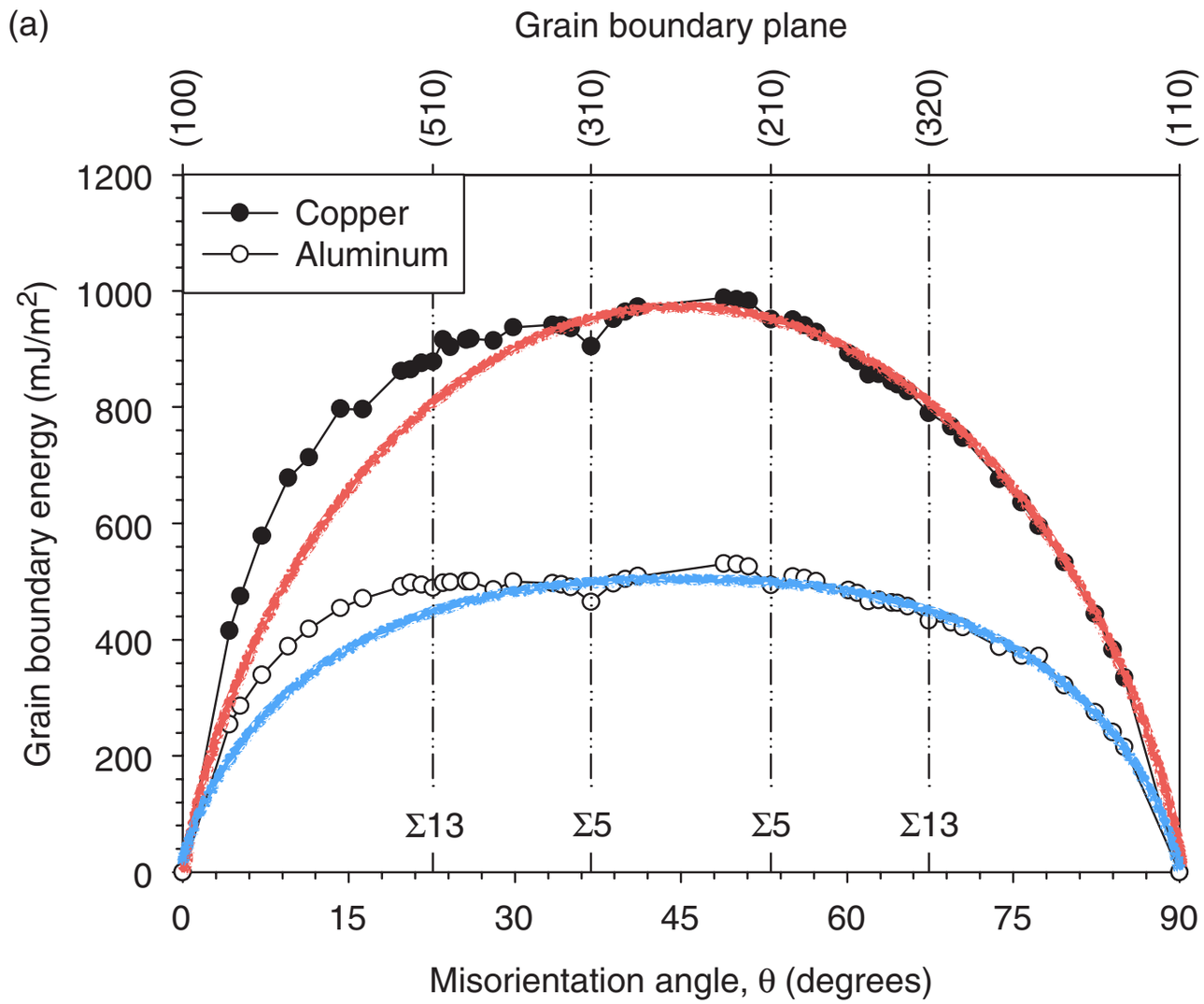
$$D = \frac{b}{\theta}$$

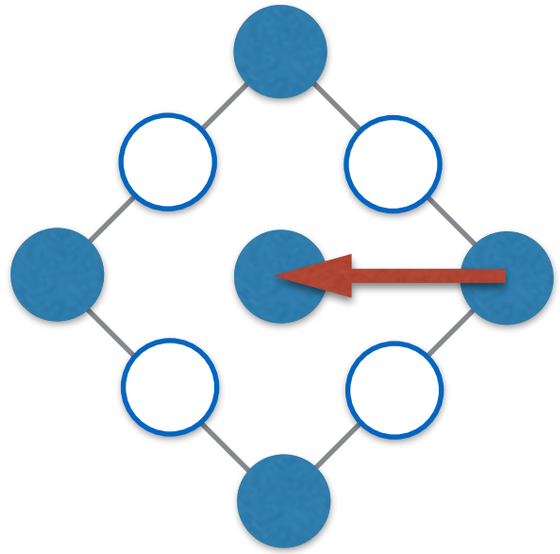
$$dE_{\mathrm{II}} = -\frac{\mathbf{b}^2 \tau_0}{2} \frac{d\theta}{\theta}$$

$$E_{\mathrm{d}} = \int_{r_{\mathrm{core}}}^{r_\theta} dE_{\mathrm{II}}$$

$$E_{\mathrm{b}} = E_{\mathrm{d}}\theta/b \fallingdotseq E_0\theta(A - \log\theta)$$







"Asymmetric tilt grain boundary structure and energy in copper and aluminium",
M. A. Tschopp and D. L. Mcdowell, Phil. Mag.,
Vol. 87 (2007), 3871–3892.
They used EAM potentials.

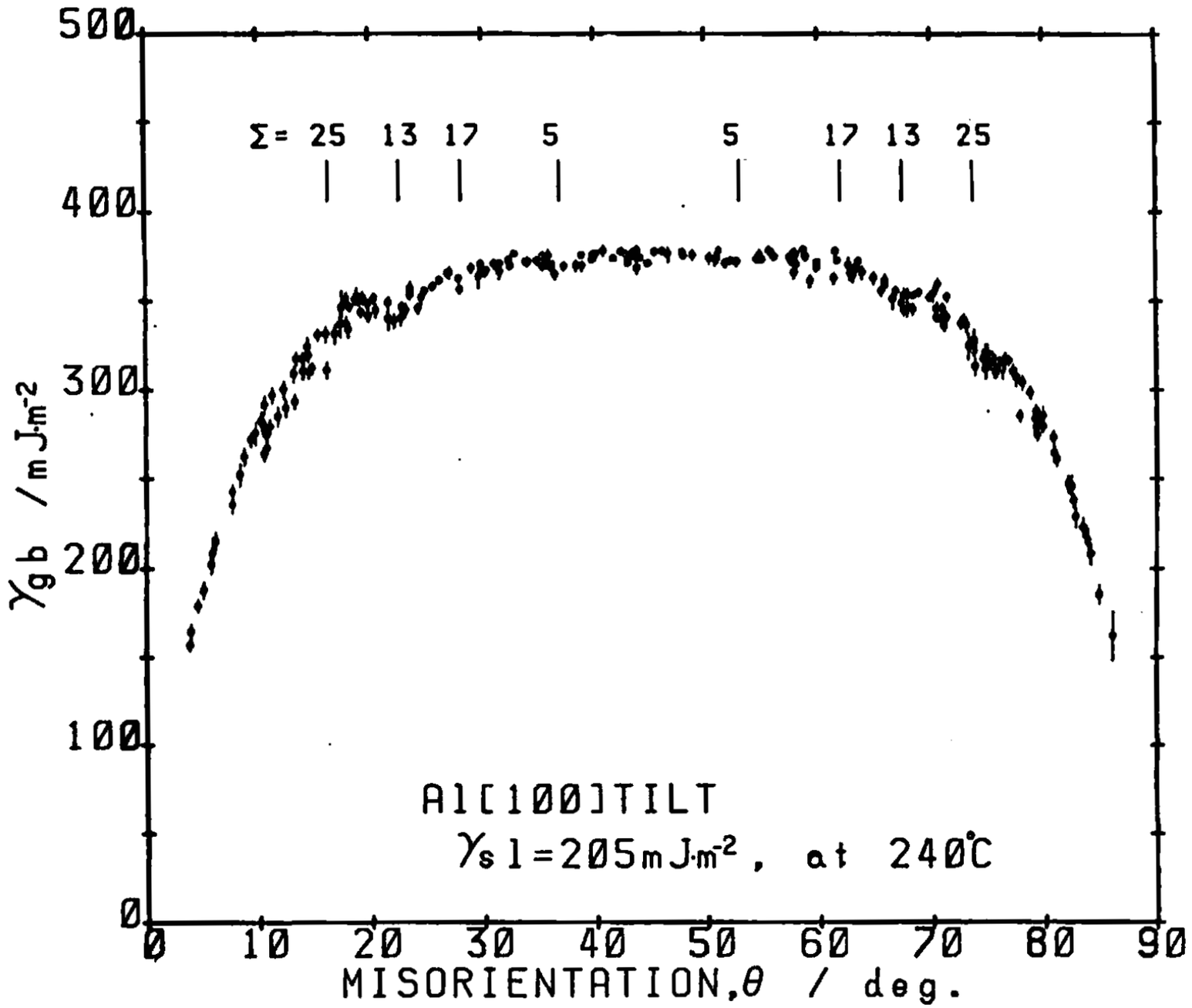
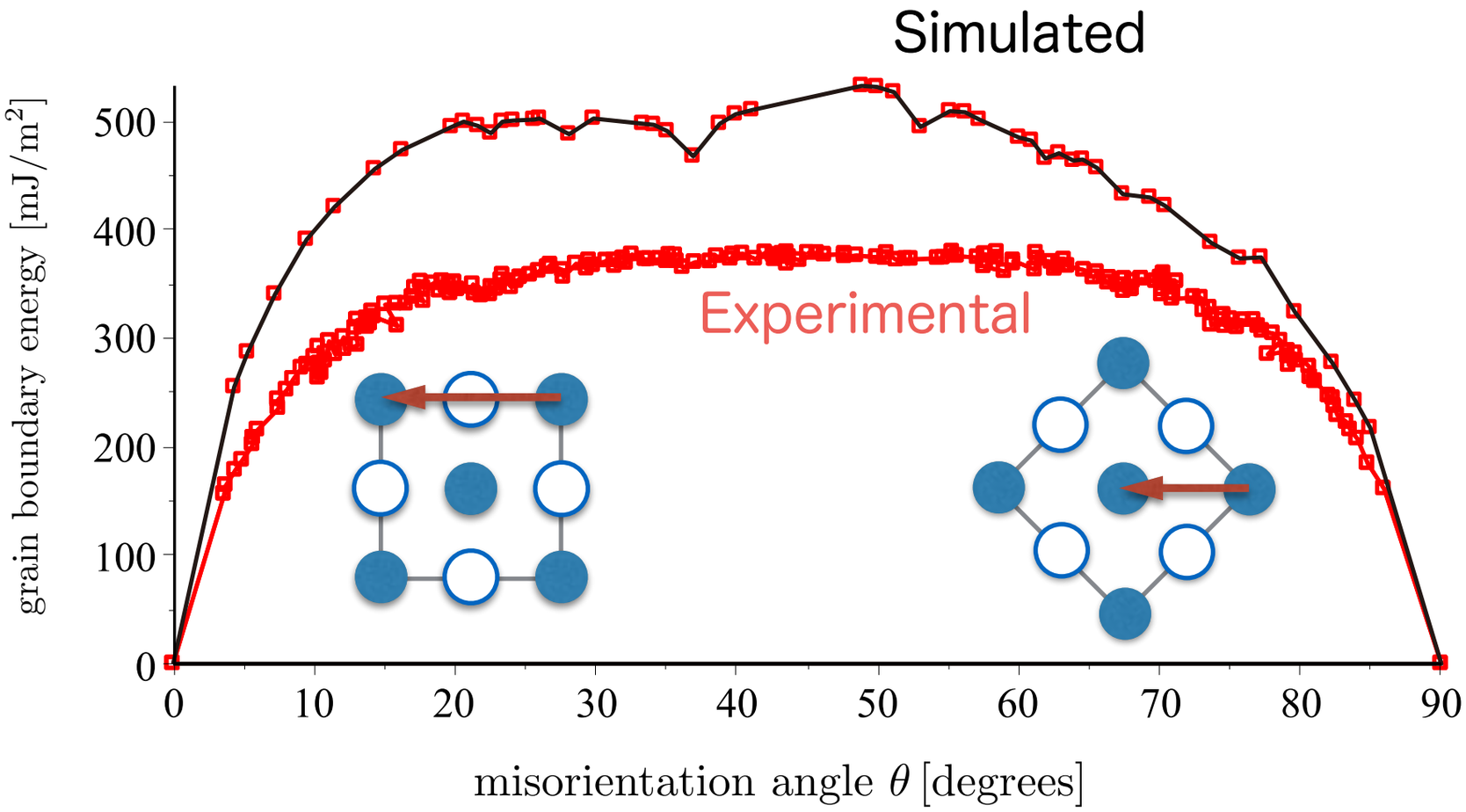
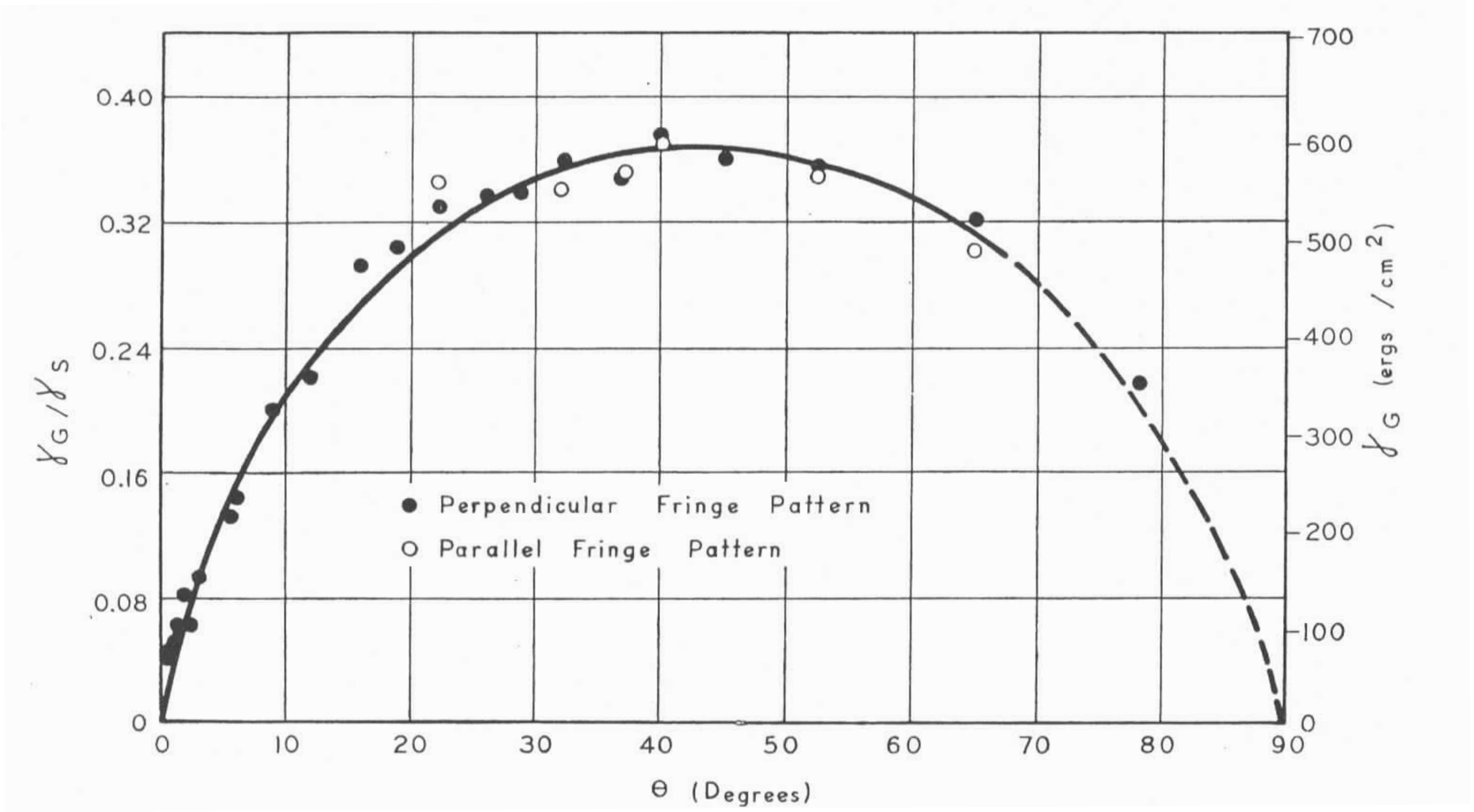


Fig.5-9 Grain boundary energy, γgb, as a function of θ for Al[100] tilt boundary, where γsl =205mJ·m^{-2}.

“アルミニウムの粒界エネルギーに関する研究”,大槻, 徹 (京都大学, 1990-07-23), 博士論文, p.115.

A. Otuki, J. Material Science, 40(2005), 3219.


Simulated
Experimental
grain boundary energy [mJ/m^2]
500
400
300
200
100
0
0
10
20
30
40
50
60
70
80
90
misorientation angle θ [degrees]



"Absolute interfacial energies of [001] tilt and twist grain boundaries in copper." N.A.Gjostein and F.N.Rhines, Acta Metallurgica, Vol. 7, May 1959, 319.

Fig.4. Dependencies of grain boundary energy on misorientation for [001] tilt boundaries at 1065C. Solid line represents the curve calculated from equation (1), using the large angle parameters.

G. C. Hasson and C. Goux, Scripta Met., 5 (1971), 889.

Measured

Computed

Al

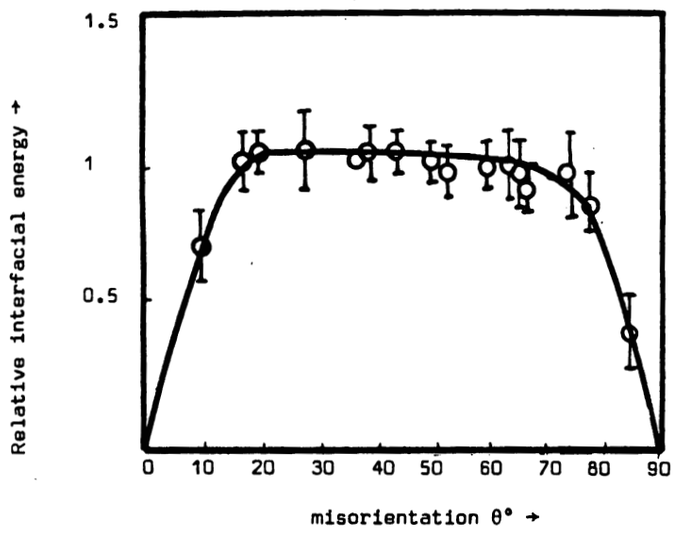


FIG. 1

Measured relative energies of [100] tilt boundaries in aluminium as a function of the misorientation θ (between [001] directions) The 37° [100] tilt boundary is used as reference for the energies.

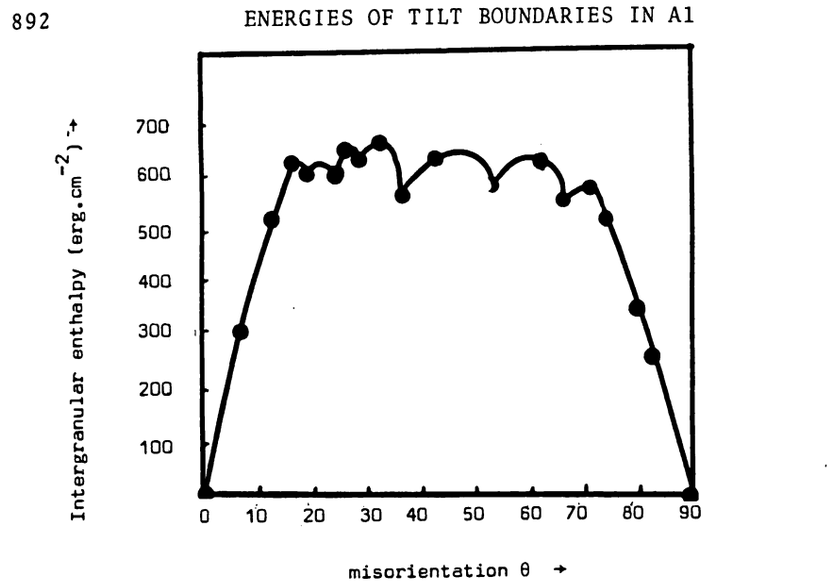
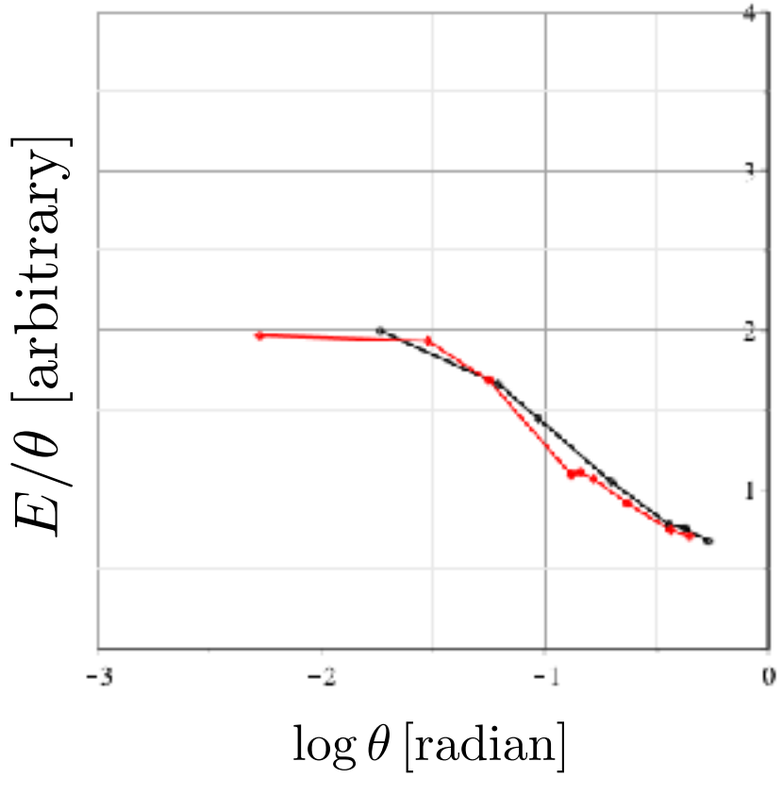
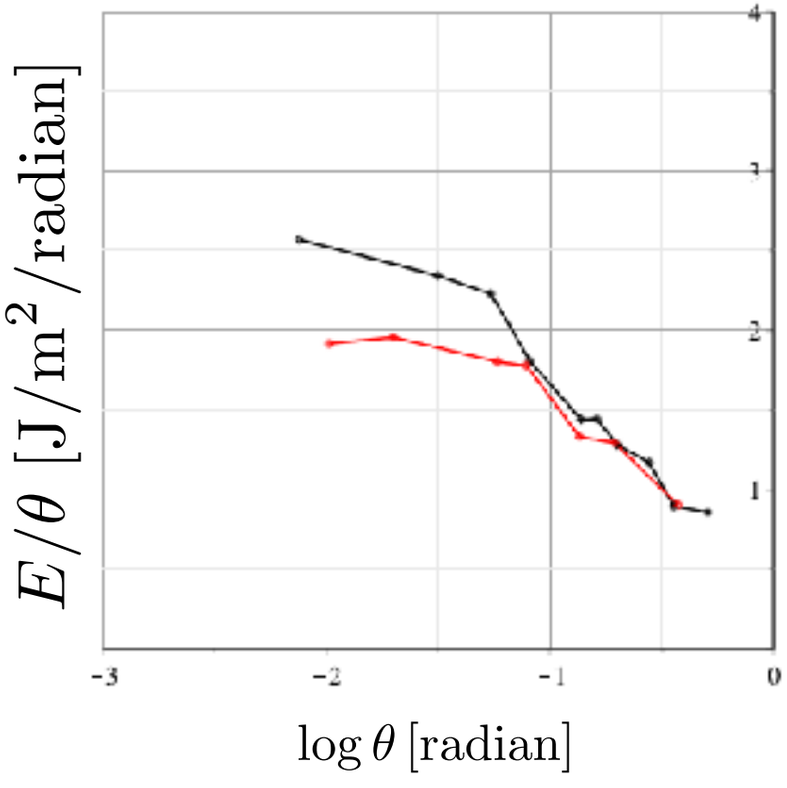


FIG. 3

Computed intergranular enthalpy of [100] tilt boundaries in aluminium as a function of misorientation θ (between [001] directions)

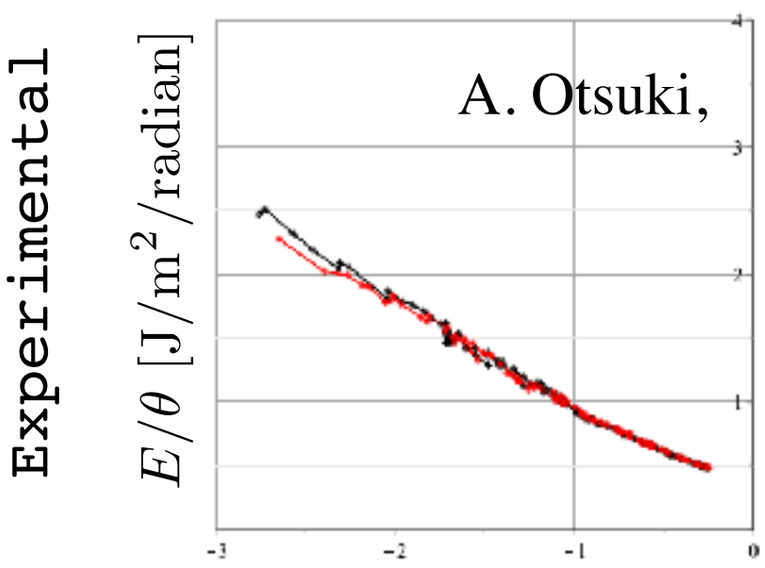


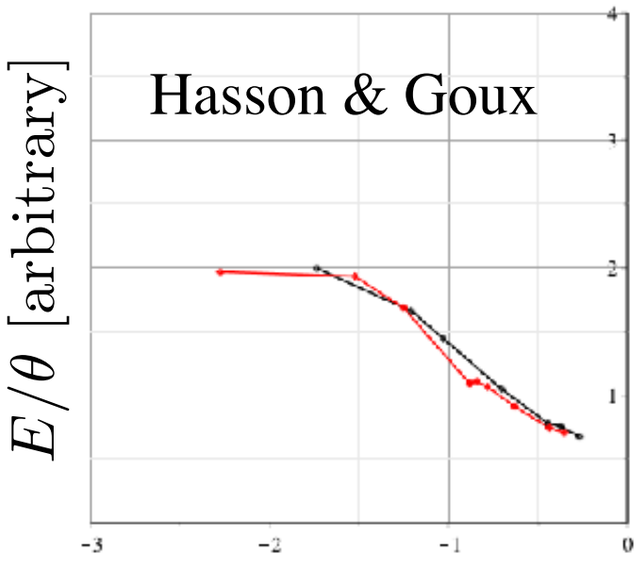


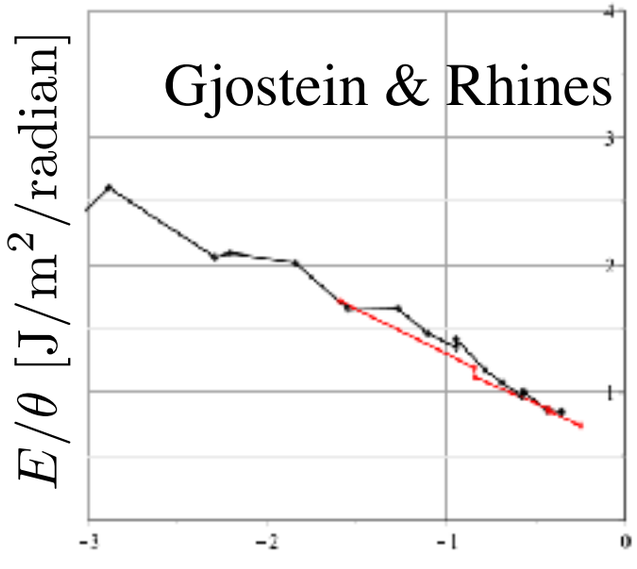
$$E = E_0\theta(A - \log\theta)$$

$$\frac{E}{\theta} = B - C\log\theta$$

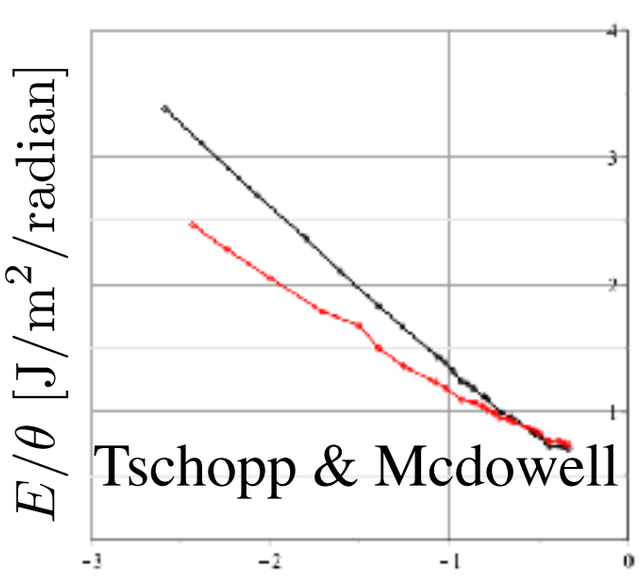
Experimental

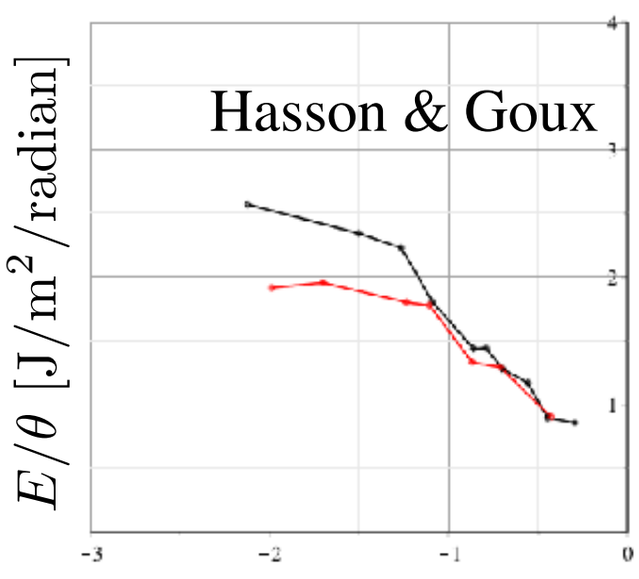


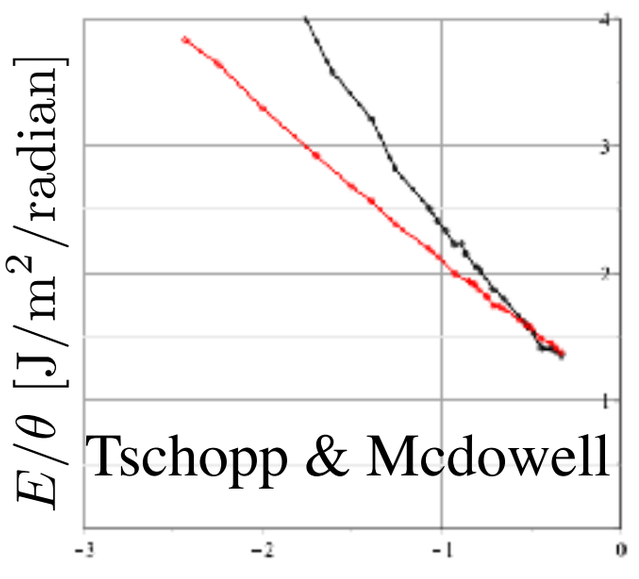




Calculated







VASP calculations for tilt boundaries

Al

VASP calc. conditions

Pseudo Potentail:PAW
Relaxations: outer relax by hand
fix calc after relaxations
INCAR
  Energy Cut off:273.15eV
   IBRION = 2   #Relax ions with conjugate-gradient
    ISIF = 2   #Relax ions, calc stress
   EDIFF = 1.0e-05 #criteria for electronic SC-loop
   EDIFFG = -0.02   #criteria for ionic relaxation loop
KPOINT
Use automatic
  length=50 due to no d-electron for Al

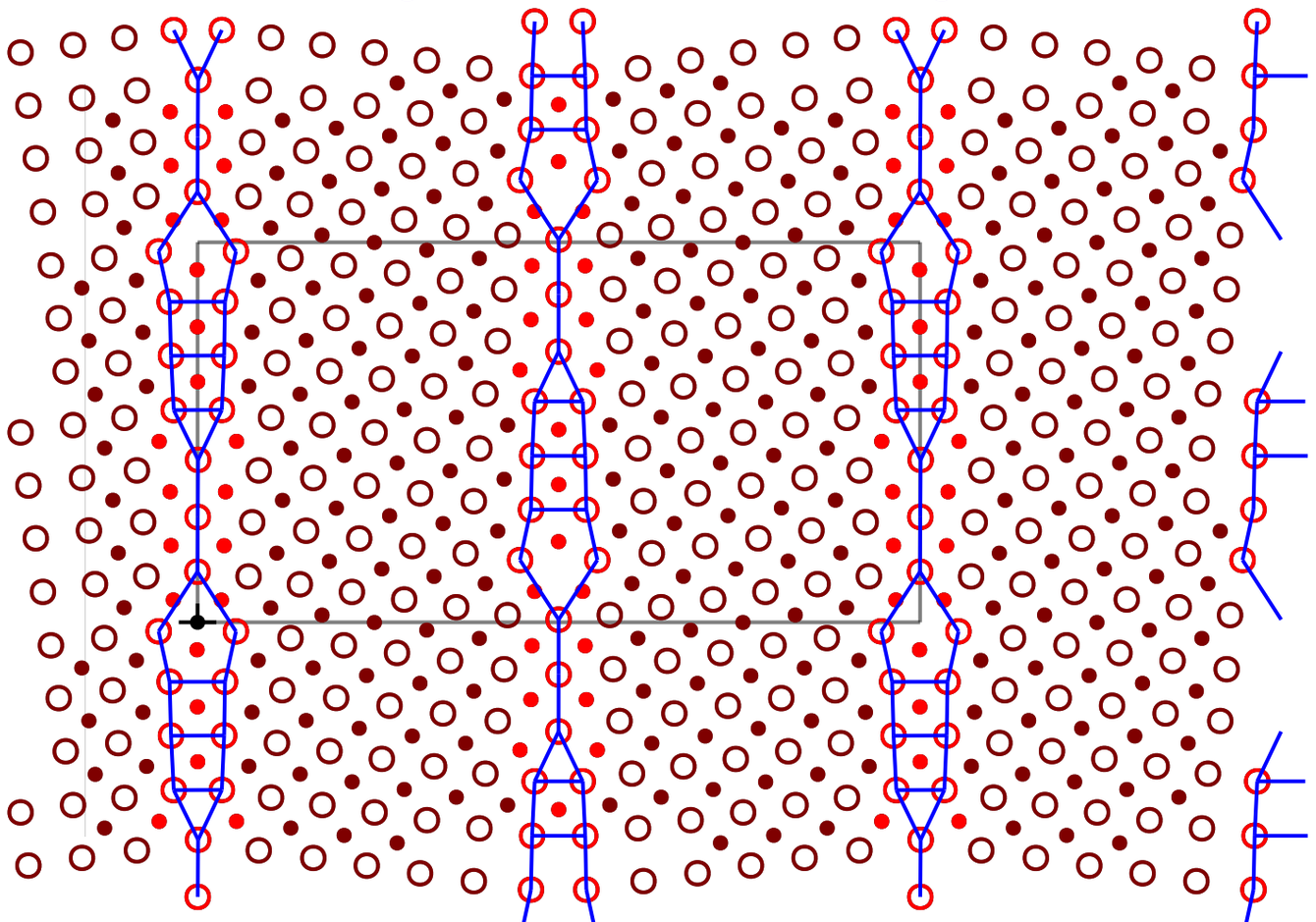
100

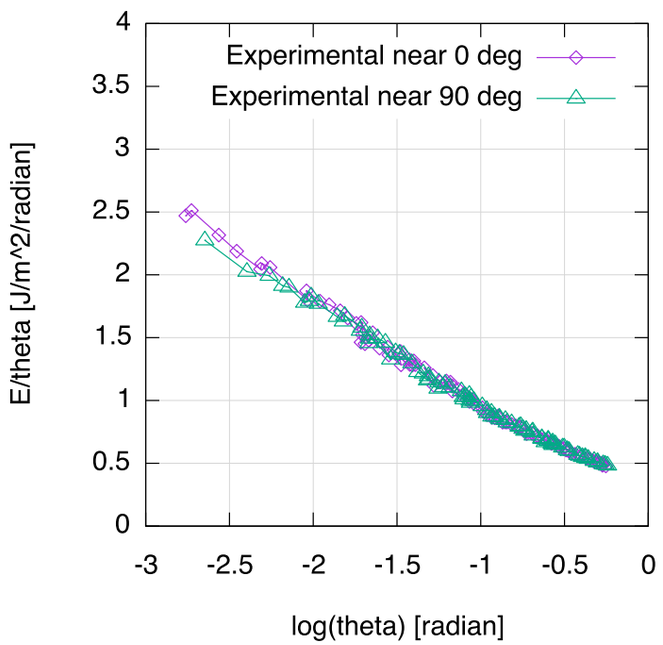
EAM analysis

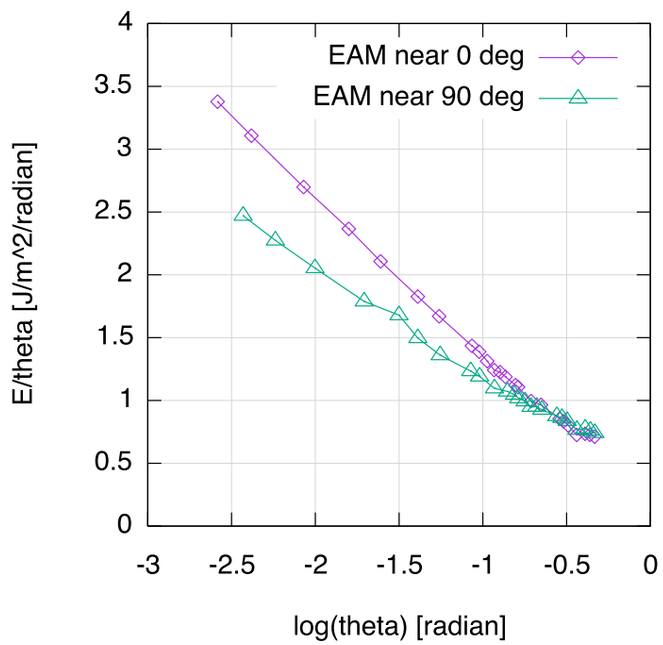
POSCAR_0_4417_88_-8_0

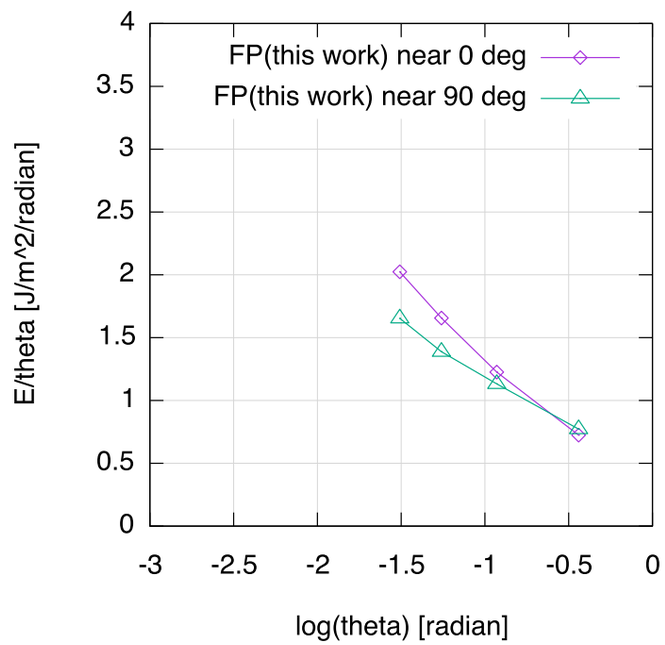
boundary structure

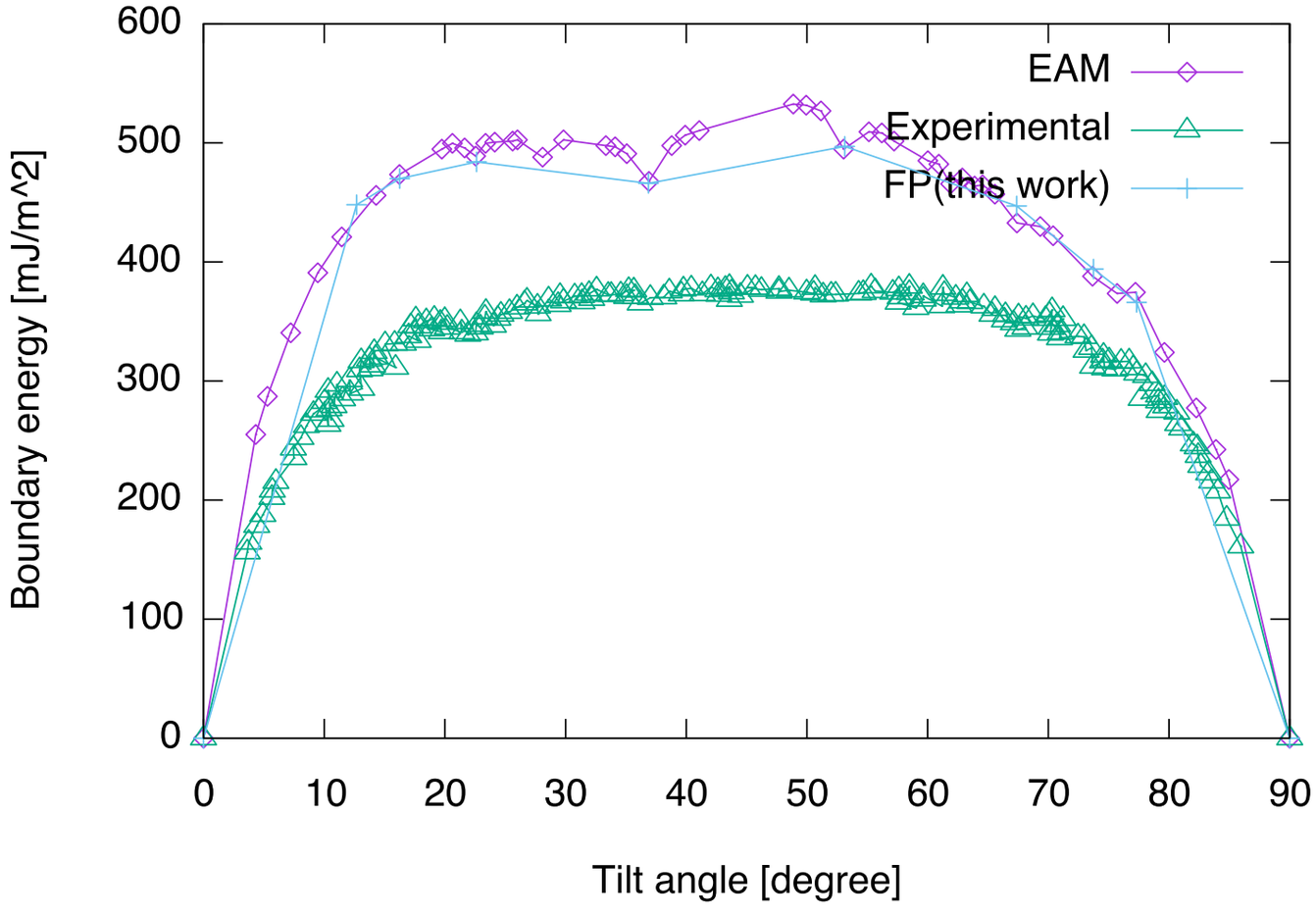
$$\theta = 16.26^\circ,$$
$$73.74^\circ$$




Experimental near 0 deg
Experimental near 90 deg
E/theta [J/m^2/radian]
log(theta) [radian]
4
3.5
3
2.5
2
1.5
1
0.5
0
-3
-2.5
-2
-1.5
-1
-0.5
0


EAM near 0 deg
EAM near 90 deg
E/theta [J/m^2/radian]
log(theta) [radian]
4
3.5
3
2.5
2
1.5
1
0.5
0
-3
-2.5
-2
-1.5
-1
-0.5
0


FP(this work) near 0 deg
FP(this work) near 90 deg
E/theta [J/m^2/radian]
log(theta) [radian]
4
3.5
3
2.5
2
1.5
1
0.5
0
-3
-2.5
-2
-1.5
-1
-0.5
0

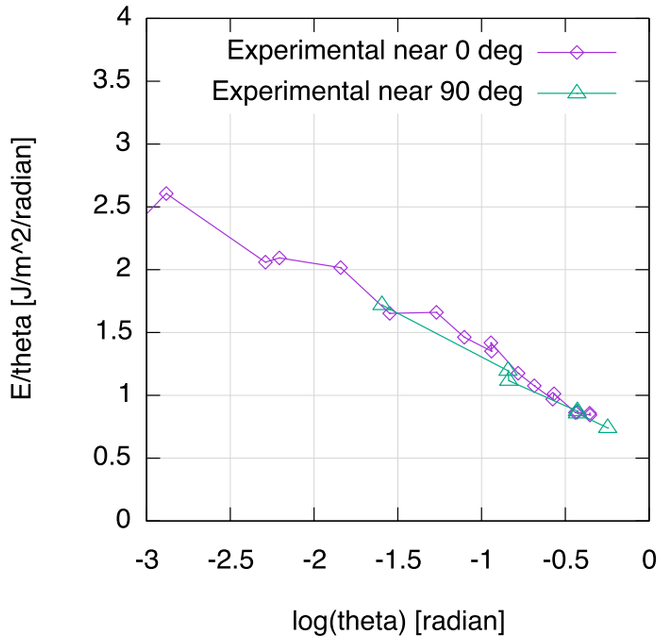

EAM
Experimental
FP(this work)
Boundary energy [mJ/m^2]
Tilt angle [degree]
600
500
400
300
200
100
0
0
10
20
30
40
50
60
70
80
90

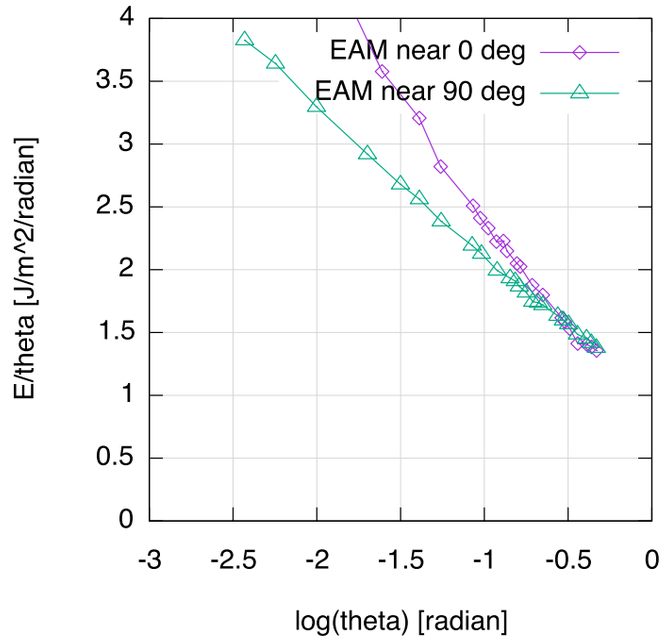
VASP calculations for tilt boundaries

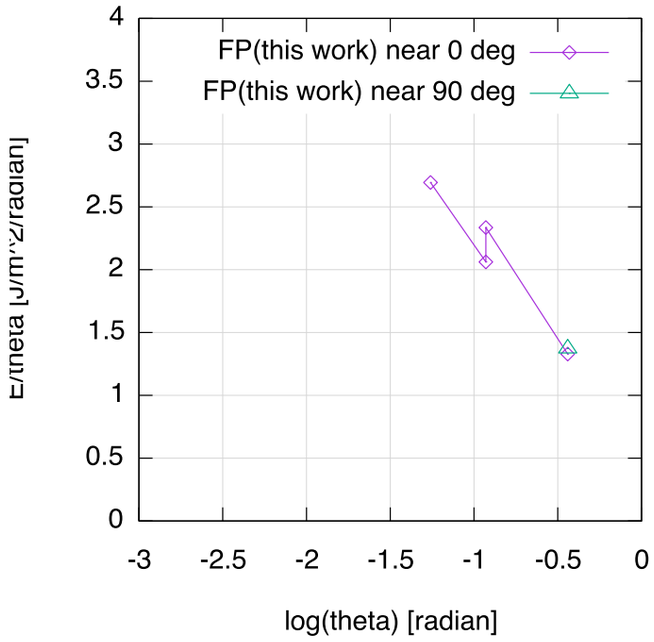
Cu

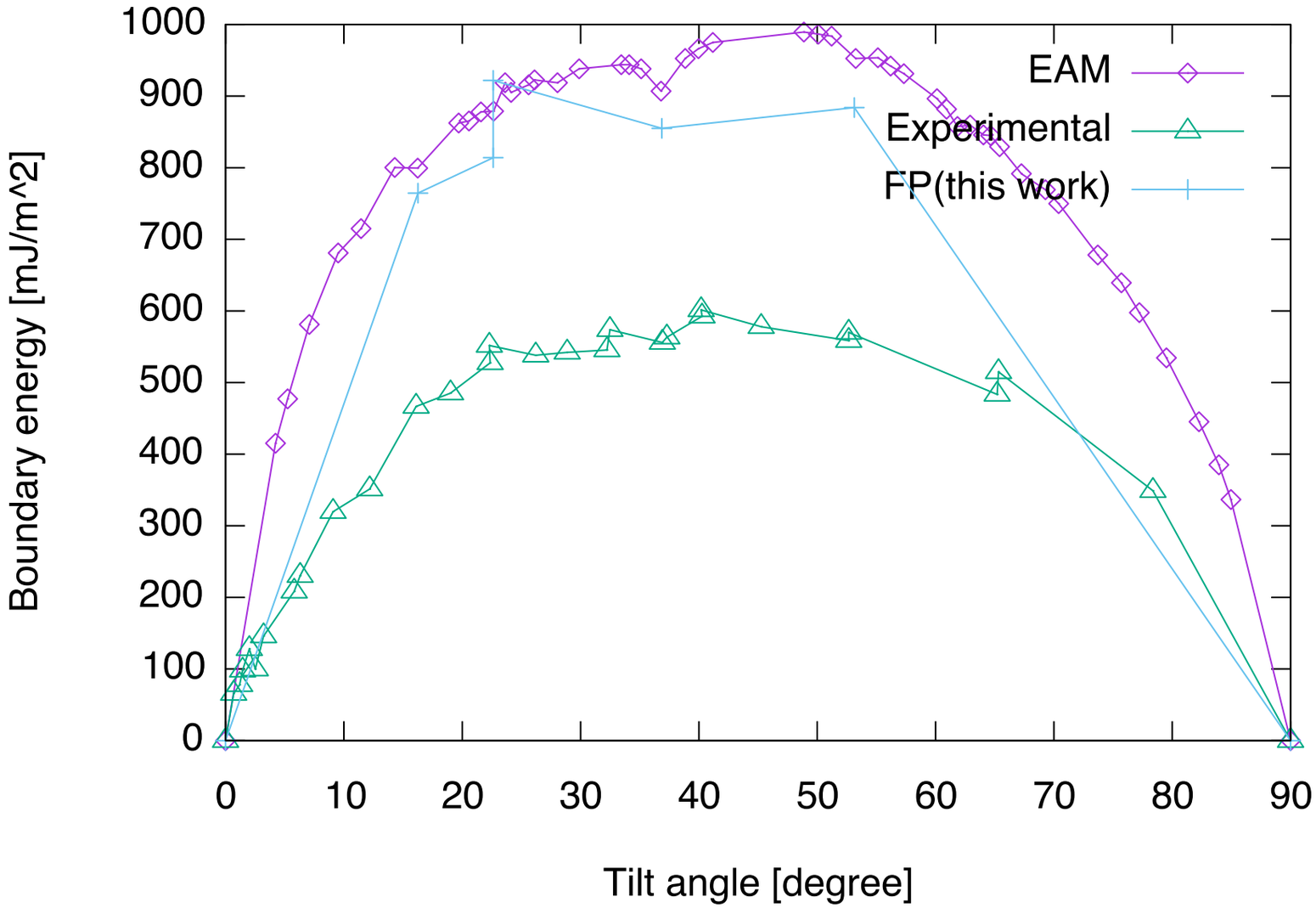
VASP calc. conditions

Pseudo Potentail:PAW-PBE
Relaxations: outer relax by hand
fix calc after relaxations
INCAR
  Energy Cut off:273.214eV
  IBRION = 2   #Relax ions with conjugate-gradient
  ISIF = 2   #Relax ions, calc stress
  EDIFF = 1.0e-05
       #criteria for electronic SC-loop
  EDIFFG = -0.02
       #criteria for ionic relaxation loop
KPOINT
  Use automatic
  length=100 due to d-electron


Experimental near 0 deg
Experimental near 90 deg
E/theta [J/m^2/radian]
log(theta) [radian]


EAM near 0 deg
EAM near 90 deg
E/theta [J/m^2/radian]
log(theta) [radian]


FP(this work) near 0 deg
FP(this work) near 90 deg
log(theta) [radian]


EAM
Experimental
FP(this work)
Boundary energy [mJ/m^2]
Tilt angle [degree]

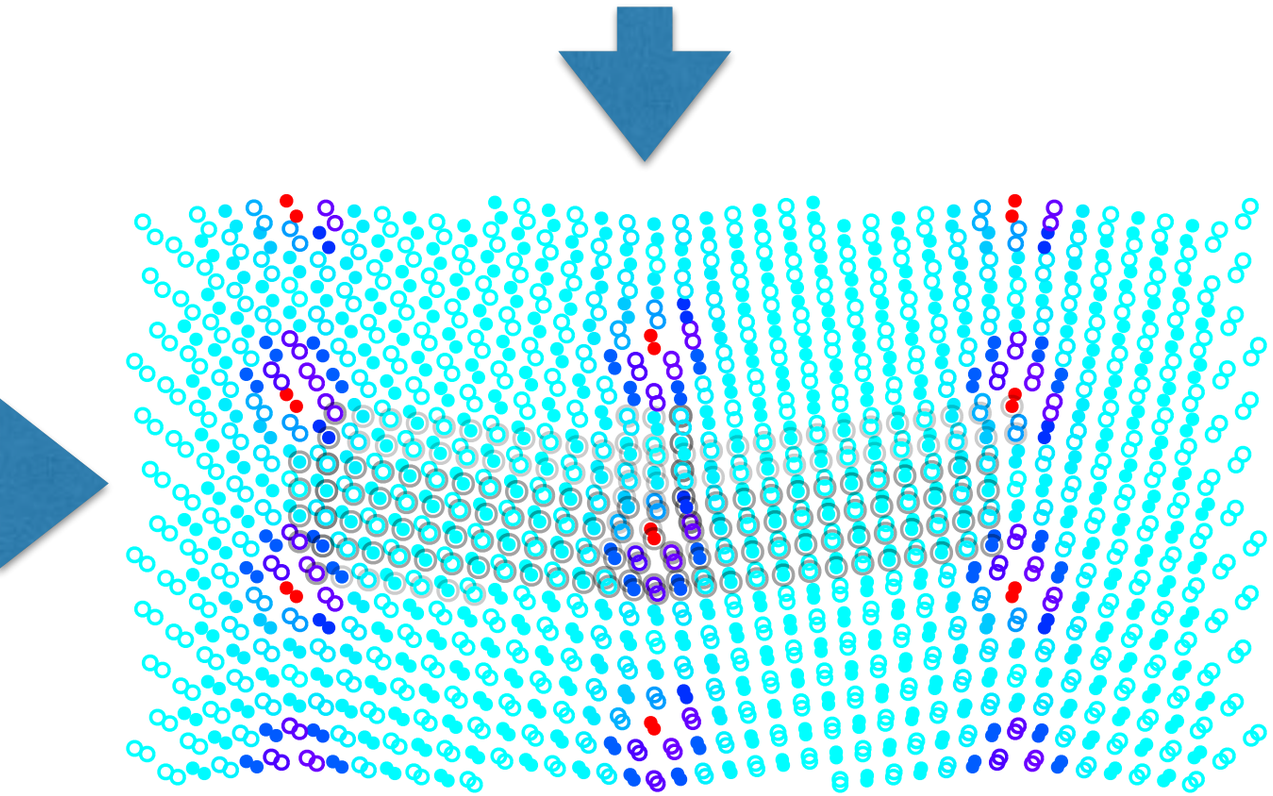
EAM analysis: local energy, strain field

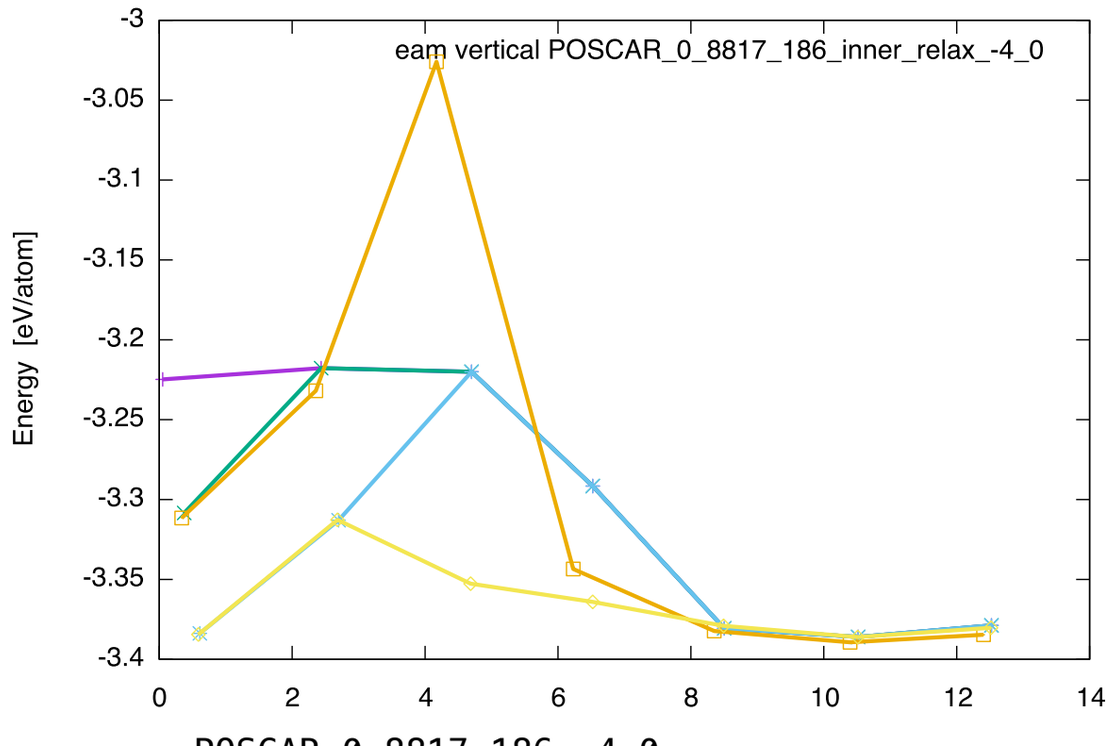
local energy

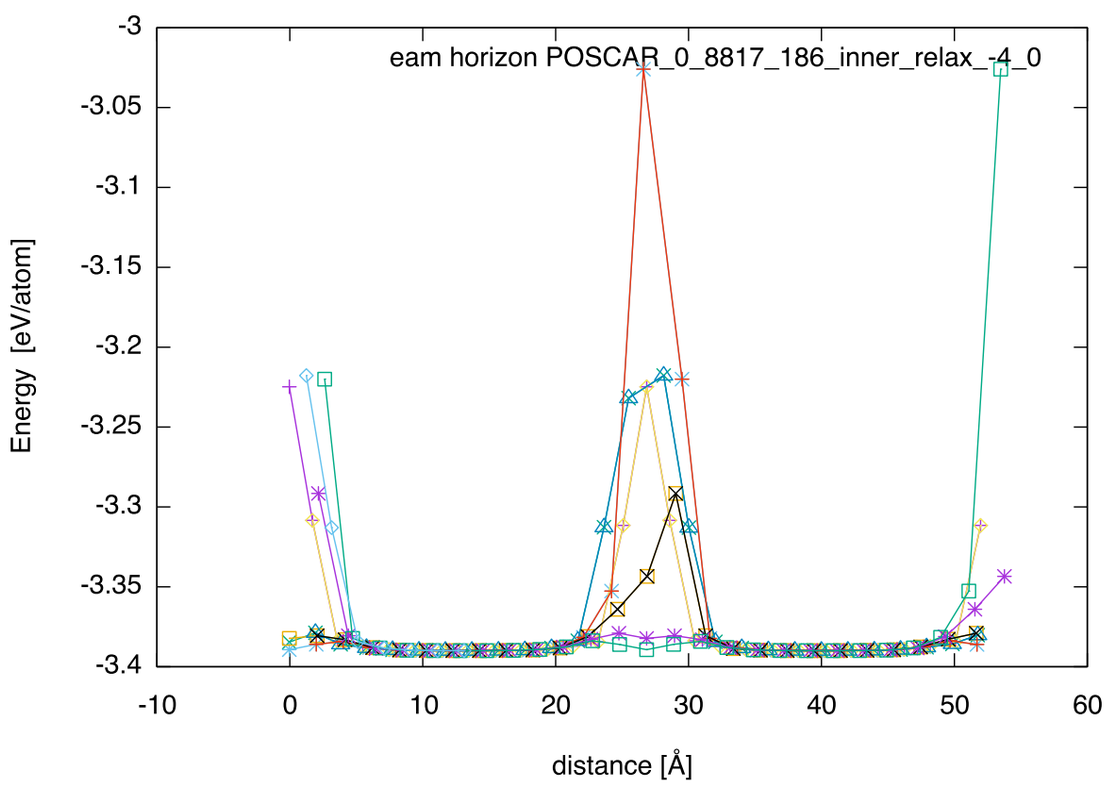
- local energy and force from the first principles
  - Under construction by M. Kohyama(AIST), Y. Shiihara(Tokyo->Toyota-TI)
  - R Kobayashi(Nagoya TI)
- using a fitted EAM potential
  - first nearest neighbor
  - Cohesive energy(3.39eV)
  - equilibrium distance(r0)
  - vacancy formation energy(0.8eV)
  - p=3.0 at r0

$$E_i = A \sum_j \exp(-p\, r_{ij}) - \sqrt{\rho}$$

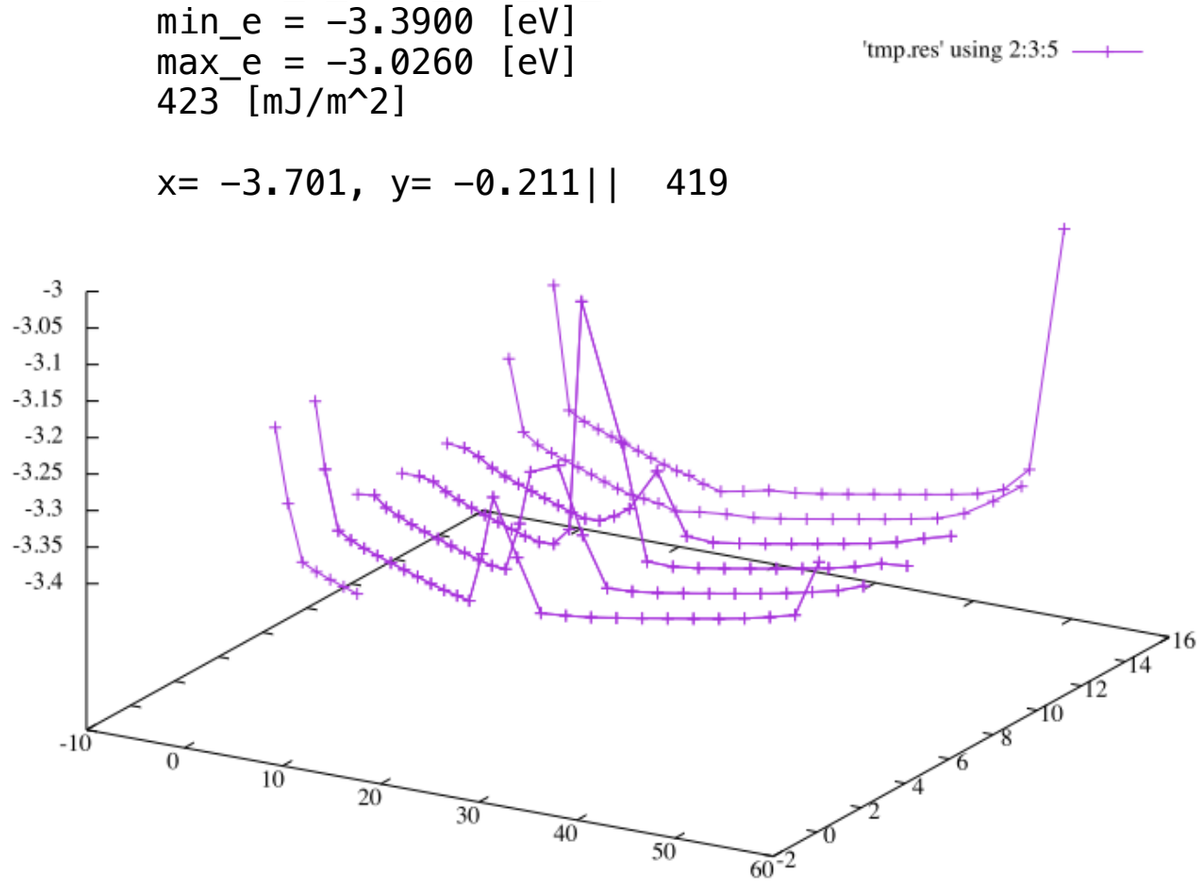
$$\rho = \sum_j \{B \exp(-q\, r_{ij})\}^2$$

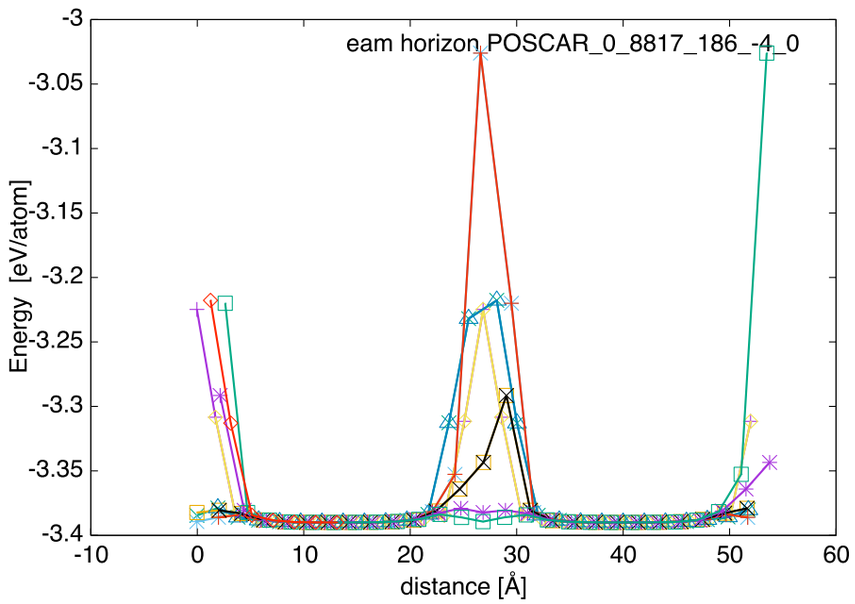


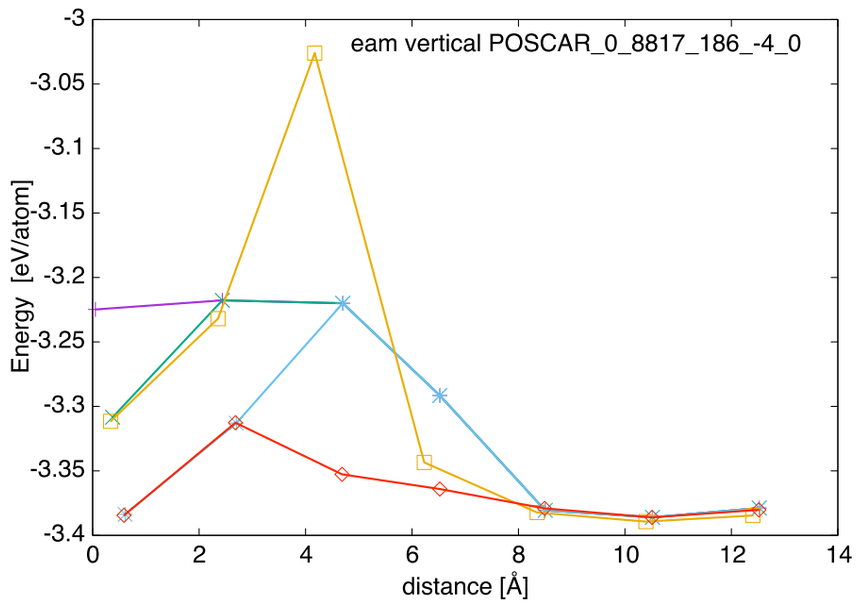




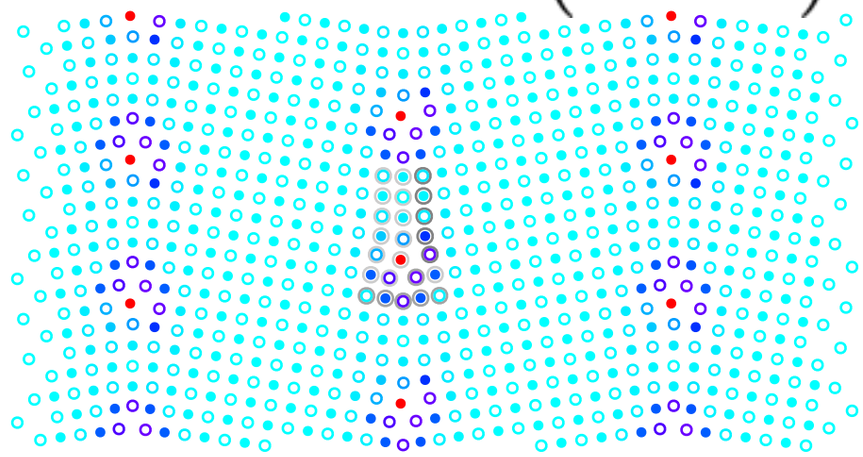

```
min_e = -3.3900 [eV]
max_e = -3.0260 [eV]
423 [mJ/m^2]

x= -3.701, y= -0.211||  419
```

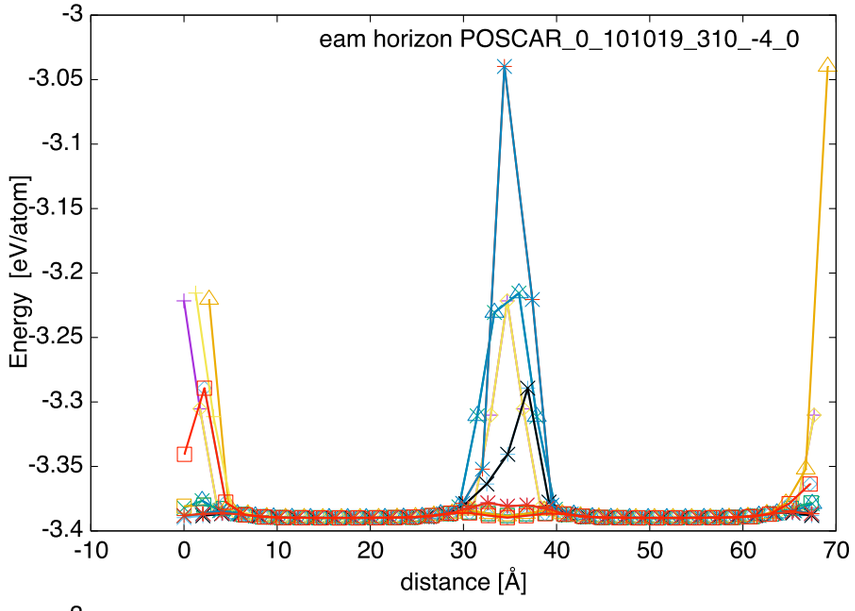


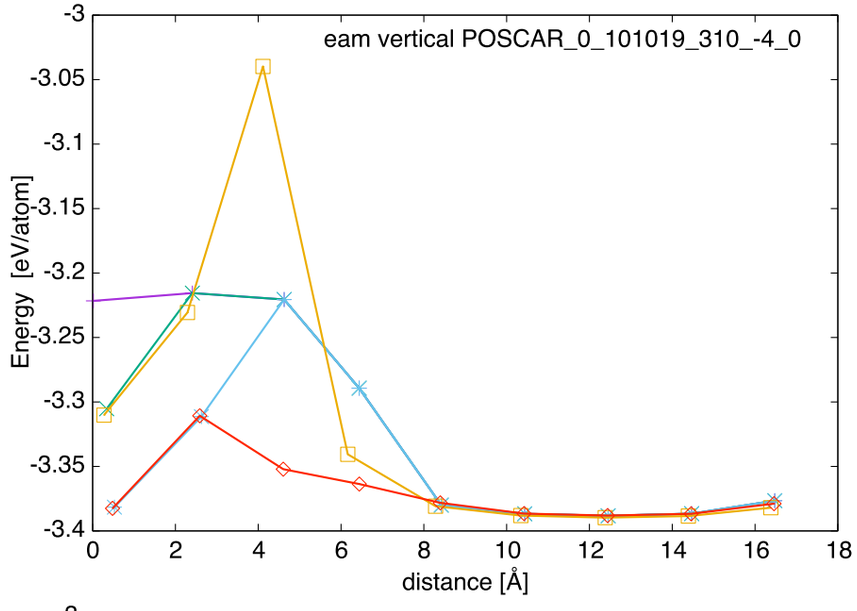




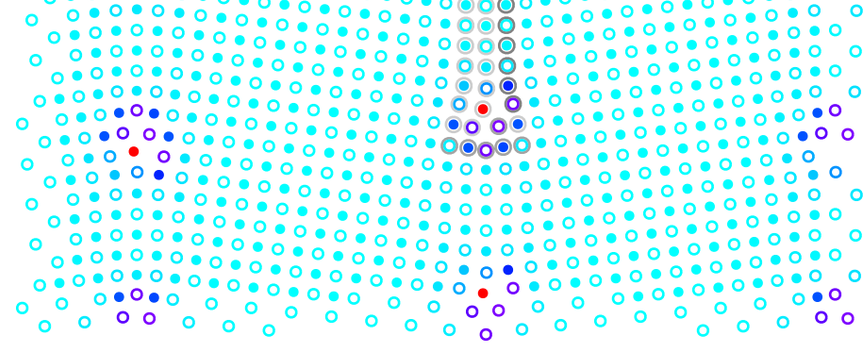
$\theta = 16.26°(n = 7)$

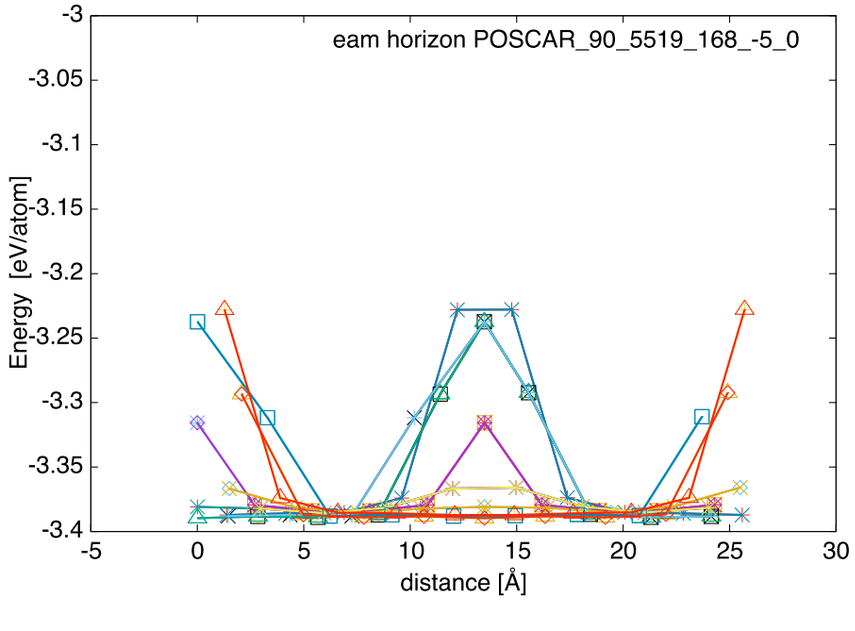


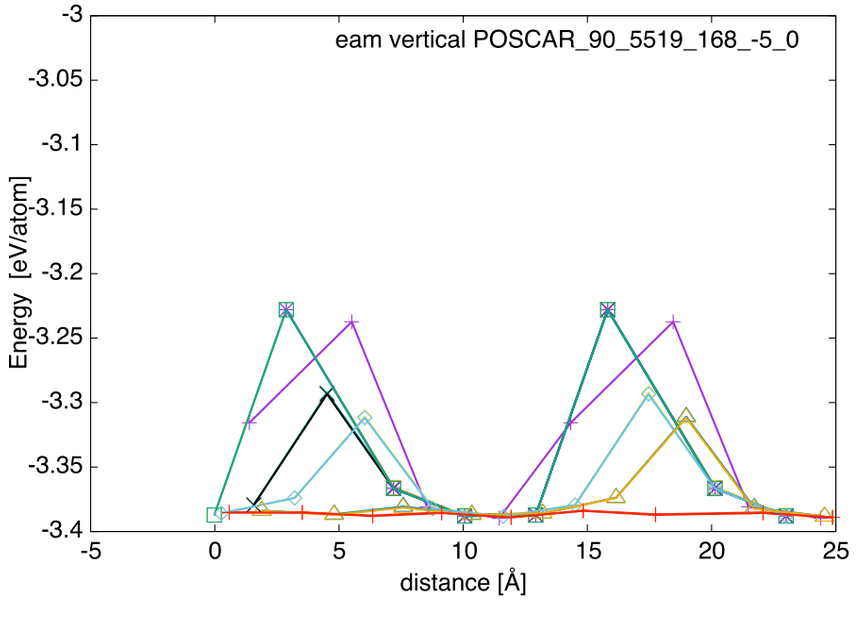




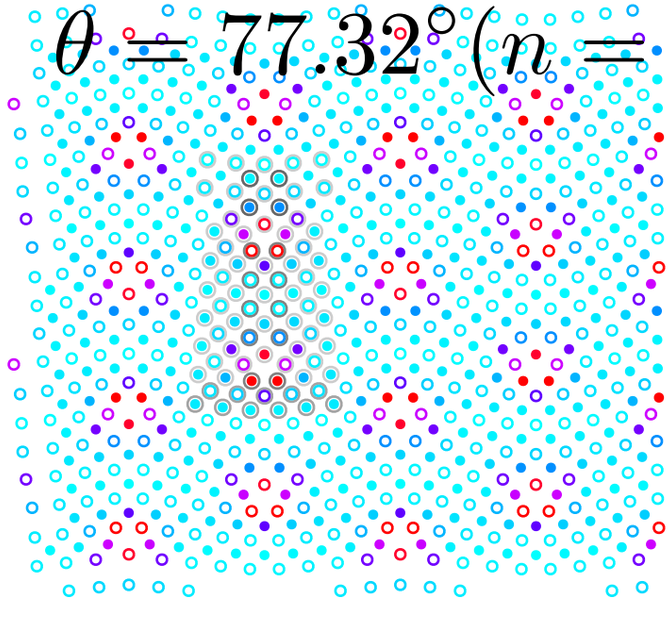
$\theta = 12.68°(n = 9)$

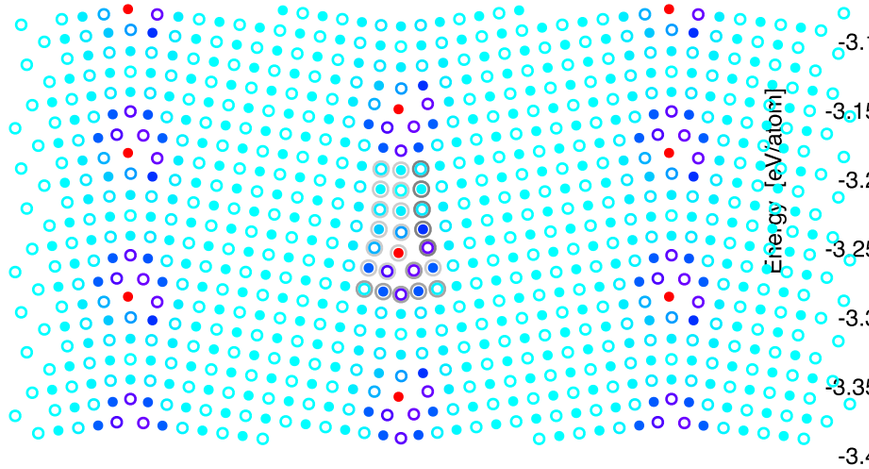


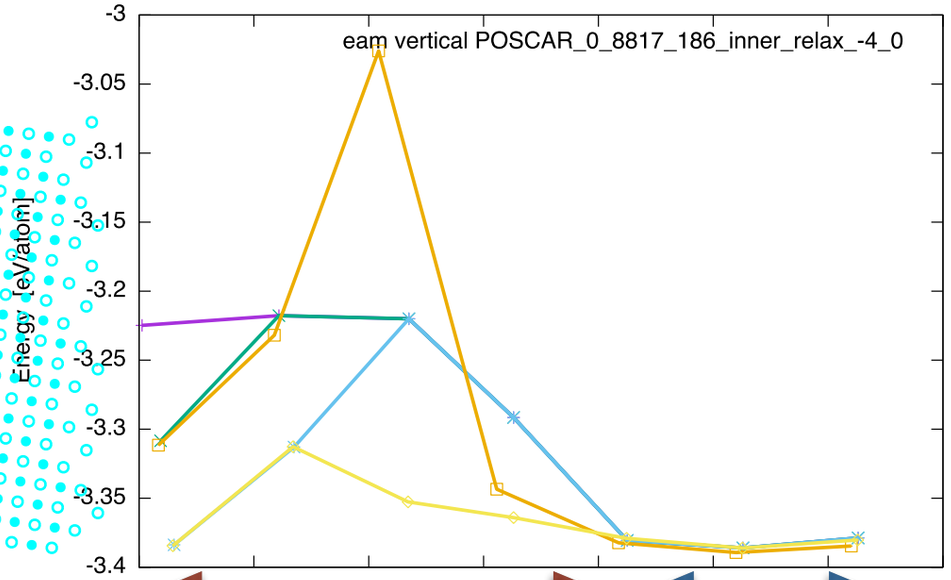


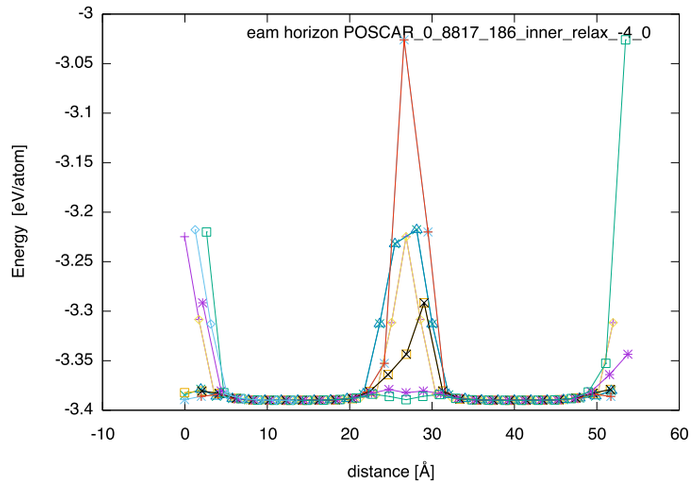


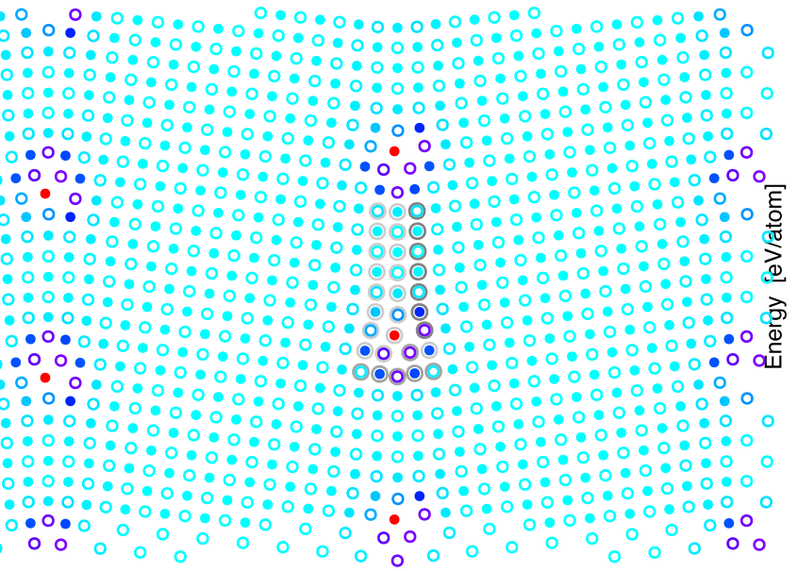
$\theta = 77.32°(n = 9)$

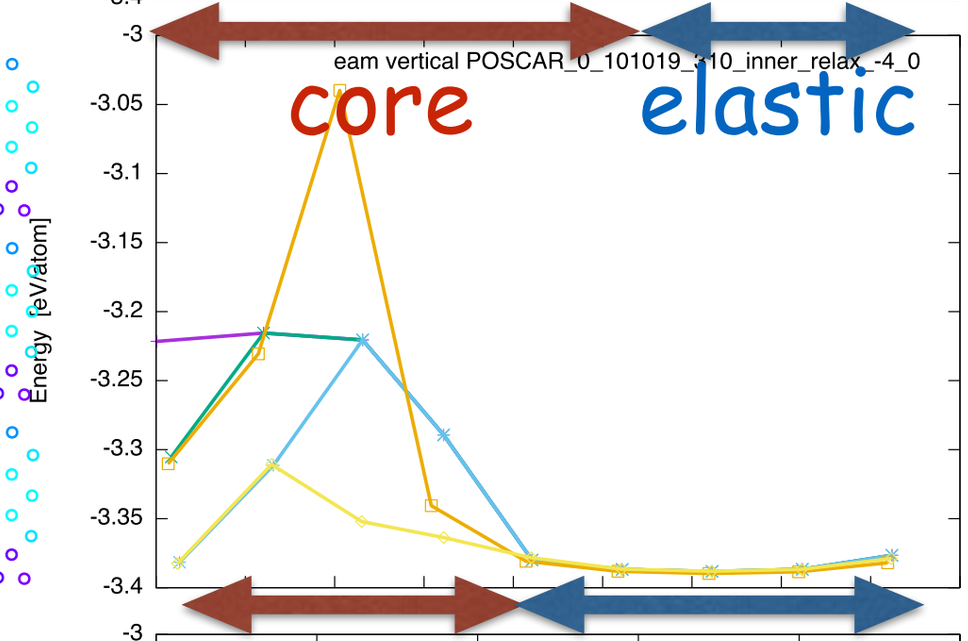


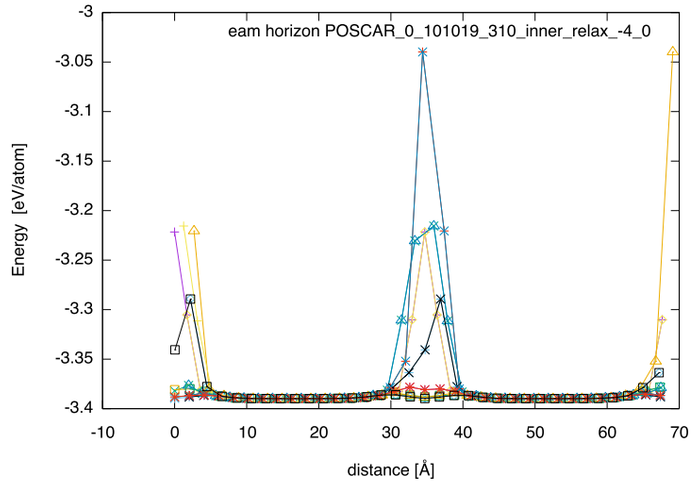


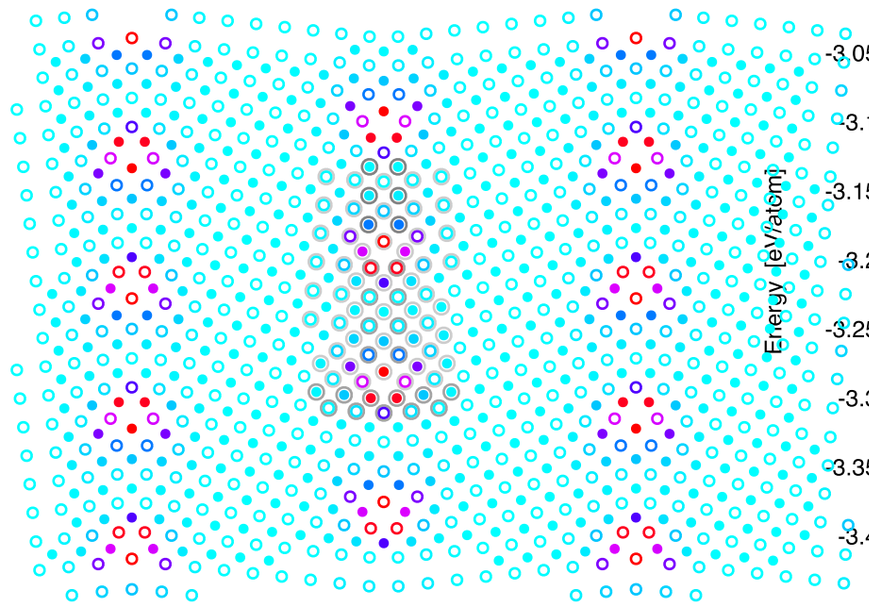

eam vertical POSCAR_0_8817_186_inner_relax_-4_0
Energy [eV/atom]
-3
-3.05
-3.1
-3.15
-3.2
-3.25
-3.3
-3.35
-3.4

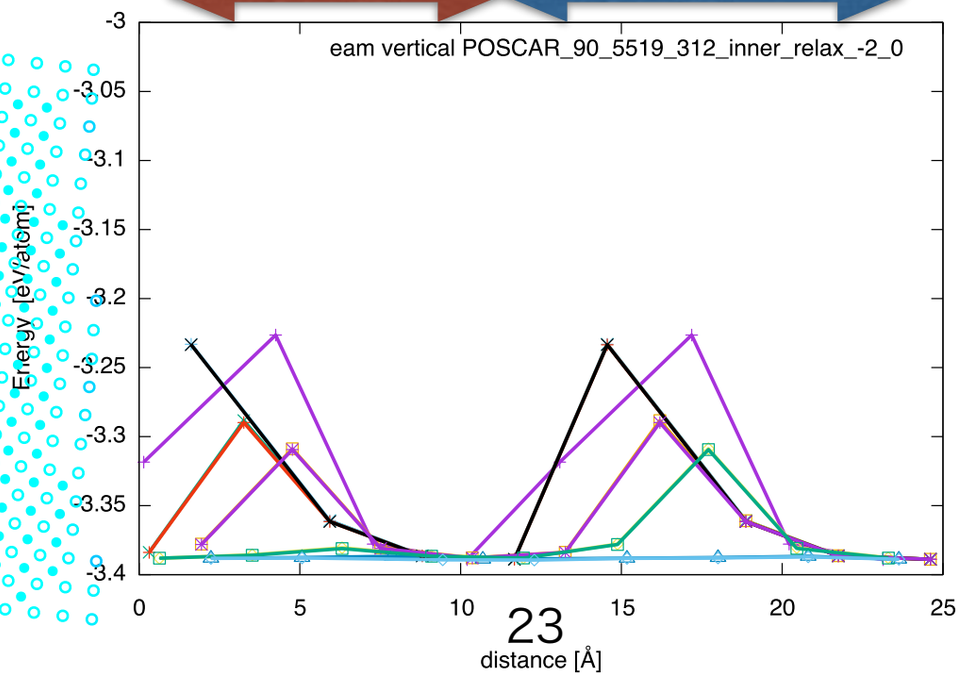

eam horizon POSCAR_0_8817_186_inner_relax_-4_0
Energy [eV/atom]
-3
-3.05
-3.1
-3.15
-3.2
-3.25
-3.3
-3.35
-3.4
-10
0
10
20
30
40
50
60
distance [Å]

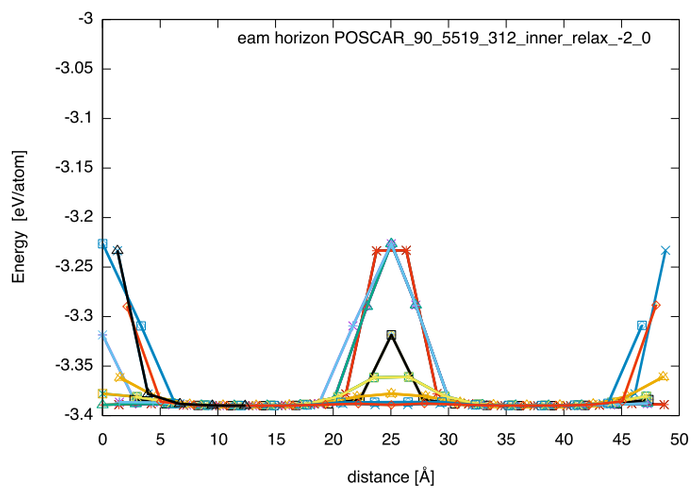


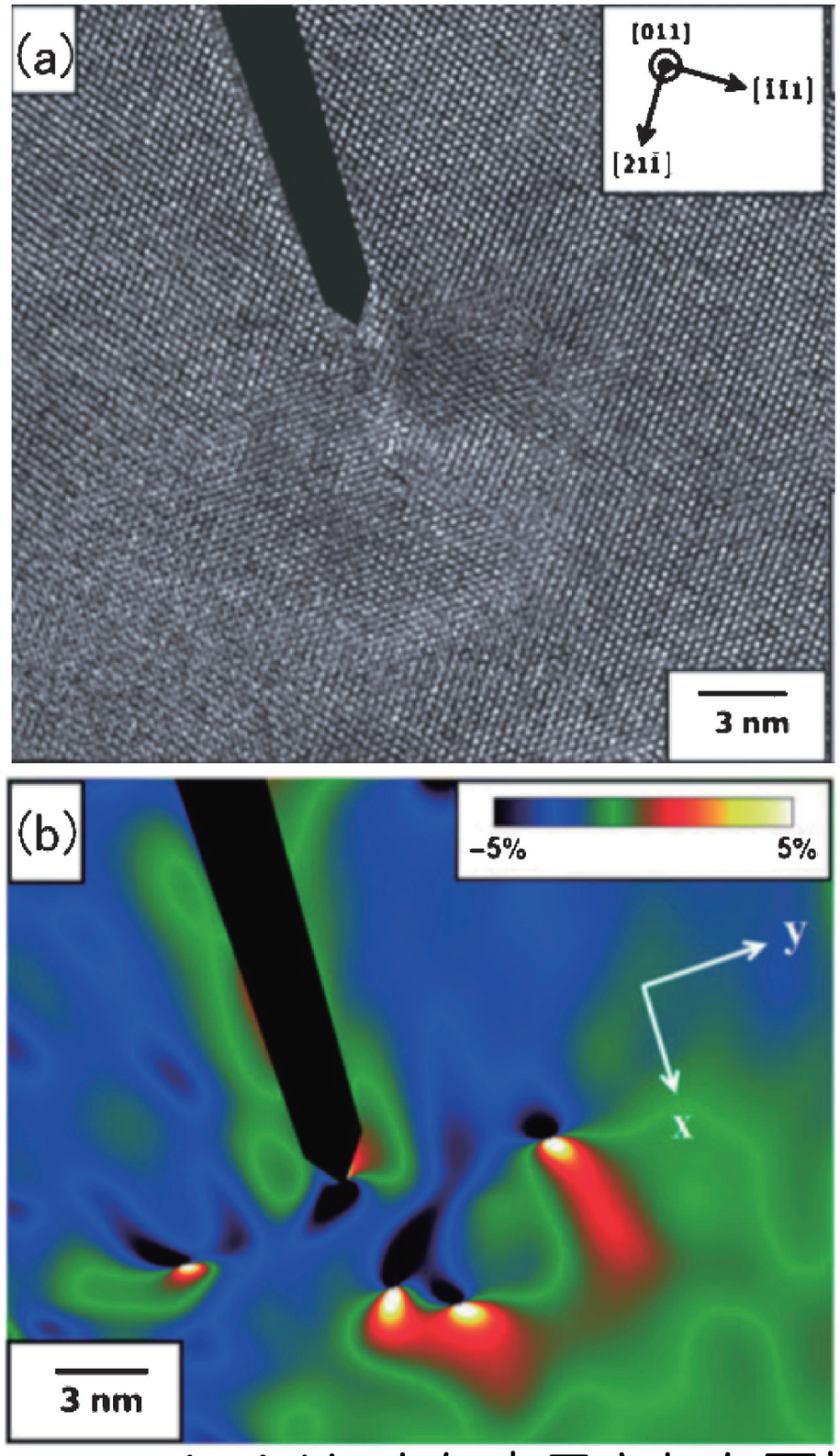

eam vertical POSCAR_0_101019_310_inner_relax_-4_0
core
elastic
Energy [eV/atom]
-3
-3.05
-3.1
-3.15
-3.2
-3.25
-3.3
-3.35
-3.4


eam horizon POSCAR_0_101019_310_inner_relax_-4_0
Energy [eV/atom]
-3
-3.05
-3.1
-3.15
-3.2
-3.25
-3.3
-3.35
-3.4
-10
0
10
20
30
40
50
60
70
distance [Å]



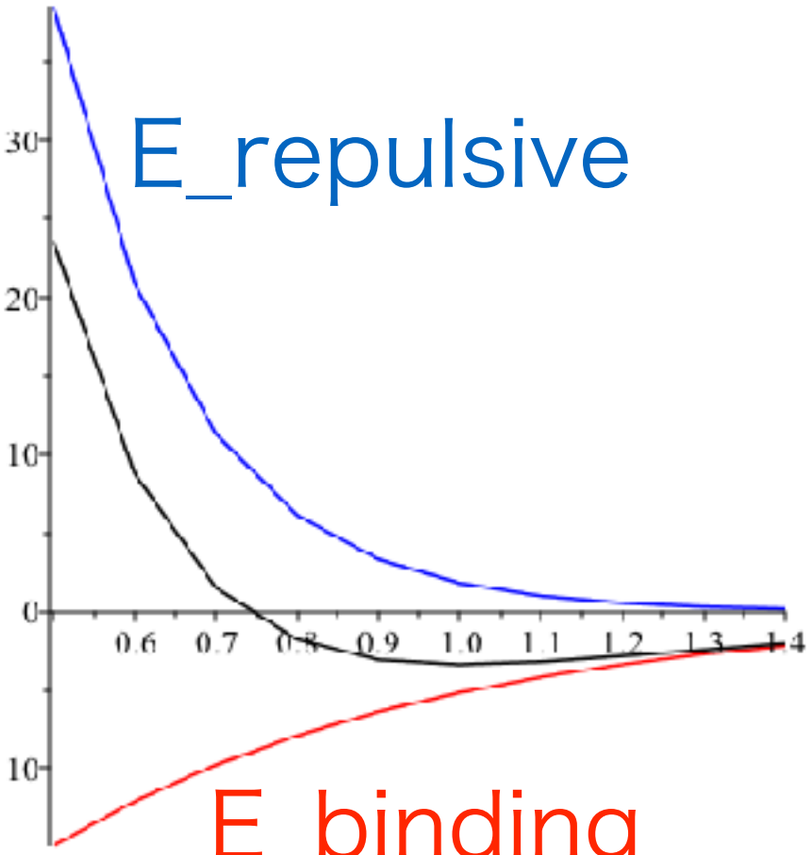

eam vertical POSCAR_90_5519_312_inner_relax_-2_0
Energy [eV/atom]
-3
-3.05
-3.1
-3.15
-3.2
-3.25
-3.3
-3.35
-3.4
0
5
10
15
20
25
distance [Å]

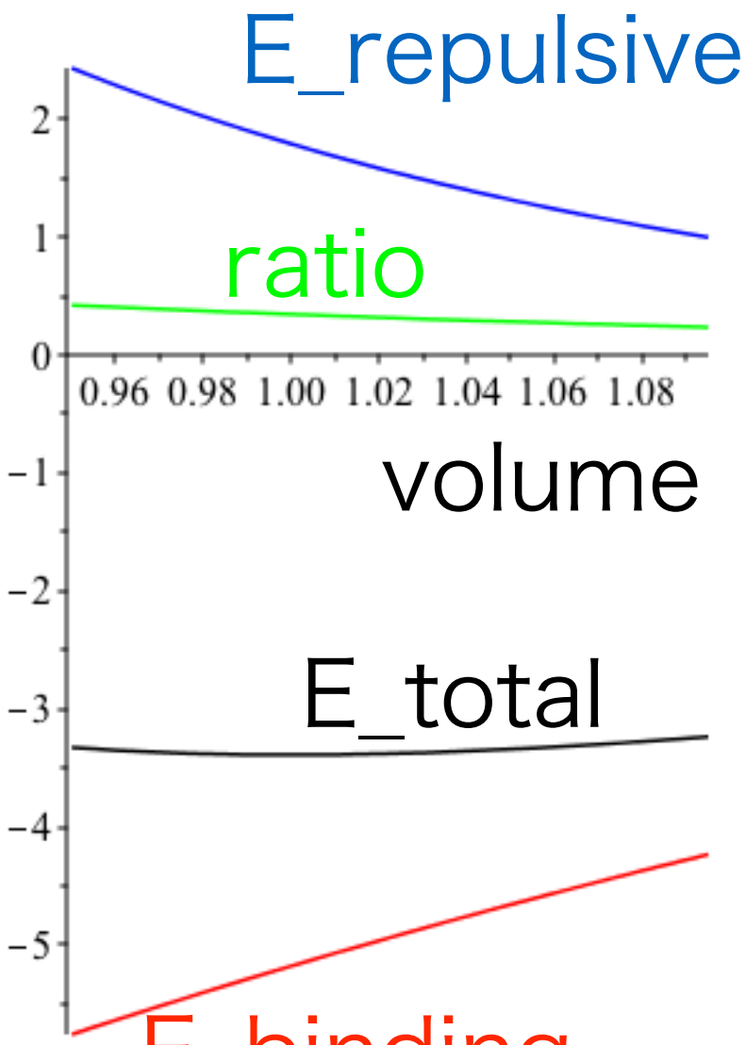

eam horizon POSCAR_90_5519_312_inner_relax_-2_0
Energy [eV/atom]
-3
-3.05
-3.1
-3.15
-3.2
-3.25
-3.3
-3.35
-3.4
0
5
10
15
20
25
30
35
40
45
50
distance [Å]

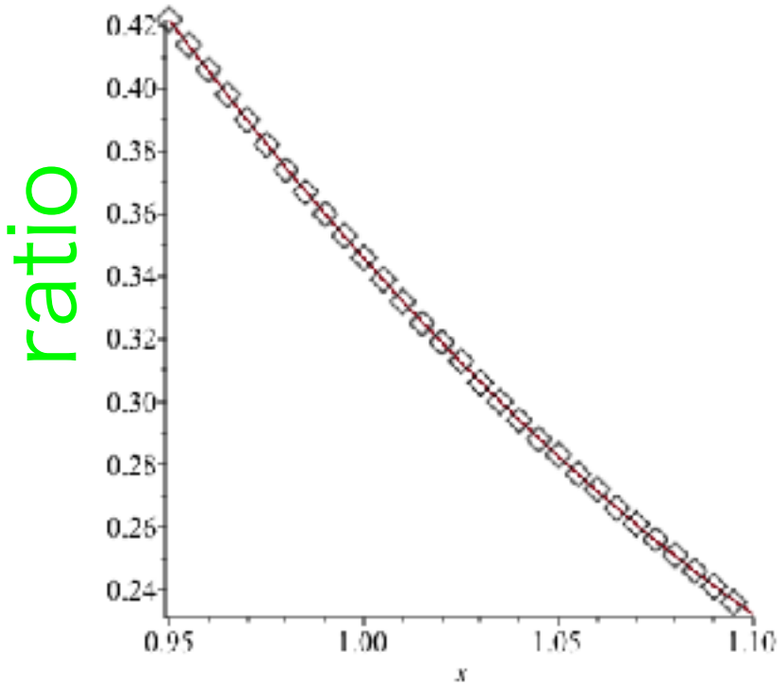


GPA(geometrical phase analysis)により表示された可視化クラック先端の歪場.

「亀裂先端転位と脆性 延性遷移挙動」,田中將己 定松直 東田賢二，まてりあ，56 巻 (2017) 10 号 p. 597-603.


E_repulsive
E_binding
30
20
10
0
10
0.6
0.7
0.8
0.9
1.0
1.1
1.2
1.3
1.4


E_repulsive
ratio
E_total
E_binding
volume
2
1
0
−1
−2
−3
−4
−5
0.96
0.98
1.00
1.02
1.04
1.06
1.08


ratio
volume
0.42
0.40
0.38
0.36
0.34
0.32
0.30
0.28
0.26
0.24
0.95
1.00
1.05
1.10
x

$$E_i = E_{\text{repulsive}} + E_{\text{binding}}$$

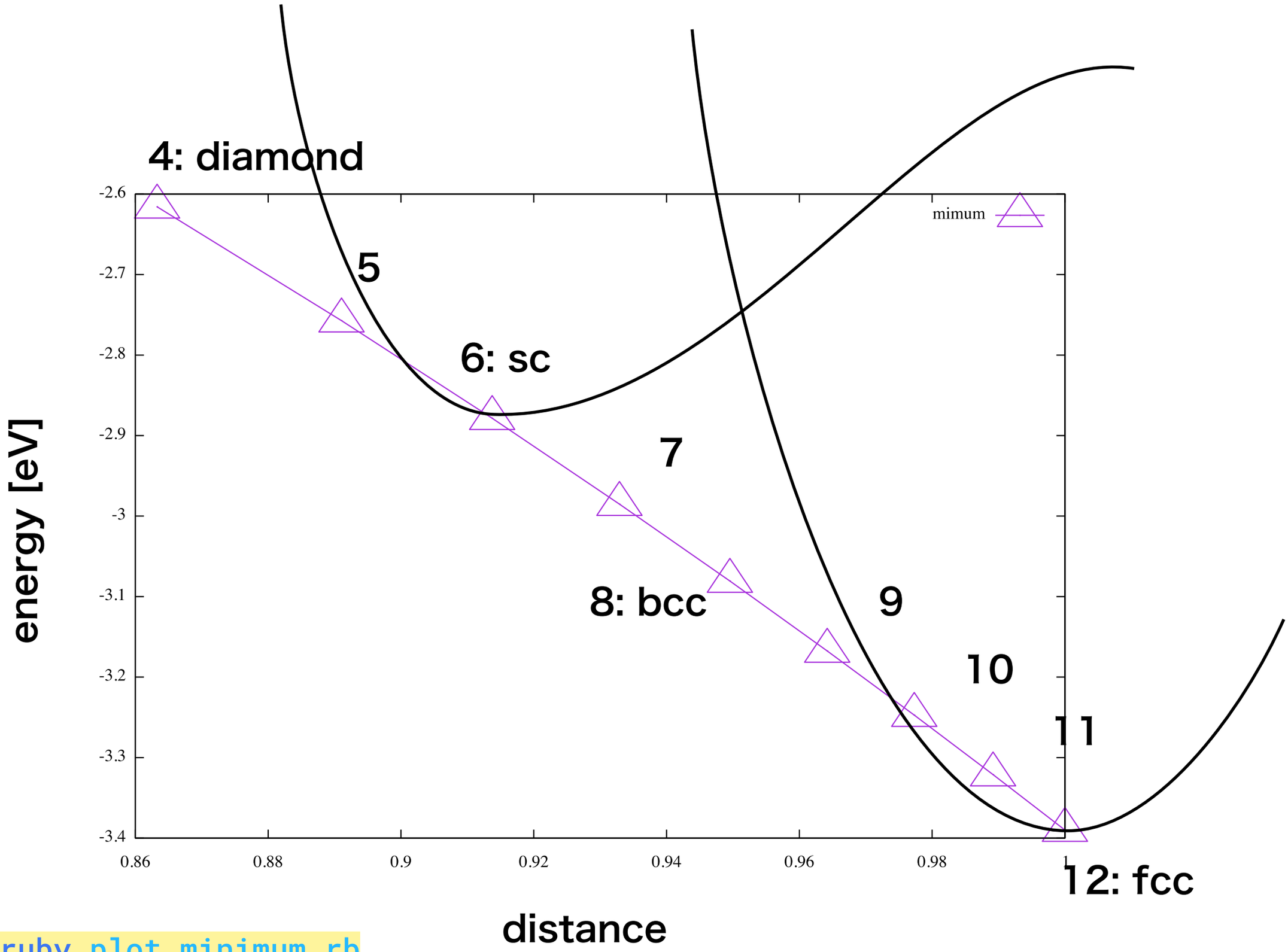
$$= \sum_j \phi(r_{ij}) - \sqrt{\sum_j h(r_{ij})^2}$$

$$\phi(r_{ij}) = A0 \exp(-p r_{ij})$$

$$h(r_{ij}) = B0 \exp(-q r_{ij})$$

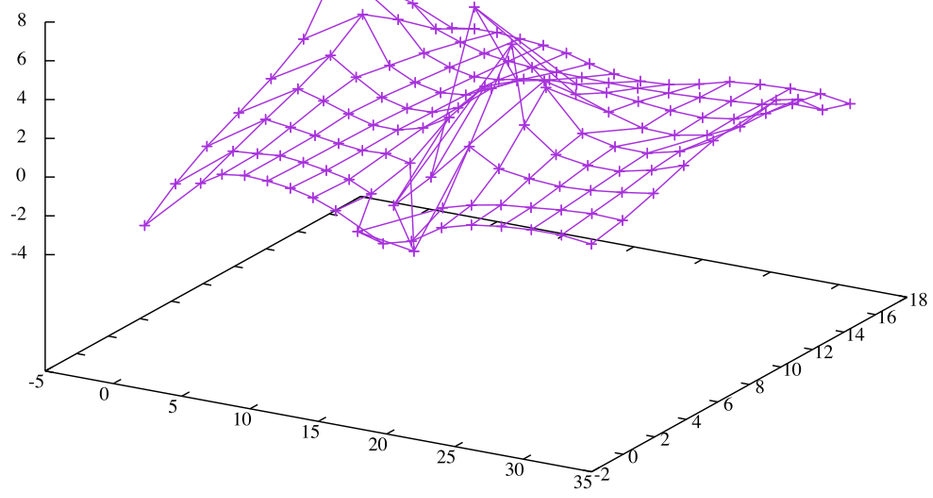
$$E_{\text{total}} = n A_0 \exp(-p r_0) - \sqrt{n B_0^2 \exp(-2 q r_0)}$$

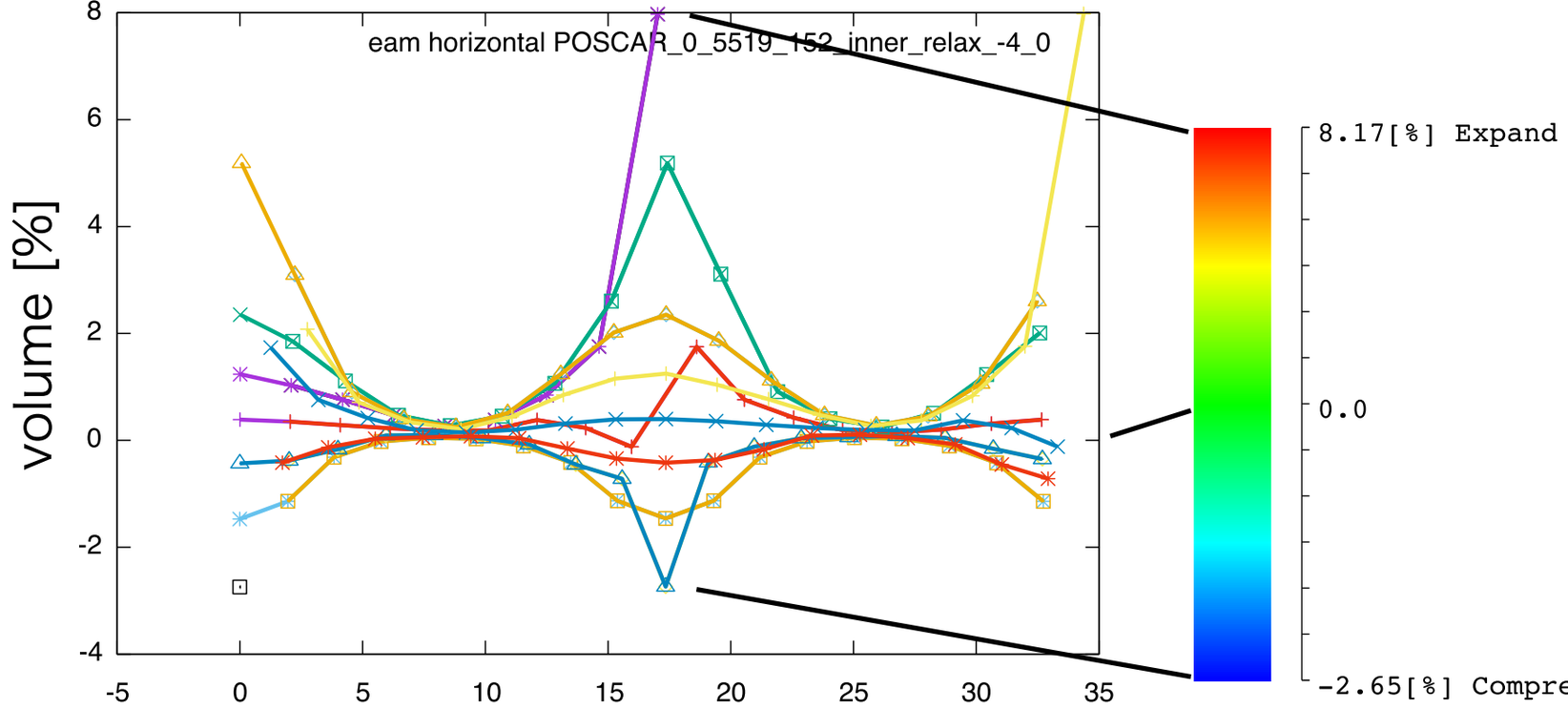
Minimum energy and distance for Al EAM

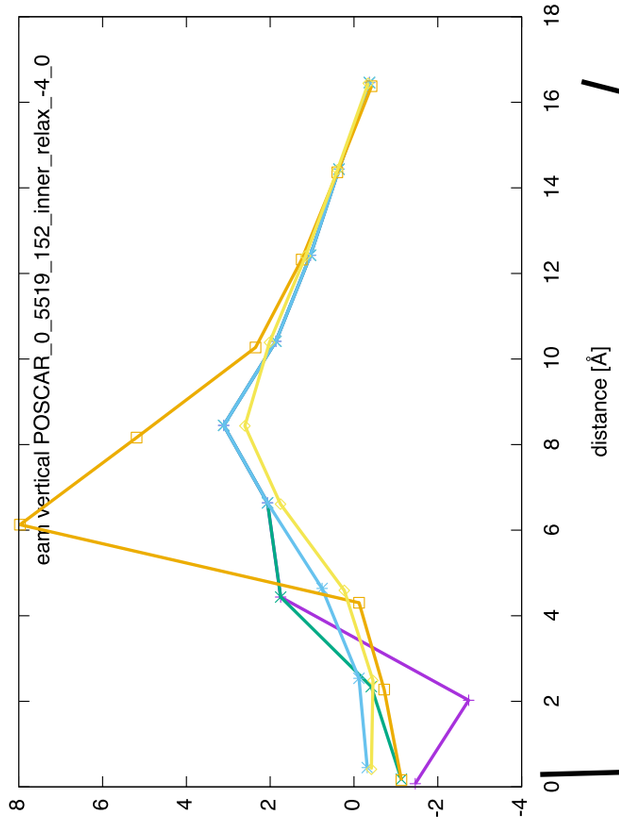



```
> ruby plot_minimum.rb
```

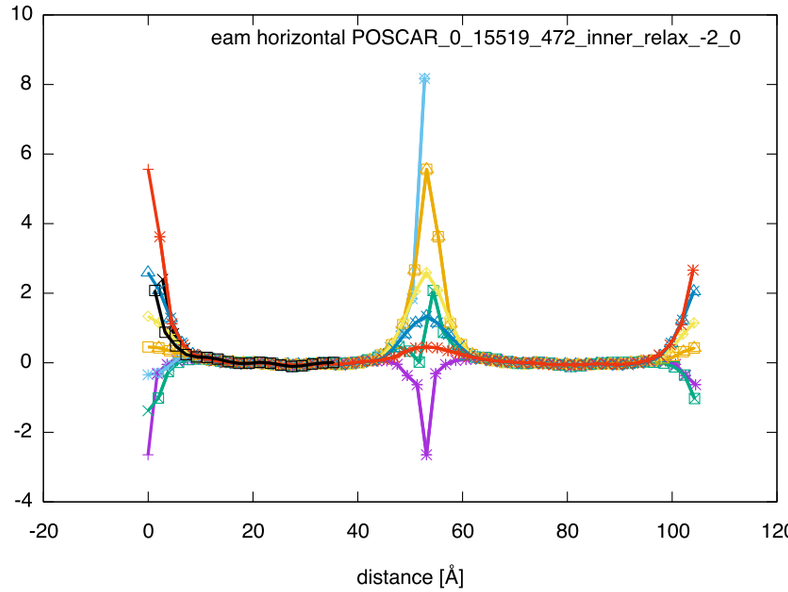
'data3d_sorted.dat' using 1:2:3

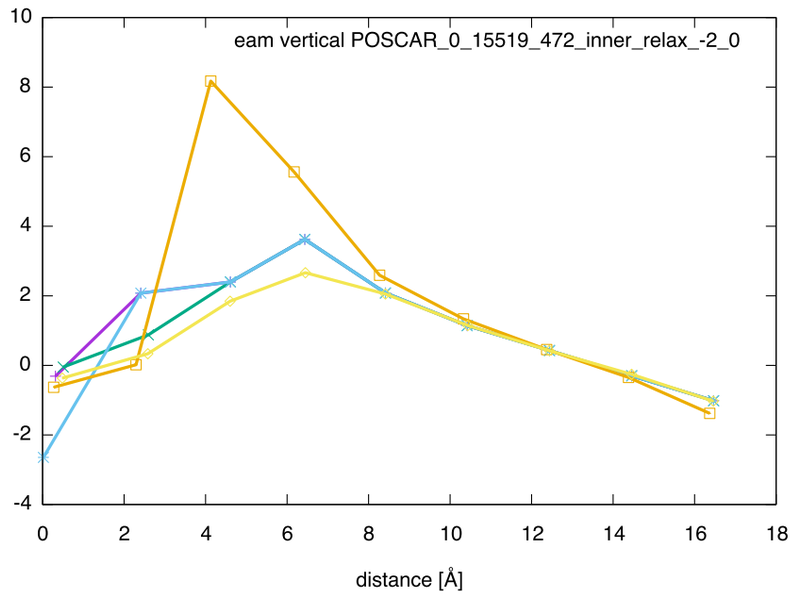


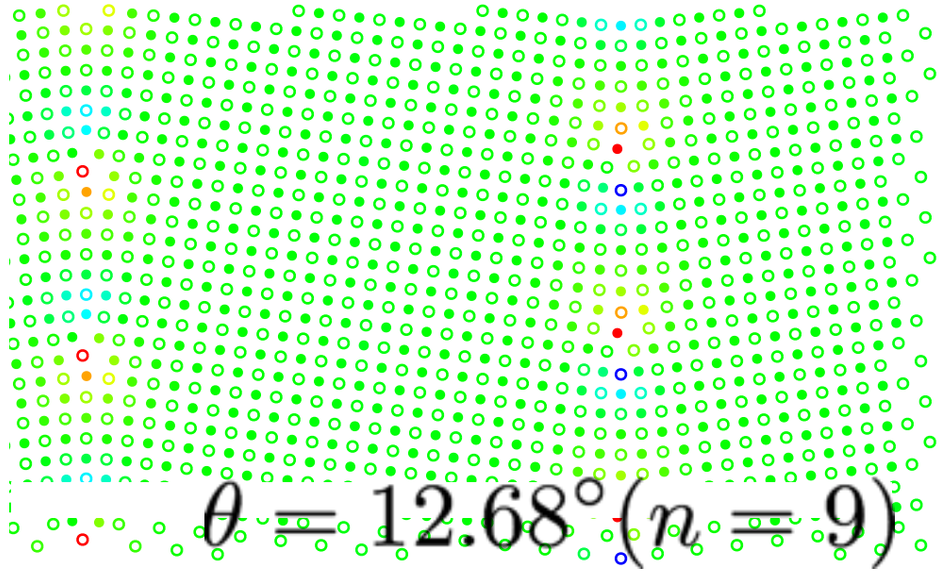


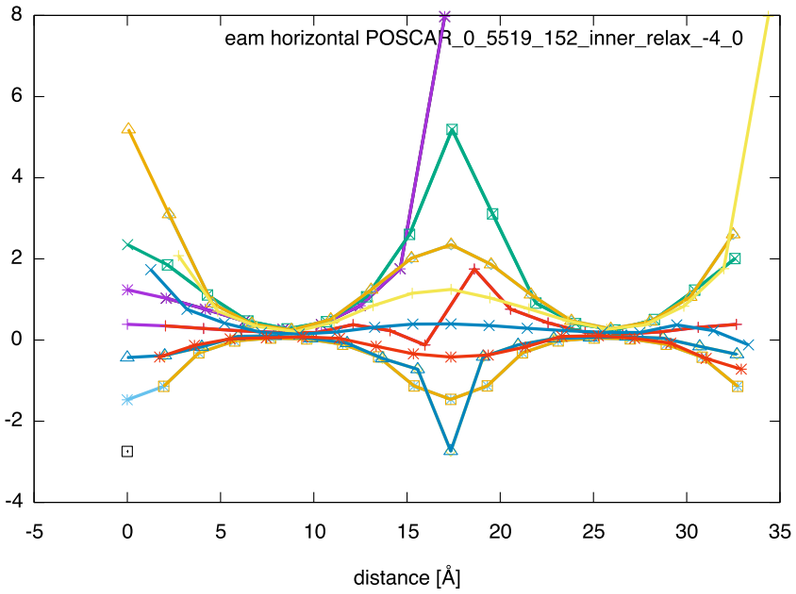


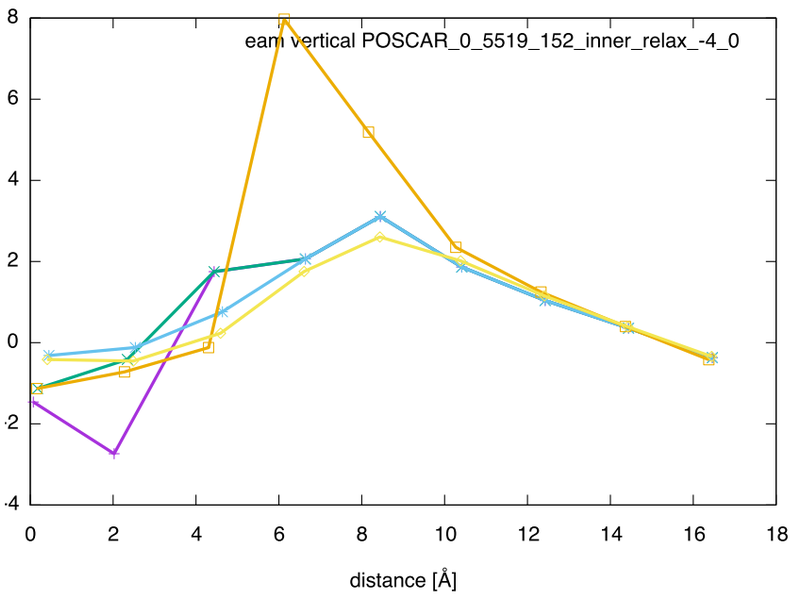
$\theta = 12.68^\circ\,(n = 9)$

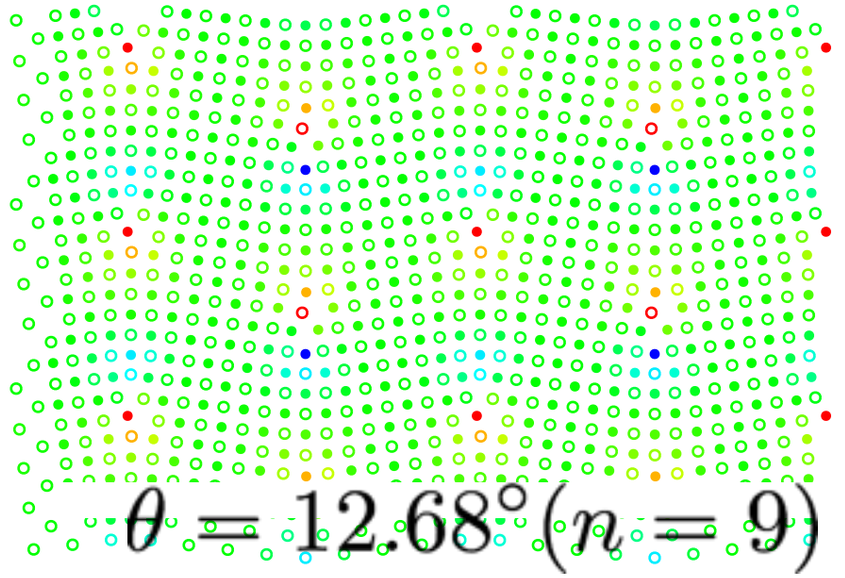

eam horizontal POSCAR_0_15519_472_inner_relax_-2_0
distance [Å]

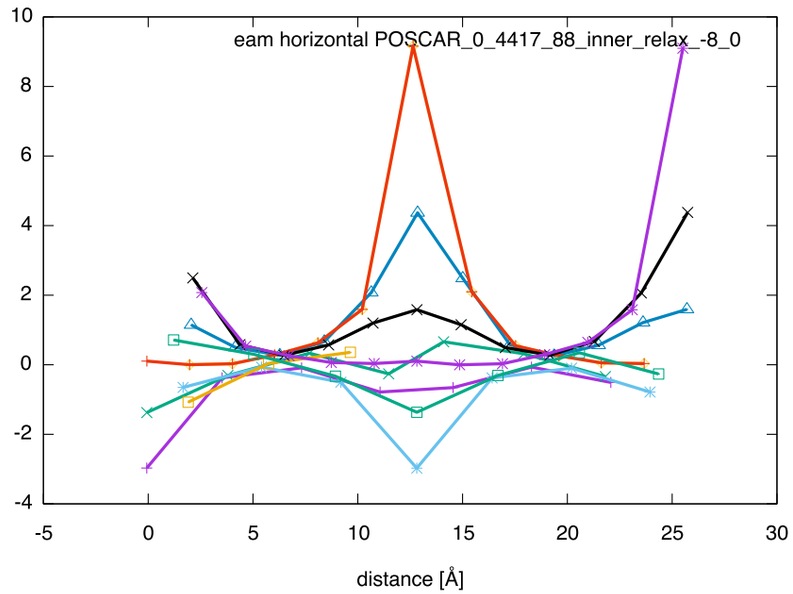

eam vertical POSCAR_0_15519_472_inner_relax_-2_0
distance [Å]

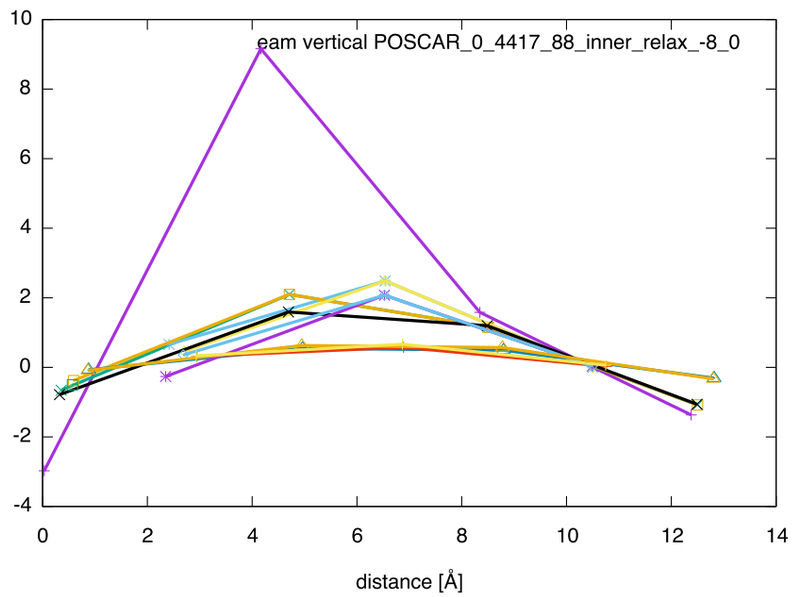

$\theta = 12.68°(n = 9)$

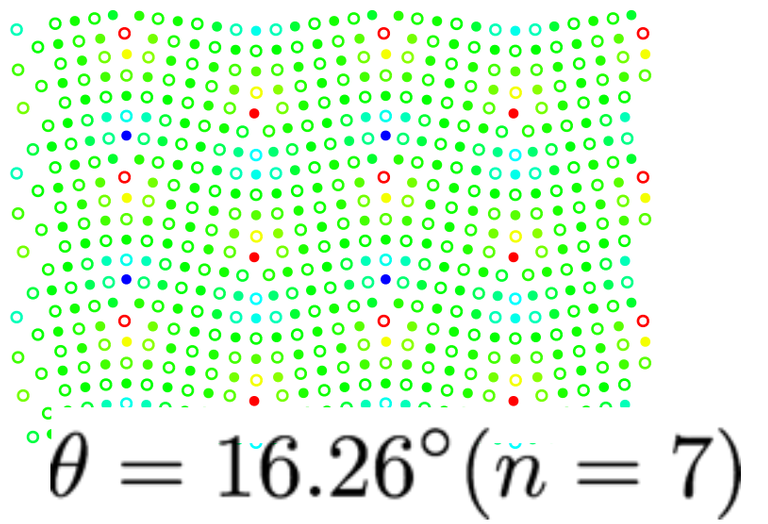

eam horizontal POSCAR_0_5519_152_inner_relax_-4_0
distance [Å]

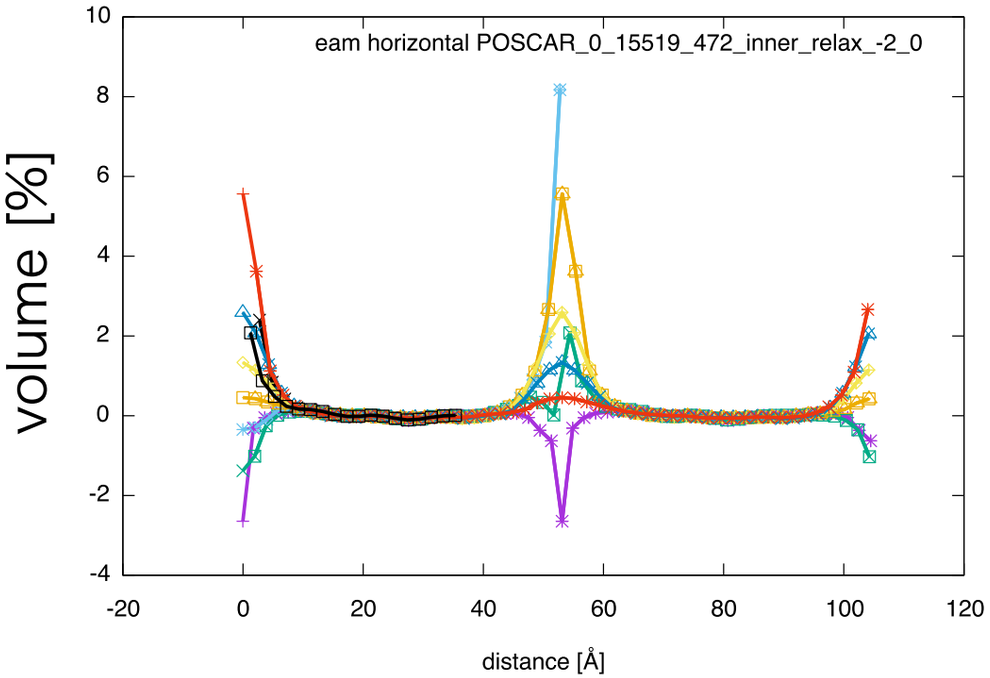

eam vertical POSCAR_0_5519_152_inner_relax_-4_0
distance [Å]

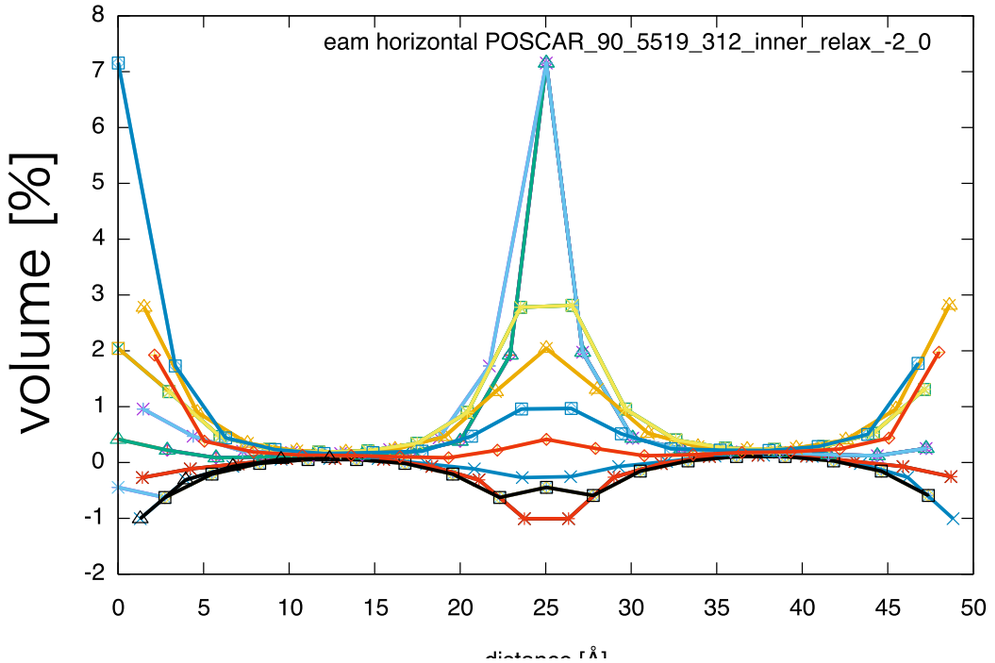

$\theta = 12.68°(n = 9)$

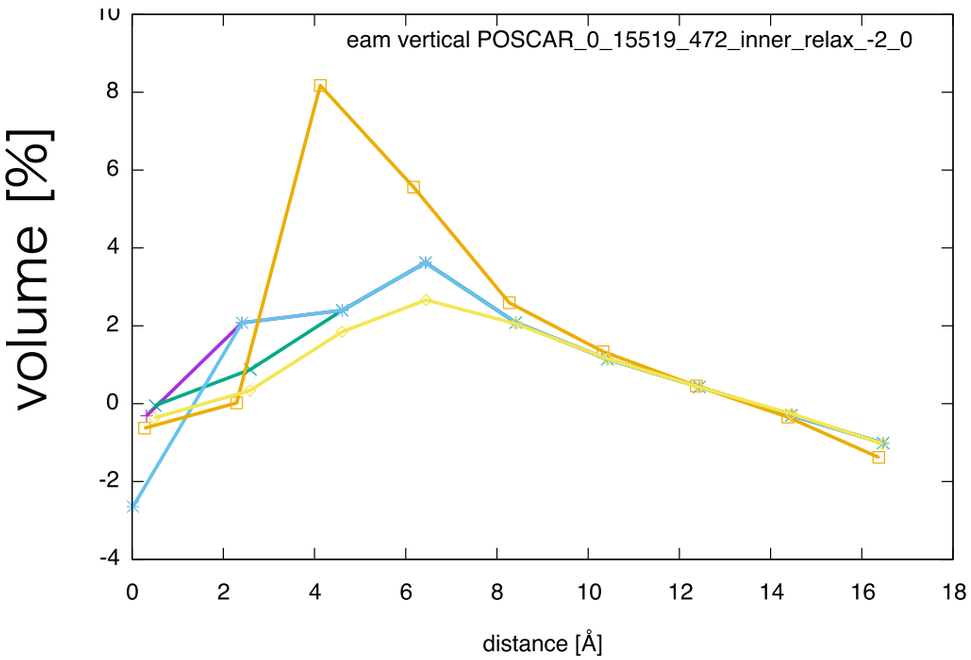

eam horizontal POSCAR_0_4417_88_inner_relax_-8_0
distance [Å]

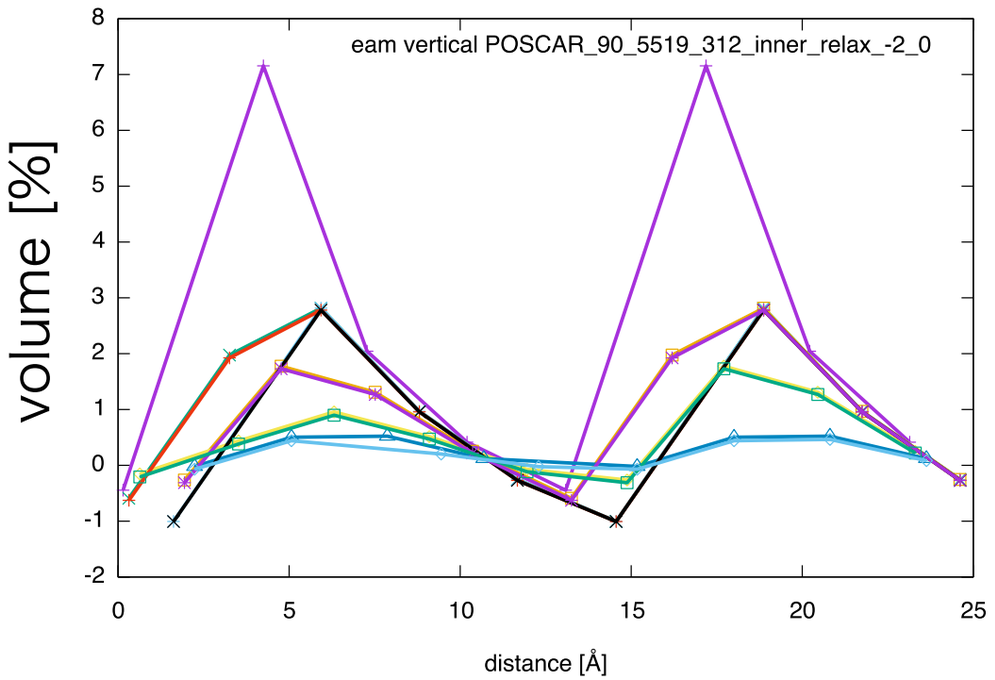

eam vertical POSCAR_0_4417_88_inner_relax_-8_0
distance [Å]

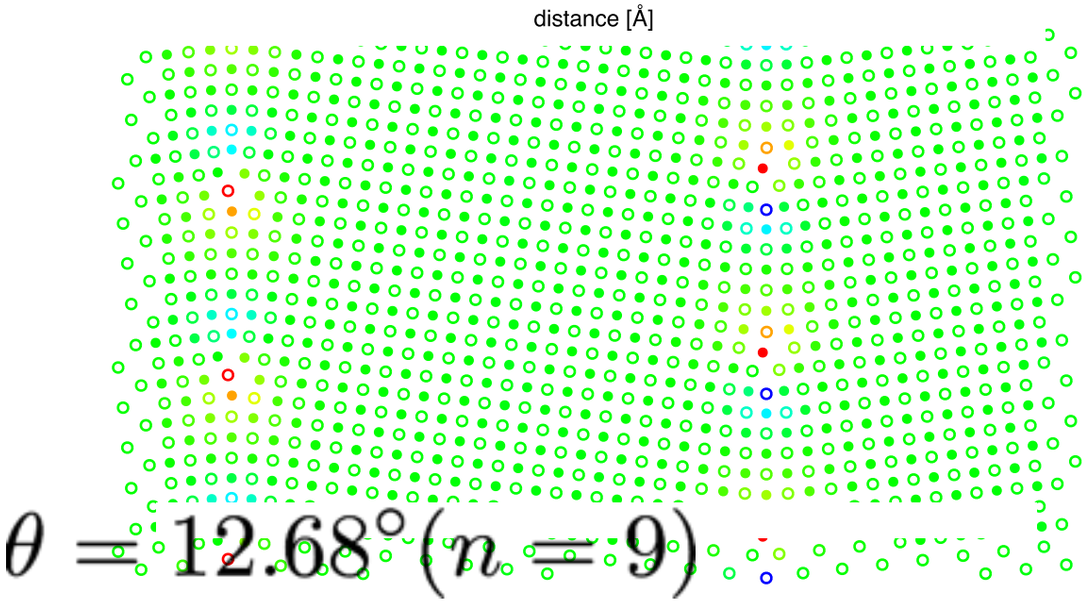

$\theta = 16.26°(n = 7)$

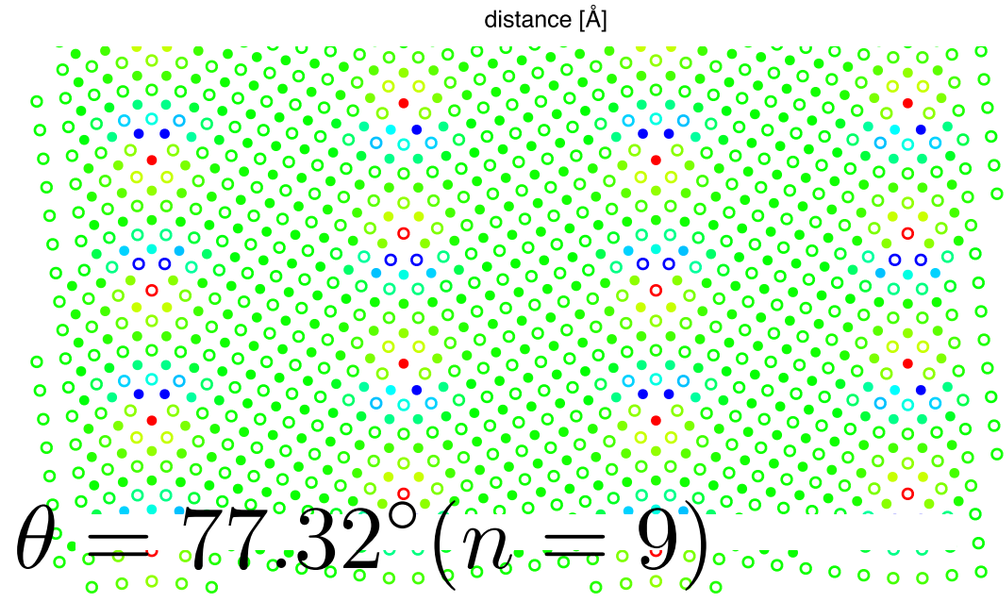

eam horizontal POSCAR_0_15519_472_inner_relax_-2_0
volume [%]
distance [Å]


eam horizontal POSCAR_90_5519_312_inner_relax_-2_0
volume [%]


eam vertical POSCAR_0_15519_472_inner_relax_-2_0
volume [%]
distance [Å]


eam vertical POSCAR_90_5519_312_inner_relax_-2_0
volume [%]
distance [Å]


θ = 12.68°(n = 9)


θ = 77.32°(n = 9)

Temporary conclusions

- Small angle Al and Cu(100) tilt boundary shows difference on the slopes at 0 and 90 degrees.
- Inconsistent with experiments results.
- Need smaller angle, larger super cell, model.