# meam.f ; MEAM92 program ( FORTRAN77 )

by Kunio TAKAHASHI

- Program for my personal usage

  This may not be fast.
  You may have to modify it,
  for your own purpose...

- Parameter file (meamPF)

  Many comments included...
  so you can modify it

- Data file format (3 types)
  - normal format

**ex.)**

```
C four Si atoms
 0
+0.00E+000  +0.00E+000  +0.00E+000  Si
+2.35E-010  +0.00E+000  +0.00E+000  Si
+0.50E-010  +2.04E-010  +0.00E+000  Si
+0.50E-010  +6.78E-011  +1.92E-010  Si
```

  - Format for reconstruction
  - SPD format

```
D:¥ORNlecture¥>meam

 ###################################
 Modified Embedded Atom Method
              by Kunio TAKAHASHI
 M.I.Baskes,Phys.Rev.B,46,2727(1992)
 ###################################
 STATUS OF CALCULTION
Type of screening function : default =  1 (MEAM92)      :  1
Type of rho expansion      : default =  0 (MEAM92)      :  0
Parameter File Name        : default = "meamPF" (MEAM92) :meamPF
 MENU
 1 : Total energy calculation
 2 : Energetics in uniform dilation&compression
 3 : Make scalable position data file for enegetics
 4 : Rose energy calculation vs distance
 5 : Argument of F(rho) in equilibrium states
 6 : Distribution of rho as a fuction of distance
 7 : Check of calculation process 2 (above)
 8 : Energy v.s. x,y,z deviation of a atom
 9 : Energy v.s. 1,2,3 deviation of a atom
10 : Reconstruction calculation
11 : Param.convert from "meamf" to "meamPF.*"(plan)
12 :   ...not defined yet ...
 A : Change screening function
 B : Change expansion function of rho
 C : Change MEAM Parameter File
 Q : Quit
 Input 1,2,3,..., or Q
```

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## Data file format (3 type)

### normal format

**ex.)**

```
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 0
+0.00E+000    +0.00E+000    +0.00E+000    Si
+2.35E-010    +0.00E+000    +0.00E+000    Si
+0.50E-010    +2.04E-010    +0.00E+000    Si
+0.50E-010    +6.78E-011    +1.92E-010    Si
```

### SPD format

**ex.)**

```
Scalable position data file
C 5 atoms in a diamond structure
C The nearest neighbour distance is 1 (normalized)
+0.00E+00     +0.00E+00     +0.00E+00
 +0.00E+00    +0.00E+00     +1.00E+00
 +9.43E-01    +0.00E+00     -3.33E-01
 -4.71E-01    +8.16E-01     -3.33E-01
 -4.71E-01    -8.16E-01     -3.33E-01
```

### Format for reconstruction

**ex.)**

```
C <four Si atoms for reconstruction calculation>
C Starting with "C","%","c",and"#" mean being comment.
 1          0          .¥PF¥meamPF.YG
 +0.00E+000    +0.00E+000    +0.00E+000    Si -7 1
 +2.35E-010    +0.00E+000    +0.00E+000    Si -1 1
 +0.50E-010    +2.06E-010    +0.00E+000    Si  0 1
 +0.50E-010    +6.78E-011    +1.92E-010    Si  0 1
```

## Example 1

- Try total energy calculation
  - ex, $Si_2$ , $Si_5$ ,,,

ex.)
C "five Si atoms"
1

| | | | |
|---|---|---|---|
| +0.00E+000 | +0.00E+000 | +0.00E+000 | Si |
| +0.00E+000 | +0.00E+000 | +2.35E-010 | Si |
| +2.22E-010 | +0.00E+000 | -7.83E-011 | Si |
| -1.11E-010 | +1.92E-010 | -7.83E-011 | Si |
| -1.11E-010 | -1.92E-010 | -7.83E-011 | Si |

Type of screening
=1, for MEAM92

Type of expansion for electronic density
=0, for MEAM92

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

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

## Example 2

- Make a SPD data
  - ex. $Si_{29}$. Data file ;Si29.spd
- Energetics for dilation
  - read above SPD data files
- Graph of the energetics

## Example 3

- Try reconstruction calculation
  - ex, $Si_5$ ,,,

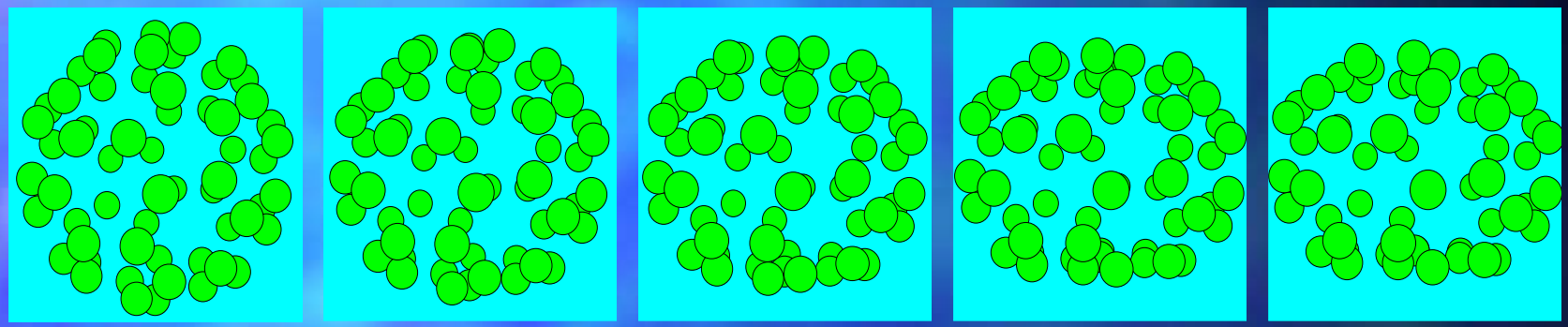
ex.)
C <five Si atoms for reconstruction calculation>
C "five Si atoms"
1 0 meamPF

| | | | | | |
|---|---|---|---|---|---|
| +0.00E+000 | +0.00E+000 | +0.00E+000 | Si | 0 | 1 |
| +0.00E+000 | +0.00E+000 | +2.35E-010 | Si | -1 | 1 |
| +2.22E-010 | +0.00E+000 | -7.83E-011 | Si | -5 | 1 |
| -1.11E-010 | +1.92E-010 | -7.83E-011 | Si | -7 | 1 |
| -1.11E-010 | -1.92E-010 | -7.83E-011 | Si | -7 | 1 |

- Visualization (Aview, etc…)

## Example 4 ( Deformation of C60 )

- Visualization



0% 10% 20% 30% 35%