**Library file**

# elt lat z ielement atwt

# alpha b0 b1 b2 b3 alat esub asub

# t0 t1 t2 t3 rozero ibar

'Pd' 'fcc' 12 1 106.420

6.4264647750 5.15 2.20 6.00 2.20 3.8890872965 3.91 0.94

1 4.50 1.47 4.85 1.00 3

'Al' 'fcc' 12 1 26.982

4.6855976824 3.20 2.60 6.00 2.60 4.0446507884 3.36 1.16

1 3.05 0.51 7.75 1.00 3

'Co' 'hcp' 12 1 58.933

5.2356147485 3.50 0.00 0.00 4.00 2.5000000000 4.41 0.90

1 3.50 5.00 -1.00 1.00 3

'Cu' 'fcc' 12 1 63.546

5.1548300830 3.83 2.20 6.00 2.20 3.6133156519 3.54 0.94

1 2.72 3.04 1.95 1.00 3

'Fe' 'bcc' 8 1 55.847

5.1571615396 4.15 1.00 1.00 1.00 2.8636573352 4.29 0.56

1 2.60 1.80 -7.20 1.00 3

'Mo' 'bcc' 8 1 89.960

5.8381780760 5.95 9.00 3.00 1.00 3.1465589671 6.81 0.61

1 2.00 7.75 -7.00 1.00 3

'Ni' 'fcc' 12 1 58.690

5.0842175782 2.56 1.50 6.00 1.50 3.5213917703 4.45 0.94

1 3.60 1.80 4.36 1.00 3

'Ti' 'hcp' 12 1 47.880

4.7194566335 2.70 1.00 3.00 1.00 2.9200000000 4.87 0.66

1 6.80 -2.00 -12.00 1.00 3

**MEAM file for the Pd-Al**

rc = 4.5

delr = 0.1

augt1 = 0

erose\_form = 2

ialloy = 2

zbl(1,1) = 0

nn2(1,1) = 1

attrac(1,1) = 0.05

repuls(1,1) = 0.05

Cmin(1,1,1) = 1.69

Cmax(1,1,1) = 2.8

Ec(1,1) = 3.91

re(1,1) = 2.75

zbl(2,2) = 0

nn2(2,2) = 1

attrac(2,2) = 0.05

repuls(2,2) = 0.05

Cmin(2,2,2) = 0.49

Cmax(2,2,2) = 2.8

Ec(2,2) = 3.36

re(2,2) = 2.86

zbl(1,2) = 0

nn2(1,2) = 1

rho0(1) = 1

rho0(2) = 1

Ec(1,2) = 4.245

re(1,2) = 2.58

alpha(1,2) = 5.29420825650716

attrac(1,2) = 0.05

repuls(1,2) = 0.05

Cmin(1,1,2) = 0.3

Cmin(2,2,1) = 0.3

Cmin(1,2,1) = 1

Cmin(1,2,2) = 1

Cmin(2,1,1) = 1

Cmin(2,1,2) = 1

Cmax(1,1,2) = 2.8

Cmax(2,2,1) = 1.44

Cmax(1,2,1) = 1.44

Cmax(1,2,2) = 2.8

Cmax(2,1,1) = 1.44

Cmax(2,1,2) = 2.8

lattce(1,2) = 'b2'

**MEAM file for the Pd-Co**

rc = 4.5

delr = 0.1

augt1 = 0

erose\_form = 2

ialloy = 2

zbl(1,1) = 0

nn2(1,1) = 1

attrac(1,1) = 0.05

repuls(1,1) = 0.05

Cmin(1,1,1) = 1.69

Cmax(1,1,1) = 2.8

Ec(1,1) = 3.91

re(1,1) = 2.75

zbl(2,2) = 0

nn2(2,2) = 1

attrac(2,2) = 0

repuls(2,2) = 0

Cmin(2,2,2) = 0.49

Cmax(2,2,2) = 2

Ec(2,2) = 4.41

re(2,2) = 2.5

zbl(1,2) = 0

nn2(1,2) = 1

rho0(1) = 1

rho0(2) = 1

Ec(1,2) = 3.69

re(1,2) = 2.51

alpha(1,2) = 6.85369019222313

attrac(1,2) = 0.025

repuls(1,2) = 0.025

Cmin(1,1,2) = 0.67

Cmin(2,2,1) = 0.79

Cmin(1,2,1) = 1

Cmin(1,2,2) = 1

Cmin(2,1,1) = 1

Cmin(2,1,2) = 1

Cmax(1,1,2) = 2

Cmax(2,2,1) = 1.44

Cmax(1,2,1) = 2.8

Cmax(1,2,2) = 2.8

Cmax(2,1,1) = 2.8

Cmax(2,1,2) = 2.8

lattce(1,2) = 'b1'

**MEAM file for the Pd-Cu**

rc = 4.5

delr = 0.1

augt1 = 0

erose\_form = 2

ialloy = 2

zbl(1,1) = 0

nn2(1,1) = 1

attrac(1,1) = 0.05

repuls(1,1) = 0.05

Cmin(1,1,1) = 1.69

Cmax(1,1,1) = 2.8

Ec(1,1) = 3.91

re(1,1) = 2.75

zbl(2,2) = 0

nn2(2,2) = 1

attrac(2,2) = 0.05

repuls(2,2) = 0.05

Cmin(2,2,2) = 1.21

Cmax(2,2,2) = 2.8

Ec(2,2) = 3.54

re(2,2) = 2.555

zbl(1,2) = 0

nn2(1,2) = 1

rho0(1) = 1

rho0(2) = 1

Ec(1,2) = 3.887

re(1,2) = 2.546

alpha(1,2) = 5.5659045465104

attrac(1,2) = 0.05

repuls(1,2) = 0.05

Cmin(1,1,2) = 0.49

Cmin(2,2,1) = 0.25

Cmin(1,2,1) = 1.44

Cmin(1,2,2) = 1.44

Cmin(2,1,1) = 1.44

Cmin(2,1,2) = 1.44

Cmax(1,1,2) = 2

Cmax(2,2,1) = 2

Cmax(1,2,1) = 2.8

Cmax(1,2,2) = 2.8

Cmax(2,1,1) = 2.8

Cmax(2,1,2) = 2.8

lattce(1,2) = 'b2'

**MEAM file for the Pd-Fe**

rc = 4.5

delr = 0.1

augt1 = 0

erose\_form = 2

ialloy = 2

zbl(1,1) = 0

nn2(1,1) = 1

attrac(1,1) = 0.05

repuls(1,1) = 0.05

Cmin(1,1,1) = 1.69

Cmax(1,1,1) = 2.8

Ec(1,1) = 3.91

re(1,1) = 2.75

zbl(2,2) = 0

nn2(2,2) = 1

attrac(2,2) = 0.05

repuls(2,2) = 0.05

Cmin(2,2,2) = 0.36

Cmax(2,2,2) = 2.8

Ec(2,2) = 4.29

re(2,2) = 2.48

zbl(1,2) = 0

nn2(1,2) = 1

rho0(1) = 1

rho0(2) = 1

Ec(1,2) = 4.095

re(1,2) = 2.72

alpha(1,2) = 5.87962853471044

attrac(1,2) = 0.05

repuls(1,2) = 0.05

Cmin(1,1,2) = 1.69

Cmin(2,2,1) = 0.01

Cmin(1,2,1) = 1.8

Cmin(1,2,2) = 2

Cmin(2,1,1) = 1.8

Cmin(2,1,2) = 2

Cmax(1,1,2) = 2.8

Cmax(2,2,1) = 1.44

Cmax(1,2,1) = 2.8

Cmax(1,2,2) = 2.8

Cmax(2,1,1) = 2.8

Cmax(2,1,2) = 2.8

lattce(1,2) = 'l12'

**MEAM file for the Pd-Mo**

rc = 4.5

delr = 0.1

augt1 = 0

erose\_form = 2

ialloy = 2

zbl(1,1) = 0

nn2(1,1) = 1

attrac(1,1) = 0.05

repuls(1,1) = 0.05

Cmin(1,1,1) = 1.69

Cmax(1,1,1) = 2.8

Ec(1,1) = 3.91

re(1,1) = 2.75

zbl(2,2) = 0

nn2(2,2) = 1

attrac(2,2) = 0

repuls(2,2) = 0

Cmin(2,2,2) = 0.82

Cmax(2,2,2) = 2.5

Ec(2,2) = 6.81

re(2,2) = 2.725

zbl(1,2) = 0

nn2(1,2) = 1

rho0(1) = 1

rho0(2) = 1

Ec(1,2) = 5.31

re(1,2) = 2.695

alpha(1,2) = 6.05990121969052

attrac(1,2) = 0.025

repuls(1,2) = 0.025

Cmin(1,1,2) = 1

Cmin(2,2,1) = 0.82

Cmin(1,2,1) = 1.22

Cmin(1,2,2) = 1.22

Cmin(2,1,1) = 1.22

Cmin(2,1,2) = 1.22

Cmax(1,1,2) = 2

Cmax(2,2,1) = 2.8

Cmax(1,2,1) = 2.8

Cmax(1,2,2) = 2.8

Cmax(2,1,1) = 2.8

Cmax(2,1,2) = 2.8

lattce(1,2) = 'b2'

**MEAM file for the Pd-Ni**

rc = 4.5

delr = 0.1

augt1 = 0

erose\_form = 2

ialloy = 2

zbl(1,1) = 0

nn2(1,1) = 1

attrac(1,1) = 0.05

repuls(1,1) = 0.05

Cmin(1,1,1) = 1.69

Cmax(1,1,1) = 2.8

Ec(1,1) = 3.91

re(1,1) = 2.75

zbl(2,2) = 0

nn2(2,2) = 1

attrac(2,2) = 0.05

repuls(2,2) = 0.05

Cmin(2,2,2) = 0.81

Cmax(2,2,2) = 2.8

Ec(2,2) = 4.45

re(2,2) = 2.49

zbl(1,2) = 0

nn2(1,2) = 1

rho0(1) = 1

rho0(2) = 1

Ec(1,2) = 3.725

re(1,2) = 2.47

alpha(1,2) = 5.49688217936057

attrac(1,2) = 0.05

repuls(1,2) = 0.05

Cmin(1,1,2) = 1.69

Cmin(2,2,1) = 0.81

Cmin(1,2,1) = 1.21

Cmin(1,2,2) = 1.21

Cmin(2,1,1) = 1.21

Cmin(2,1,2) = 1.21

Cmax(1,1,2) = 2.8

Cmax(2,2,1) = 2.8

Cmax(1,2,1) = 2.8

Cmax(1,2,2) = 2.8

Cmax(2,1,1) = 2.8

Cmax(2,1,2) = 2.8

lattce(1,2) = 'b1'

**MEAM file for the Pd-Ti**

rc = 4.5

delr = 0.1

augt1 = 0

erose\_form = 2

ialloy = 2

zbl(1,1) = 0

nn2(1,1) = 1

attrac(1,1) = 0.05

repuls(1,1) = 0.05

Cmin(1,1,1) = 1.69

Cmax(1,1,1) = 2.8

Ec(1,1) = 3.91

re(1,1) = 2.75

zbl(2,2) = 0

nn2(2,2) = 1

attrac(2,2) = 0

repuls(2,2) = 0

Cmin(2,2,2) = 1

Cmax(2,2,2) = 1.44

Ec(2,2) = 4.87

re(2,2) = 2.92

zbl(1,2) = 0

nn2(1,2) = 1

rho0(1) = 1

rho0(2) = 1

Ec(1,2) = 5.1236

re(1,2) = 2.7266

alpha(1,2) = 5.19235176042731

attrac(1,2) = 0.025

repuls(1,2) = 0.025

Cmin(1,1,2) = 1.09

Cmin(2,2,1) = 0.29

Cmin(1,2,1) = 1.47

Cmin(1,2,2) = 0.17

Cmin(2,1,1) = 1.47

Cmin(2,1,2) = 0.17

Cmax(1,1,2) = 1.78

Cmax(2,2,1) = 2.2

Cmax(1,2,1) = 2.21

Cmax(1,2,2) = 1.66

Cmax(2,1,1) = 2.21

Cmax(2,1,2) = 1.66

lattce(1,2) = 'b2'