```
bravo@bravo-ThinkPad-T590:~/桌面/kmc_ABVI_surface-master$ ./exekmc
########## Initializing System... ##########
Setting:
nx= 64, ny= 64, nz= 64
The crystal structure is: BCC
v0: -0.5 0.5 0.5
v1: 0.5 -0.5 0.5
v2: 0.5 0.5 -0.5
And the number of 1st neighbors: 8
    the number of 2nd neighbors: 6

####### Generating configuration... #######
START FROM a random configuration...
The random solution configuration has been generated!
Vacancy: 0
Vacuum:  0
Atype A: 223073, pct: 85.0956%
Atype B: 39071, pct: 14.9044%
Output t0 conf files
Open history.sol & history.def with write mode

##### Energy calculation parameters #####
temperature= 2100, beta= 5.52596
correlation factor= 1.775
Vacancy mu= 6460000000000.000000 6460000000000.000000
Interstitial mu= 0.000000 0.000000
Vacancy Em= 1.623000 1.651000
Interstitial Em= 0.000000 0.000000
Rotation Er(AA, AB, BB)= 0.430000 0.000000 0.000000
Interstitial Em(AA AB BB)= 0.003000 0.120000 0.000000 (Dubey, CMS 2015)

##### Input epsilons: #####
(1st neigbor)
AA-AA: -0.190500, AA-A: 0.174000, AA-AB: -0.250500, AA-B: -0.275000, AA-BB: 0.000000
A-A:   -1.581500, A-V:  -0.489800, A-AB: 0.110400, A-B:   0.000000, A-BB: 0.000000
V-V:   0.587300, V-B:  0.000000
AB-AB: -1.397700, AB-B: -0.348600, AB-BB: 0.000000
B-B:   -1.406700, B-BB: 0.000000
BB-BB: 0.000000
(2nd neigbor)
AA-AA: -0.080400, AA-A: 0.073400, AA-AB: -0.105700, AA-B: -0.116000, AA-BB: 0.000000
A-A:   -0.667200, A-V:  -0.206700, A-AB: 0.046600, A-B:   0.000000, A-BB: 0.000000
V-V:   0.556600, V-B:  0.000000
AB-AB: -0.589700, AB-B: -0.147000, AB-BB: 0.000000
B-B:   -0.593500, B-BB: 0.000000
BB-BB: 0.000000

##### Ising formulation constants: #####
(1st neighbor)
Class 1
C44: 0.031725, C42: -0.146766, C22: 0.591858
Class 2
C43: 0.007957, C41: -0.045261, C32: -0.058357, C21: 0.296861
Class 3
C33: -0.096801, C31: 0.364526, C11: -1.379301
Class 0
C40: -0.091704, C30: -0.015742, C20: 0.538104, C10: 0.000342
C00: -0.810400, C0_ABA: 1.592700, C0_ABB: 0.643900, C0_AA: 2.349200, C0_A: -6.474000, C0_AB: -2.349200, C0_B: -2.802000, C0_BB: 2.349200
Vacuum
CMM: -0.587300, CMA: 0.489800, CMV: -0.587300, CMB: 0.000000
(2nd neighbor)
Class 1
C44: 0.039124, C42: -0.177749, C22: 0.764499
Class 2
C43: 0.003360, C41: -0.019110, C32: -0.024635, C21: 0.125310
Class 3
C33: -0.040839, C31: 0.153789, C11: -0.581914
Class 0
C40: 0.038504, C30: -0.006625, C20: -0.158954, C10: 0.000075
C00: -0.033100, C0_ABA: 0.826450, C0_ABB: 0.426150, C0_AA: 1.669800, C0_A: -2.048700, C0_AB: -1.669800, C0_B: -0.887100, C0_BB: 1.669800
Vacuum
CMM: -0.556600, CMA: 0.206700, CMV: -0.556600, CMB: 0.000000

2nd nn parameters are non-zero

########## Initializing Events ... ##########
##Generation parameters (rate_genr) 262.144 (damage/s)
##Recombination parameters: 3rd nearest-neighbor distance (FIXED in SURFACE simulations)

########## The Simulation Begins !! ##########
TIMESTEP() TIME(s) GENR()       NA() NB()       NV() NAA() NAB() NBB()  AJUMP_V% AJUMP_I%
0 0.0000000000e+00 0      223073 39071     0 0 0 0     0.000000 0.000000
100000 3.8148378182e-03 1     223072 39070     1 0 1 0     0.722031 0.000010  *** 0-defect genr: 1 ***
200000 1.9075277390e-02 5     223072 39070     1 0 1 0     0.737335 0.000005  *** 0-defect genr: 4 ***
300000 1.9075503153e-02 5     223072 39070     1 0 1 0     0.736247 0.000004
400000 3.4335191162e-02 9     223072 39070     1 0 1 0     0.737145 0.000003  *** 0-defect genr: 4 ***
500000 4.5780316682e-02 12     223072 39070     1 0 1 0     0.737241 0.000006  *** 0-defect genr: 3 ***
600000 4.9595804106e-02 13     223073 39070     0 0 1 0     0.738917 0.000005  *** 0-defect genr: 1 ***
700000 5.3410605751e-02 14     223072 39070     1 0 1 0     0.737440 0.000006  *** 0-defect genr: 1 ***
800000 6.1040224387e-02 16     223073 39070     0 0 1 0     0.737590 0.000005  *** 0-defect genr: 2 ***
900000 6.1040325324e-02 16     223073 39070     0 0 1 0     0.737590 0.000005
1000000 6.1040383091e-02 16     223073 39070     0 0 1 0     0.737590 0.000004   <Output conf files at: 1000000>
1100000 8.7745619358e-02 23     223073 39069     1 0 1 0     0.735740 0.000005  *** 0-defect genr: 7 ***
1200000 9.5376597410e-02 25     223072 39070     1 0 1 0     0.735559 0.000004  *** 0-defect genr: 2 ***
1300000 1.1063640329e-01 29     223073 39070     0 0 1 0     0.735092 0.000006  *** 0-defect genr: 4 ***
1400000 1.1445141386e-01 30     223073 39070     0 0 1 0     0.735098 0.000005  *** 0-defect genr: 1 ***
1500000 1.1445152382e-01 30     223073 39070     0 0 1 0     0.735098 0.000005
1600000 1.1826638303e-01 31     223073 39069     1 0 1 0     0.735415 0.000005  *** 0-defect genr: 1 ***
1700000 1.4115608709e-01 37     223073 39069     1 0 1 0     0.735310 0.000004  *** 0-defect genr: 6 ***
1800000 1.5260073860e-01 40     223073 39069     1 0 1 0     0.735228 0.000004  *** 0-defect genr: 3 ***
1900000 1.5260100137e-01 40     223073 39070     0 0 1 0     0.735172 0.000004
2000000 1.6404540736e-01 43     223072 39070     1 0 1 0     0.734953 0.000004  *** 0-defect genr: 3 ***   <Output conf files at: 2000000>
```

```
// System
const int    par_nx=                    64; // sizes in the 3-dimensions
const int    par_ny=                    64;
const int    par_nz=                    64;
const int    par_nMlayer=                0;

const double par_compA =               0.85;
const double par_compV=                   0; // vcc; set >1.0 to get only 1 defect
const double par_typeD=                   0; // if sinlge defect, what is the type of defect

// Simulation time parameters
const double        par_time=          100.0; // time: total
const double        time_conf=          10.0; //       output conf

const long long int par_step=            1e7; // steps: toal (minus step with no limit for this)
const long long int step_log=            1e5; //        output log
const long long int step_conf=           1e6; //        output conf
const long long int step_out=            1e5; //        compute properties
const long long int step_his=            1e5; //        output history files
```

```
// Parameters for events
const double par_dis_rec=     0.866*3; // recombination distance
const bool   par_isgenr=         true; // whether F-P genr
const double par_dpasm1=         1e-3; // dpa/s
const bool   par_trap_included= false;
const bool   par_iscaldsro=     false; // whether cal sro change
const int    par_x_sink= (int) (par_nx/2); // the location of plane sink

// Kinetic parameters
const double par_temp = 2100;
const double par_beta= 1.0/par_temp/8.617332478e-5; // 1/kbT, units: eV, K
const double par_corrfac=  2.93 - 0.00055*par_temp; // correlation factor for SIA
```

```
const double par_muiAA=          6.46e+12; // itl mu and Em and Er
const double par_muiAB=          6.46e+12;
const double par_emiAA=             0.003;
const double par_emiAB=              0.12;
const double par_erAA=               0.43;
```

TABLE IV. Self-interstitial migration parameters. The jump distance for SIA migration is $\delta = a_0\sqrt{3}/2$.

E_m^{AA}	0.003	Ref. [25]
E_r^{AA}	0.43	Ref. [25]
E_m^{AB}	0.12	Ref. [27]
f	$2.93 - 0.00055T$	Ref. [45]

```
// Bonding energy parameters
const double r21=                    0.421875; // rati

const double e0A1B=                   -1.5090; // eA1B
const double e1A1B=                   -0.0219;
const double e0A2B=                   -0.6366; // eA1B
const double e1A2B=                   -0.0092;

const double e0B1V=                   -0.4898; // eB1V
const double e1B1V=                  -0.009432;
const double e0B2V=                   -0.3311; // eB2V
const double e1B2V=                     0.036;

// bonds
const double eA1A=                    -1.5815;
const double eA2A=                    -0.6672;
const double eB1B=     (double)(-0.5935000000000000275)
const double eB2B=                    -0.5935;

const double eA1V=                    -0.4898;
const double eA2V=                    -0.2067;
const double eV1V=                     0.5873;
const double eV2V=                     0.5566;

const double eAA1A=                    0.1740;
const double eAA2A=                    0.0734;
const double eA1AB=                    0.1104;
const double eA2AB=                    0.0466;

const double eAA1B=                   -0.2750;
const double eAA2B=                   -0.1160;
const double eAB1B=                   -0.3486;
const double eAB2B=                   -0.1470;

const double eAA1AA=                  -0.1905;
const double eAA2AA=                  -0.0804;
const double eAA1AB=                  -0.2505;
const double eAA2AB=                  -0.1057;
const double eAB1AB=                  -1.3977;
const double eAB2AB=                  -0.5897;
```

TABLE I. Energetics of W-Re systems calculated with DFT.

Quantity	Value	Source
E_{coh}^{A}	8.3276	This work
E_{coh}^{B}	7.4070	This work
ΔH^{mix}	$-0.1571-0.2311X$	Ref. [27]
E_f^{V}	3.1690	This work
$E_b^{(a)}$	-0.2096	This work
$E_b^{(b)}$	-0.1520	This work
$E_b^{(c)}$	-0.3079	This work
$E_b^{(d)}$	-0.2992	This work
$E_{b,1\mathrm{nn}}^{\mathrm{V\text{-}V}}$	-0.0146	This work[3]
$E_{b,2\mathrm{nn}}^{\mathrm{V\text{-}V}}$	0.3028	This work[3]
E_f^{AA}	10.16	Ref. [46]
E_f^{AB}	9.49	Ref. [46]
$E_{b,1\mathrm{nn}}^{\mathrm{AA\text{-}B}}$	-0.52	Ref. [46]
$E_{b,1\mathrm{nn}}^{\mathrm{AB\text{-}B}}$	-0.53	Ref. [49]
$E_{b,1\mathrm{nn}}^{\mathrm{AA\text{-}AA}}$	-2.12	Ref. [50]
$E_{b,1\mathrm{nn}}^{\mathrm{AA\text{-}AB}}$	-2.12	Assumed [4]
$E_{b,1\mathrm{nn}}^{\mathrm{AB\text{-}AB}}$	-3.2	Ref. [27]
$E_m^{\mathrm{V}\to\mathrm{A}}$ (A)	1.623	This work
$E_m^{\mathrm{V}\to\mathrm{B}}$ (A)	1.651	This work
$E_m^{\mathrm{V}\to\mathrm{A}(1)}$ (Fig. 2(c))	1.7151	This work
$E_m^{\mathrm{V}\to\mathrm{A}(2)}$ (Fig. 2(c))	1.6378	This work
$E_m^{\mathrm{V}\to\mathrm{B}(3)}$ (Fig. 2(c))	1.577	This work
$E_m^{\mathrm{V}\to\mathrm{A}}$ (V)	1.623	This work
$E_m^{\mathrm{V}\to\mathrm{B}}$ (V)	1.651	This work

$\varepsilon_{\mathrm{A\text{-}A}}^{(1)}$	-1.5815	cohesive energy, eq. (9)	This work
$\varepsilon_{\mathrm{A\text{-}A}}^{(2)}$	-0.6672	cohesive energy, eq. (9)	This work
$\varepsilon_{\mathrm{B\text{-}B}}^{(1)}$	-1.4067	cohesive energy, eq. (9)	This work
$\varepsilon_{\mathrm{B\text{-}B}}^{(2)}$	-0.5935	cohesive energy, eq. (9)	This work
$\varepsilon_{\mathrm{A\text{-}B}}^{(1)}$	$-1.5090-0.0219x$	mixing energy	Ref. [27]
$\varepsilon_{\mathrm{A\text{-}B}}^{(2)}$	$-0.6366-0.0092x$	eq. (9)	Ref. [27]
$\varepsilon_{\mathrm{A\text{-}V}}^{(1)}$	-0.4898	formation energy, eq. (9)	This work
$\varepsilon_{\mathrm{A\text{-}V}}^{(2)}$	-0.2067	formation energy, eq. (9)	This work
$\varepsilon_{\mathrm{B\text{-}V}}^{(1)}$	$-0.4898-0.009432/x$	formation energy fitted to $\varepsilon_{B-V}^{(1)}=a+b/x$	This work
$\varepsilon_{\mathrm{B\text{-}V}}^{(2)}$	$-0.3311+0.036x$	formation energy fitted to $\varepsilon_{B-V}^{(1)}=a+bx$	This work
$\varepsilon_{\mathrm{V\text{-}V}}^{(1)}$	0.5873	1nn binding energy	This work
$\varepsilon_{\mathrm{V\text{-}V}}^{(2)}$	0.5566	2nn binding energy	This work
$\varepsilon_{\mathrm{AA\text{-}A}}^{(1)}$	0.1740	formation energy, eq. (9)	Ref. [46]
$\varepsilon_{\mathrm{AA\text{-}A}}^{(2)}$	0.0734	formation energy, eq. (9)	Ref. [46]
$\varepsilon_{\mathrm{AB\text{-}A}}^{(1)}$	0.1104	formation energy, eq. (9)	Ref. [46]
$\varepsilon_{\mathrm{AB\text{-}A}}^{(2)}$	0.0466	formation energy, eq. (9)	Ref. [46]
$\varepsilon_{\mathrm{AA\text{-}B}}^{(1)}$	-0.2750	binding energy	Ref. [46]
$\varepsilon_{\mathrm{AA\text{-}B}}^{(2)}$	-0.1160	eq. (9)	Ref. [46]
$\varepsilon_{\mathrm{AB\text{-}B}}^{(1)}$	-0.3486	binding energy	Ref. [49]
$\varepsilon_{\mathrm{AB\text{-}B}}^{(2)}$	-0.1470	eq. (9)	Ref. [49]
$\varepsilon_{\mathrm{AA\text{-}AA}}^{(1)}$	-0.1905	binding energy	Ref. [50]
$\varepsilon_{\mathrm{AA\text{-}AA}}^{(2)}$	-0.0804	eq. (9)	Ref. [50]
$\varepsilon_{\mathrm{AA\text{-}AB}}^{(1)}$	-0.2505	binding energy	Assumed [4]
$\varepsilon_{\mathrm{AA\text{-}AB}}^{(2)}$	-0.1057	eq. (9)	Assumed [4]
$\varepsilon_{\mathrm{AB\text{-}AB}}^{(1)}$	-1.3977	binding energy	Ref. [27]
$\varepsilon_{\mathrm{AB\text{-}AB}}^{(2)}$	-0.5897	eq. (9)	Ref. [27]