Development of the ReaxFF Reactive Force Field for Cu/Si Systems with application to Copper Cluster Formation During Cu Diffusion Inside Silicon

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Reactive MD-force field: Si/Cu force field June 11 2012 - based on Dow-Corning FF
39 ! Number of general parameters
50.0000 !Overcoordination parameter
9.4514 !Overcoordination parameter
56.6636 !Valency angle conjugation parameter
3.0000 !Triple bond stabilisation parameter
6.5000 !Triple bond stabilisation parameter
0.0000 !C2-correction
1.0701 !Undercoordination parameter
9.0000 !Triple bond stabilisation parameter
11.9083 !Undercoordination parameter
13.3822 !Undercoordination parameter
0.0000 !Triple bond stabilization energy
0.0000 !Lower Taper-radius
10.0000 !Upper Taper-radius
2.8793 !Not used
33.8667 !Valency undercoordination
5.8971 !Valency angle/lone pair parameter
1.0563 !Valency angle
2.0384 !Valency angle parameter
6.1431 !Not used
6.9290 !Double bond/angle parameter
0.3989 !Double bond/angle parameter: overcoord
3.9954 !Double bond/angle parameter: overcoord
-2.4837 !Not used
5.8374 !Torsion/BO parameter
10.0000 !Torsion overcoordination
1.8820 !Torsion overcoordination
-1.2327 !Conjugation 0 (not used)
2.1861 !Conjugation
1.5591 !vdWaals shielding

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  0.0100 !Cutoff for bond order (*100)
  0.7151 !Valency angle conjugation parameter
  2.7425 !Overcoordination parameter
 12.5819 !Overcoordination parameter
  2.1533 !Valency/lone pair parameter
  0.5000 !Not used
 20.0000 !Not used
  5.0000 !Molecular energy (not used)
  0.0000 !Molecular energy (not used)
  1.4155 !Valency angle conjugation parameter
 3    ! Nr of atoms; cov.r; valency;a.m;Rvdw;Evdw;gammaEEM;cov.r2;#
        alfa;gammavdW;valency;Eunder;Eover;chiEEM;etaEEM;n.u.
        cov r3;Elp;Heat inc.;n.u.;n.u.;n.u.;n.u.
        ov/un;val1;n.u.;val3,vval4
Si   2.0175   4.0000  28.0600   2.0473   0.1835   0.7777   1.2962   4.0000
    12.3588   1.2523   4.0000  21.7115 139.9309   4.2885   6.1868   0.0000
    -1.0000   0.0000 128.2031   8.7895  23.9298   0.8381   0.8563   0.0000
    -4.7525   2.1607   1.0338   4.0000   2.5791   0.0000   0.0000   0.0000
Cu   1.8424   1.0000  63.5460   1.8399   0.1899   0.8218   0.1000   1.0000
    12.4221   4.7107   1.0000   0.0000   0.0000   4.8038   7.3852   0.0000
    -1.0000   0.0000  78.0000   6.2293   5.2294   0.1542   0.8563   0.0000
    -5.0396   2.9867   1.0338   8.0000   2.5791   0.0000   0.0000   0.0000
X   -0.1000   2.0000   1.0080   2.0000   0.0000   1.0000  -0.1000   6.0000
    10.0000   2.5000   4.0000   0.0000   0.0000   8.5000   1.5000   0.0000
    -0.1000   0.0000 127.6226   8.7410  13.3640   0.6690   0.9745   0.0000
   -11.0000   2.7466   1.0338   6.2998   2.8793   0.0000   0.0000   0.0000
 3      ! Nr of bonds; Edis1;LPpen;n.u.;pbe1;pbo5;13corr;pbo6
                pbe2;pbo3;pbo4;n.u.;pbo1;pbo2;ovcorr
 1  1  78.0276  54.0531  30.0000   0.5398  -0.3000   1.0000  16.0000   0.0476
       0.2865  -0.8055   7.1248   1.0000  -0.0681   8.6957   0.0000   0.0000
 1  2  92.2603   0.0000   0.0000  -0.2343  -0.2000   0.0000  16.0000   0.1843
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      3.8737  -0.2000  15.0000   1.0000  -0.0966   4.5425   0.0000   0.0000
2  2 115.9289   0.0000   0.0000  -0.1272  -0.2000   0.0000  16.0000   0.3956
      2.3229  -0.2000  15.0000   1.0000  -0.0756   5.2802   0.0000   0.0000
1    ! Nr of off-diagonal terms; Ediss;Ro;gamma;rsigma;rpi;rpi2
1  2   0.1999   2.2638  10.2775   1.7291  -1.0000  -1.0000
5    ! Nr of angles;at1;at2;at3;Thetao,o;ka;kb;pv1;pv2;val(bo)
1  1  1  71.0490  32.4076   1.2648   0.0000   0.0133   0.0000   1.2899
1  1  2  72.7292  14.2411   1.7353   0.0000   0.0100   0.0000   1.5918
1  2  1  47.4577   5.1156   4.9750   0.0000   0.9242   0.0000   1.9624
1  2  2  32.1164   1.3775   1.1554   0.0000   0.7425   0.0000   1.3695
2  1  2  79.5321   0.0249   2.6130   0.0000   0.1256   0.0000   1.0400
0    ! Nr of torsions;at1;at2;at3;at4;;V1;V2;V3;V2(BO);vconj;n.u;n
0    ! Nr of hydrogen bonds;at1;at2;at3;Rhb;Dehb;vhb1
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