Modification of 2NN MEAM parameters for diamond structure in LAMMPS

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Problem of 2NN MEAM in LAMMPS

- If a reference structure was diamond and the C_{min} value was lower than 0.5, LAMMPS calculation shows different result with KISSMD calculation.

- In those case, the pair potential is affected by screening function because second-nearest neighbors were considered.

- Something is wrong with that in LAMMPS.

- 2NN MEAM codes in LAMMPS should be modified.
  Path : Lammps-DDMMYY/lib/meam/meam_setup_done.F

Modification of 2NN MEAM parameters in LAMMPS

(meam_setup_done.F)

```
c neighbor screening function for lattice type "latt"

      subroutine get_Zij2(Zij2,a,S,latt,cmin,cmax)
      implicit none
      integer Zij2
      real*8 a,S,cmin,cmax
      character*3 latt
      real*8 rratio,C,x,sijk
      integer numscr

      if (latt.eq.'bcc') then
        Zij2 = 6
        a = 2.d0/sqrt(3.d0)
        numscr = 4
      else if (latt.eq.'fcc') then
        Zij2 = 6
        a = sqrt(2.d0)
        numscr = 4
      else if (latt.eq.'dia') then
        Zij2 = 0
        a = sqrt(8.d0/3.d0)
        numscr = 4
        if (cmin.lt.0.500001) then
c          call error('can not do 2NN MEAM for dia')
        endif
      else if (latt.eq.'hcp') then
        Zij2 = 6
        a = sqrt(2.d0)
        numscr = 4
      else if (latt.eq.'b1') then
        Zij2 = 12
        a = sqrt(2.d0)
        numscr = 2
      else
c        call error('Lattice not defined in get_Zij2.')
      endif

c Compute screening for each first neighbor
      C = 4.d0/(a*a) - 1.d0
      x = (C-cmin)/(cmax-cmin)
      call fcut(x,sijk)
c There are numscr first neighbors screening the second neighbors
      S = sijk**numscr

      return
      end
```

Variable	Value	Notes
Zij2	0 → 12	Number of second-nearest neighbor
a	sqrt(8/3)	R2/R1
numscr	4 → 1	Square of screening function

```
c
      elseif(lattice.eq.'HCP_A3') then
c
        a2(n)    = dsqrt(2.d0)
        Z(n)     = 12.0d0
        scr = screen(0.5d0,0.5d0,Cmax(n,n,n),Cmin(n,n,n))
        scr_2nn = scr * scr * scr * scr
        Z2(n) = 6.0d0 * scr_2nn
        ZR2 = Z2(n) / Z(n)
        alat = Re(n)
        omega(n,n) = alat * alat * alat / a2(n)
c
      elseif(lattice.eq.'DIA_A4') then
c
        a2(n)    = 4.d0 / dsqrt(6.d0)
        Z(n)     = 4.0d0
        scr_2nn = screen(0.375d0,0.375d0,Cmax(n,n,n),Cmin(n,n,n))
        Z2(n) = 12.0d0 * scr_2nn
c        print *, n, Z2(n)
        ZR2 = Z2(n) / Z(n)
        alat = 4.d0 * Re(n) / dsqrt(3.d0)
        omega(n,n) = alat * alat * alat / 8.d0
c
```

Modification of 2NN MEAM parameters in LAMMPS

(meam_setup_done.F)

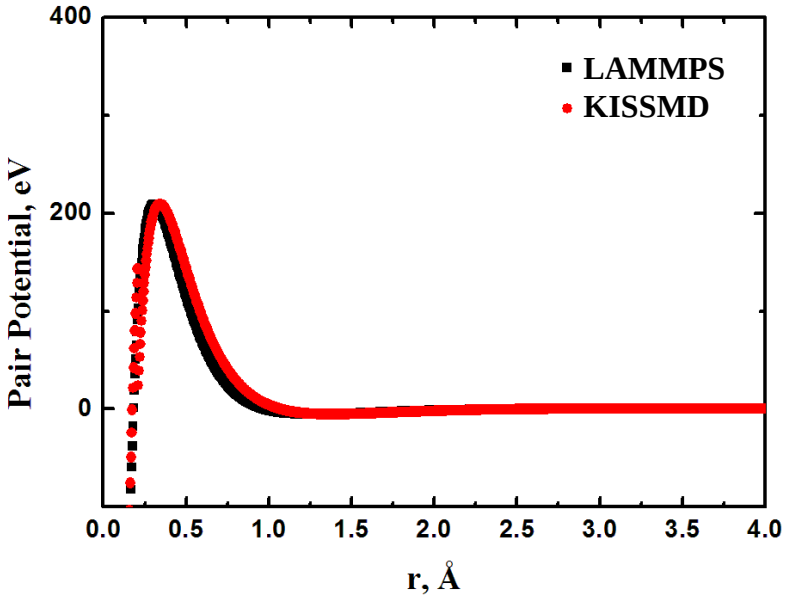
```
c     The B1, B2,  and L12 cases with NN2 have a trick to them; we need to
c     compute the contributions from second nearest neighbors, like a-a
c     pairs, but need to include NN2 contributions to those pairs as
c     well.
            if (lattce_meam(a,b).eq.'b1'.or.
     &          lattce_meam(a,b).eq.'b2'.or.
     &          lattce_meam(a,b).eq.'l12'.or.
     &          lattce_meam(a,b).eq.'dia') then
              rarat = r*arat

c             phi_aa
              phiaa = phi_meam(rarat,a,a)
              call get_Zij(Z1,lattce_meam(a,a))
              call get_Zij2(Z2,arat,scrn,lattce_meam(a,a),
     &             Cmin_meam(a,a,a),Cmax_meam(a,a,a))
              nmax = 10
              if (scrn.gt.0.0) then
                do n = 1,nmax
                  phiaa = phiaa +
     &                 (-Z2*scrn/Z1)**n * phi_meam(rarat*arat**n,a,a)
                enddo
              endif

c             phi_bb
              phibb = phi_meam(rarat,b,b)
              call get_Zij(Z1,lattce_meam(b,b))
              call get_Zij2(Z2,arat,scrn,lattce_meam(b,b),
     &             Cmin_meam(b,b,b),Cmax_meam(b,b,b))
              nmax = 10
              if (scrn.gt.0.0) then
                do n = 1,nmax
                  phibb = phibb +
     &                 (-Z2*scrn/Z1)**n * phi_meam(rarat*arat**n,b,b)
                enddo
              endif
c              if(nv2.eq.2) then
c                 print *, phiaa
c                 print *, phir(j,nv2)
c              endif
c              print *, phiaa, phibb
              if (lattce_meam(a,b).eq.'b1'.
     &            or.lattce_meam(a,b).eq.'b2'
     &            or.lattce_meam(a,b).eq.'dia') then
c     Add contributions to the B1 or B2 potential
                call get_Zij(Z1,lattce_meam(a,b))
                call get_Zij2(Z2,arat,scrn,lattce_meam(a,b),
     &               Cmin_meam(a,a,b),Cmax_meam(a,a,b))
                phir(j,nv2) = phir(j,nv2) -
```

add

add



Si-N MEAM potential (KISSMD vs. LAMMPS)

Si-N Potential : α, β, γ - Si_3N_4 structure

Type	Property		KISSMD	Lammps
α-Si_3N_4 (type)	Lattice constant (Å)	a	**7.751**	**7.759**
		c	**5.619**	**5.617**
	Formation energy(eV/atom)		**-1.218**	**-1.218**
	Volume of cells(Å^3)		**292.4**	**292.8**
	Melting Temperature(K)		**3200**	
	Bulk modulus *B* (GPa)		**206.5 (**B′=4.132**)**	
	C_{11} (GPa)		**431.6**	**429.1**
	C_{12} (GPa)		**153.8**	**151.2**
	C_{13} (GPa)		**47.9**	**48.5**
	C_{33} (GPa)		**494.9**	**491.4**
	C_{44} (GPa)		**190.5**	**189.2**
	C_{66} (GPa)		**138.8**	**139.4**

Type	Property		KISSMD	Lammps
β-Si_3N_4 (type)	Lattice constant (Å)	a	**7.539**	**7.496**
		c	**2.981**	**2.983**
	Formation energy(eV/atom)		**-1.32**	**-1.32**
	Volume of cells(Å^3)		**144.62**	**144.71**
	Bulk modulus *B* (GPa)		**214.3 (**B′=1.43**)**	
	C_{11} (GPa)		**412.5**	**409.3**
	C_{12} (GPa)		**161.0**	**174.3**
	C_{13} (GPa)		**33.3**	**37.2**
	C_{33} (GPa)		**653.6**	**647.0**
	C_{44} (GPa)		**153.3**	**153.3**
	C_{66} (GPa)		**125.7**	**120.7**

Type	Property	KISSMD	Lammps
γ-Si_3N_4 (type)	Lattice constant (Å)	**7.981**	**7.985**
	Formation energy(eV/atom)	**0.0443**	**0.0444**
	Volume of cells(Å^3)	**444.81**	**445.53**
	Bulk modulus *B* (GPa)	**263.1 (**B′=4.609**)**	
	C_{11} (GPa)	**473.9**	**471.7**
	C_{12} (GPa)	**157.7**	**156.6**
	C_{44} (GPa)	**364.5**	**351.0**

C-N MEAM Potential (KISSMD vs. LAMMPS)

C-N Potential : C_3N_4 structure

Property		α-C_3N_4 (MEAM)	Lammps	β-C_3N_4 (MEAM)	Lammps	γ-C_3N_4	Lammps
Lattice constant (Å)	a	**6.387**	**6.388**	**5.994**	**5.994**	**6.82**	**6.82**
	c	**4.63**	**4.63**	**2.489**	**2.489**		
Formation energy(eV/atom)		**-0.321**	**-0.321**	**-0.499**	**-0.499**	**1.962**	**1.962**
Volume of cells(Å^3)		**81.78**	**81.82**	**39.67**	**39.67**	**39.66**	**39.66**
Bulk modulus *B* (GPa)		**427**		**456**		**373**	

Property		Cubic-C_3N_4 (MEAM)	Lammps	Pseudocubic-C_3N_4 (MEAM)	Lammps
Lattice constant (Å)	a	**5.475**	**5.475**	**3.54**	**3.54**
Formation energy(eV/atom)		**0.628**	**0.628**	**0.658**	**0.658**
Volume of cells(Å^3)		**41.03**	**41.03**	**19.07**	**19.07**
Bulk modulus *B* (GPa)		**392**		**350**	
C_{11} (GPa)		**857.4**	**857.3**		
C_{12} (GPa)		**159.0**	**159.3**		
C_{44} (GPa)		**238.8**	**238.7**		

Property		Graphitic-C_3N_4 (MEAM)	Lammps
Lattice constant (Å)	a	**5.056**	**5.056**
	c	**6.996**	**6.996**
Formation energy(eV/atom)		**0.1434**	**0.1434**

Si-C-N MEAM potential (KISSMD vs. LAMMPS)

Si-C-N Potential : $Si_xC_yN_z$ structure

Property		α-Si_2CN_4 (KISSMD)	Lammps	α-SiC_2N_4 (KISSMD)	Lammps	β-Si_2CN_4 (KISSMD)	Lammps	β-SiC_2N_4 (KISSMD)	Lammps
Lattice constant (Å)	a	**7.355**	**7.357**	**6.863**	**6.863**	**7.197**	**7.197**	**6.559**	**6.558**
	c	**5.235**	**5.236**	**4.912**	**4.912**	**2.683**	**2.683**	**2.586**	**2.585**
Formation energy(eV/atom)		**-0.836**	**-0.837**	**-0.5532**	**-0.5533**	**-0.9593**	**-0.9593**	**-0.6624**	**-0.6627**
Volume of cells(Å^3)		**244.06**	**244.29**	**199.79**	**199.79**	**119.62**	**119.63**	**98.21**	**98.15**
Bulk modulus *B* (GPa)		**253** (B´=4.11)		**312** (B´=4.29)		**268.7** (B´=4.191)		**352.9** (B´=6.184)	

Property		Cubic-SiC_2N_4 (KISSMD)	Lammps	Cubic-SiCN (KISSMD)	Lammps	Orthorhombic-Si_2CN_4 (KISSMD)	Lammps
Lattice constant (Å)	a	**6.943**	**6.943**	**4.672**	**4.672**	**5.47**	**5.47**
	b					**14.32**	**14.32**
	c					**4.88**	**4.88**
Formation energy(eV/atom)		**-0.468**	**-0.468**	**0.764**	**0.764**	**-0.953**	**-0.953**

Property		Pseudocubic-SiC_2N_4 (KISSMD)	Lammps	Pseudocubic-Si_2CN_4 (KISSMD)	Lammps
Lattice constant (Å)	a	**3.62**	**3.62**	**4.01**	**4.01**
	c	**3.96**	**3.96**	**3.93**	**3.93**
Formation energy(eV/atom)		**-0.076**	**-0.076**	**-0.424**	**-0.426**
Bulk modulus *B* (GPa)		**277.3**		**225.5**	
Volume of cells		**51.88**	**51.88**	**62.49**	**62.48**