

Paper where functions presented:

Baskes, M.I., *Modified embedded-atom potentials for cubic materials and impurities*. Physical Review B (Condensed Matter), 1992. 46(5): p. 2727-42.

Papers that use these functions for pure Si:

Improved modified embedded-atom method potentials for gold and silicon

Ryu, S. ; Weinberger, C.R. ; Baskes, M.I. ; Cai, W.

Modelling and Simulation in Materials Science and Engineering (2009) Vol.17, iss.7 075008

Swadener, J.G., M.I. Baskes, and M. Nastasi, *Stress-induced platelet formation in silicon: A molecular dynamics study*. Physical Review B, 2005. 72(20): p. 201202. (Slightly modified parameters)

Molecular dynamics simulation of silicon sputtering: Sensitivity to the choice of potential

Thijsse, B.J. ; Klaver, T.P.C. ; Haddeman, E.F.C.

Applied Surface Science (Jun 15 2004) Vol.231-232, p.29-38

Macroscopic measure of the cohesive length scale: fracture of notched single-crystal silicon

Bailey, N.P. ; Sethna, J.P.

Physical Review B (Condensed Matter and Materials Physics) (15 Nov. 2003) vol.68, no.20, p.205204-1-8

A modified embedded atom method study of the high pressure phases of silicon

Badis, N ; Feraoun, H ; Aourag, H ; Certier, M

MATERIALS CHEMISTRY AND PHYSICS (MAY 26 2003) Vol.80, iss.2, p.405-40

Swadener, J.G., M.I. Baskes, and M. Nastasi, *Molecular dynamics simulation of brittle fracture in silicon*. Physical Review Letters, 2002. 89(8): p. 085503-1.

Relationship between the modified embedded-atom method and Stillinger-Weber potentials in calculating the structure of silicon

Thijsse, B.J.

Physical Review B (Condensed Matter and Materials Physics) (15 May 2002) vol.65, no.19, p.195207/1-5

Baskes, M.I., *Calculation of the behaviour of Si ad-dimers on Si(001)*. Modelling and Simulation in Materials Science and Engineering, 1997. 5(2): p. 149-58.

COMPARISON OF SEMIEMPIRICAL POTENTIAL FUNCTIONS FOR SILICON AND GERMANIUM

COOK, SJ ; CLANCY, P

PHYSICAL REVIEW B (APR 1 1993) Vol.47, iss.13, p.7686-7699

MEAM Parameters (eV, Å):

Reference Structure	$E_c$	a	$\alpha$	A	$\beta_0$	$\beta_1$	$\beta_2$	$\beta_3$	$t_1$	$t_2$	$t_3$	$C_{max}$	$C_{min}$	$r_{cut}$
Diamond Cubic	4.63	5.431	4.87	1.0	4.40	5.5	5.5	5.5	3.13	4.47	-1.80	2.8	2.0	4.3

f-partial electron density was not corrected as in Eq. 8d in 1992 PRB (legend=0 (DYNAMO), augt1=1 (LAMMPS))

Test results using DYNAMO:

				MEAM	
Diamond cubic	-4.629999993	potential	energy		eV/atom
	20.02393325	volume			Å <sup>3</sup>
	10.86199973	x	period	2.352	NN distance (Å)
				5.431	a (Å)
0.001 uniform expansion	-4.629945268	potential	energy	97	Bulk modulus (GPa)
0.001 uniform compression	-4.629944909	potential	energy		
c_44 0.001 shear	-4.62998088	potential	energy	76	Shear modulus (GPa)
(c_11-c_12)/2 0.001 shear	-4.629987591	potential	energy	50	Shear modulus (GPa)
(100) surface 64 atoms	-4.228991933	potential	energy	1740	Surface energy (mJ/m <sup>2</sup> )
	10.862	y	period		Y=Z={100}
(110) surface 72 atoms	-4.323324646	potential	energy	1412	Surface energy (mJ/m <sup>2</sup> )
	11.520890495	y	period		Y={110}
	10.861999726	z	period		Z={100}
(111) surface 144 atoms	-4.47115444	potential	energy	1194	Surface energy (mJ/m <sup>2</sup> )
	11.52089024	y	period		Y={110}
	13.30317783	z	period		Z={112}
0,0,2.217 displacement	-4.323938545	potential	energy	15.37	SF energy (mJ/m <sup>2</sup> )
0,-1.920,1.109 displacement	-4.321851694	potential	energy	15.59	SF energy (mJ/m <sup>2</sup> )
					Vacancy formation energy
Vacancy MD 5 ps 64 atoms	-4.577182244	potential	energy	3.33	energy
	299.9101	average	T		K
	-53.49453	average	P		bar
	20.26985	average	V		Å <sup>3</sup>
					Specific heat
	-4.587896	average	potential	0.156	(meV/atom/K)

					Linear thermal expansion
	10.90628	average	period	13	$10^{-6}$
	350.0637	average	T		K
	-32.25689	average	P		bar
	20.30939	average	V		$\text{\AA}^3$
	-4.580097	average	potential		ev/atom
	10.91337	average	period		$\text{\AA}$
$\beta$ -tin	-4.316107485	potential	energy	0.31	Energy relative to DC
	9.999298406	x	period	2.588	NN distance ( $\text{\AA}$ )
				2.500	a ( $\text{\AA}$ )
	10.84128723	z	period	1.084	c/a
bcc	-4.246460391	potential	energy	0.38	Energy relative to DC
	15.95199483	x	period	2.763	NN distance ( $\text{\AA}$ )
				3.190	a ( $\text{\AA}$ )
Simple cubic	-4.213845041	potential	energy	0.42	Energy relative to DC
	10.61223773	x	period	2.653	NN distance ( $\text{\AA}$ )
				2.653	a ( $\text{\AA}$ )
dimer	-2.473092215	potential	energy	2.16	Energy relative to DC
				2.448	NN distance ( $\text{\AA}$ )
fcc	-4.130246995	potential	energy	0.50	Energy relative to DC
	16.59847758	x	period	2.934	NN distance ( $\text{\AA}$ )
				4.150	a ( $\text{\AA}$ )
hcp	-4.136108481	potential	energy	0.49	
	11.75578552	x	period	2.939	NN distance ( $\text{\AA}$ )
				2.939	a ( $\text{\AA}$ )
	14.30825008	z	period	1.623	c/a