

# michael Baskes

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

123 papers	19,949 citations	45 h-index	127 g-index
127 ext. papers	21,249 ext. citations	3.4 avg, IF	6.68 L-index

#	Paper	IF	Citations
123	Development of 2NN MEAM potential for FeAl and atomistic investigation of surface and interface properties of the inhibition layer in galvanized Fe. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2022</b> , 30, 045001	2	0
122	Molecular dynamics simulations of phospholipid bilayer mechanoporation under different strain states—comparison between GROMACS and LAMMPS. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2021</b> , 29, 055015	2	0
121	Coherent phase decomposition in the PdBi system. <i>Journal of Materials Science</i> , <b>2020</b> , 55, 4864-4882	4.3	5
120	Correlating damage progression to fragmentation at high strain rates using molecular dynamics. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2020</b> , 28, 025009	2	0
119	Modified embedded-atom method potential for high-temperature crystal-melt properties of TiNi alloys and its application to phase field simulation of solidification. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2020</b> , 28, 015006	2	11
118	Molecular dynamics investigation of grain boundaries and surfaces in U <sub>3</sub> Si <sub>2</sub> . <i>Journal of Nuclear Materials</i> , <b>2019</b> , 514, 290-298	3.3	14
117	Molecular dynamics simulations showing 1-palmitoyl-2-oleoyl-phosphatidylcholine (POPC) membrane mechanoporation damage under different strain paths. <i>Journal of Biomolecular Structure and Dynamics</i> , <b>2019</b> , 37, 1346-1359	3.6	6
116	Mechanical instabilities in the modeling of phase transitions of titanium. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2018</b> , 26, 065002	2	13
115	A multi-state modified embedded atom method potential for titanium. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2017</b> , 25, 015010	2	2
114	A modified Embedded-Atom Method interatomic potential for uranium-silicide. <i>Journal of Nuclear Materials</i> , <b>2017</b> , 495, 267-276	3.3	20
113	Commentary on Modified embedded atom method potentials for hcp metals—M I Baskes and R A Johnson (1994) <i>Modelling Simul. Mater. Sci. Eng.</i> The early basis for modeling hcp materials using MEAM. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2017</b> , 25, 071002	2	2
112	A modified embedded-atom method interatomic potential for ionic systems: 2NNMEAM+Qeq. <i>Physical Review B</i> , <b>2016</b> , 93,	3.3	11
111	Hierarchical Bridging Between Ab Initio and Atomistic Level Computations: Calibrating the Modified Embedded Atom Method (MEAM) Potential (Part A). <i>Jom</i> , <b>2015</b> , 67, 143-147	2.1	8
110	Hierarchical Bridging Between Ab Initio and Atomistic Level Computations: Sensitivity and Uncertainty Analysis for the Modified Embedded-Atom Method (MEAM) Potential (Part B). <i>Jom</i> , <b>2015</b> , 67, 148-153	2.1	10
109	Phase-Field Crystal Model for Fe Connected to MEAM Molecular Dynamics Simulations. <i>Jom</i> , <b>2014</b> , 66, 429-436	2.1	29
108	Structural, elastic, and thermal properties of cementite (Fe <sub>3</sub> C) calculated using a modified embedded atom method. <i>Physical Review B</i> , <b>2014</b> , 89,	3.3	66
107	An interatomic potential for saturated hydrocarbons based on the modified embedded-atom method. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 6233-49	3.6	35

106	The embedded atom method ansatz: validation and violation. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2014</b> , 22, 025025	2	2
105	Atomistic Ordering in Body Centered Cubic Uranium-Zirconium Alloy. <i>Materials Research Society Symposia Proceedings</i> , <b>2013</b> , 1514, 27-35		4
104	First principles calculations of the structure and elastic constants of Pu and Uranium. <i>Journal of Nuclear Materials</i> , <b>2013</b> , 433, 143-151	3.3	75
103	Atomistic Calculations of Hydrogen Interactions with Ni3Al Grain Boundaries and Ni/Ni3Al Interfaces <b>2013</b> , 77-90		1
102	Atomistic Investigations of Intrinsic and Extrinsic Point Defects in bcc Uranium <b>2013</b> , 231-247		1
101	Modified embedded atom method potential for Al, Si, Mg, Cu, and Fe alloys. <i>Physical Review B</i> , <b>2012</b> , 85,	3.3	201
100	Atomistic properties of Uranium. <i>Journal of Physics Condensed Matter</i> , <b>2012</b> , 24, 075401	1.8	28
99	The role of interface structure in spallation of a layered nanocomposite. <i>Jom</i> , <b>2011</b> , 63, 74-77	2.1	34
98	Modified embedded atom method study of the mechanical properties of carbon nanotube reinforced nickel composites. <i>Physical Review B</i> , <b>2010</b> , 81,	3.3	26
97	Semi-Empirical Potential Methods for Atomistic Simulations of Metals and Their Construction Procedures. <i>Journal of Engineering Materials and Technology, Transactions of the ASME</i> , <b>2009</b> , 131,	1.8	12
96	A deformation gradient tensor and strain tensors for atomistic simulations. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2008</b> , 16, 015001	2	68
95	Bridge structure for the graphene/Ni(111) system: A first principles study. <i>Physical Review B</i> , <b>2008</b> , 77,	3.3	149
94	Influence of interfacial dislocations on hysteresis loops of ferroelectric films. <i>Journal of Applied Physics</i> , <b>2008</b> , 104, 104110	2.5	38
93	Modified embedded-atom method interatomic potentials for the MgAl alloy system. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	54
92	Self-Irradiation Cascade Simulations in Plutonium Metal: Model Behavior at High Energy. <i>Journal of Computer-Aided Materials Design</i> , <b>2007</b> , 14, 357-365		11
91	Effect of Elastic Anisotropy and Inhomogeneity on Coring Structure Evolution in Pu-Ga Alloys Phase-field modeling. <i>Journal of Computer-Aided Materials Design</i> , <b>2007</b> , 14, 389-402		2
90	Atomistic simulations of Ga atom ordering in Pu 5 at. % Ga alloys. <i>Journal of Computer-Aided Materials Design</i> , <b>2007</b> , 14, 379-388		20
89	Multistate modified embedded atom method. <i>Physical Review B</i> , <b>2007</b> , 75,	3.3	45

88	Atomistic simulations of shock induced microstructural evolution and spallation in single crystal nickel. <i>Journal of Applied Physics</i> , <b>2007</b> , 101, 043504	2.5	56
87	Phase-field modeling of microvoid evolution under elastic-plastic deformation. <i>Applied Physics Letters</i> , <b>2007</b> , 90, 081921	3.4	19
86	Dr Smith goes to Los Alamos <b>2006</b> , 11, 8-25		
85	Kinetics of the Nucleation and Growth of Helium Bubbles in bcc Iron. <i>Materials Research Society Symposia Proceedings</i> , <b>2006</b> , 929, 1		
84	The Role of Metallic Bonding in the Crystallographic Pitting of Magnesium. <i>Journal of the Electrochemical Society</i> , <b>2006</b> , 153, B358	3.9	32
83	Atomistic model of helium bubbles in gallium-stabilized plutonium alloys. <i>Physical Review B</i> , <b>2006</b> , 73,	3.3	64
82	Modified embedded-atom method interatomic potentials for Ti and Zr. <i>Physical Review B</i> , <b>2006</b> , 74,	3.3	145
81	Spallation of single crystal nickel by void nucleation at shock induced grain junctions. <i>Journal of Materials Science</i> , <b>2006</b> , 41, 7838-7842	4.3	12
80	Lattice vibrations in Plutonium: Molecular dynamics calculation. <i>Physical Review B</i> , <b>2005</b> , 72,	3.3	29
79	Monte Carlo simulations of segregation in Pt-Ni catalyst nanoparticles. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 024706	3.9	113
78	Stress-induced platelet formation in silicon: A molecular dynamics study. <i>Physical Review B</i> , <b>2005</b> , 72,	3.3	27
77	Surface structures of cubo-octahedral Pt-Mo catalyst nanoparticles from Monte Carlo simulations. <i>Journal of Physical Chemistry B</i> , <b>2005</b> , 109, 11683-92	3.4	32
76	Compact and dissociated dislocations in aluminum: implications for deformation. <i>Physical Review Letters</i> , <b>2005</b> , 94, 125502	7.4	52
75	MEAM molecular dynamics study of lead free solder for electronic packaging applications. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2005</b> , 13, 1279-1290	2	14
74	Formation mechanism of wide stacking faults in nanocrystalline Al. <i>Applied Physics Letters</i> , <b>2004</b> , 84, 3564-3566	3.5	52
73	Nucleation and growth of deformation twins in nanocrystalline aluminum. <i>Applied Physics Letters</i> , <b>2004</b> , 85, 5049-5051	3.4	174
72	Non-classical nucleation in supercooled nickel. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2004</b> , 12, 1063-1068	2	30
71	Monte Carlo simulations of segregation in Pt-Re catalyst nanoparticles. <i>Journal of Chemical Physics</i> , <b>2004</b> , 121, 5410-22	3.9	53

70	An atomistic study of solid/liquid interfaces in binary systems. <i>Jom</i> , <b>2004</b> , 56, 45-48	2.1	11
69	On the Lennard-Jones EAM potential. <i>Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences</i> , <b>2004</b> , 460, 1649-1672	2.4	14
68	Shock Hugoniot and Melt Curve for a Modified Embedded Atom Method Model of Gallium. <i>AIP Conference Proceedings</i> , <b>2004</b> ,	0	2
67	Accelerated Molecular Dynamics Study of Vacancies in Pu. <i>AIP Conference Proceedings</i> , <b>2003</b> ,	0	7
66	An atomistic study of solid/liquid interfaces and phase equilibrium in binary systems. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , <b>2003</b> , 34, 435-439	2.3	20
65	Using the modified embedded-atom method to calculate the properties of Pu-Ga alloys. <i>Jom</i> , <b>2003</b> , 55, 41-50	2.1	36
64	A multiscale analysis of fixed-end simple shear using molecular dynamics, crystal plasticity, and a macroscopic internal state variable theory. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2003</b> , 11, 265-286	2	54
63	Nucleation of kink pairs on partial dislocations: A new model for solution hardening and softening. <i>Philosophical Magazine</i> , <b>2003</b> , 83, 1329-1346	1.6	35
62	Semiempirical atomic potentials for the fcc metals Cu, Ag, Au, Ni, Pd, Pt, Al, and Pb based on first and second nearest-neighbor modified embedded atom method. <i>Physical Review B</i> , <b>2003</b> , 68,	3.3	368
61	Deformation mechanism in nanocrystalline Al: Partial dislocation slip. <i>Applied Physics Letters</i> , <b>2003</b> , 83, 632-634	3.4	335
60	Predicted transport properties of liquid plutonium. <i>Physical Review B</i> , <b>2003</b> , 67,	3.3	14
59	Torsion/Simple Shear of Single Crystal Copper. <i>Journal of Engineering Materials and Technology, Transactions of the ASME</i> , <b>2002</b> , 124, 322-328	1.8	21
58	Interpretations of Indentation Size Effects. <i>Journal of Applied Mechanics, Transactions ASME</i> , <b>2002</b> , 69, 433-442	2.7	219
57	Calculations of the Structure and Properties of Rapidly Quenched Ni/Zr Alloys. <i>Materials Research Society Symposia Proceedings</i> , <b>2002</b> , 754, 1		
56	Molecular dynamics simulation of brittle fracture in silicon. <i>Physical Review Letters</i> , <b>2002</b> , 89, 085503	7.4	123
55	Atomistic model of gallium. <i>Physical Review B</i> , <b>2002</b> , 66,	3.3	52
54	Stacking-fault energy and yield stress asymmetry in molybdenum disilicide. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , <b>2001</b> , 81, 1079-1097		17
53	Determining the range of forces in empirical many-body potentials using first-principles calculations. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , <b>2001</b> , 81, 991-1008		25

52	Properties of liquid nickel: A critical comparison of EAM and MEAM calculations. <i>Physical Review B</i> , <b>2001</b> , 65,	3.3	78
51	Atomistic model of plutonium. <i>Physical Review B</i> , <b>2000</b> , 62, 15532-15537	3.3	83
50	Morphology and dynamics of 2D Sn-Cu alloys on (100) and (111) Cu surfaces. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>2000</b> , 8, 335-344	2	23
49	Second nearest-neighbor modified embedded-atom-method potential. <i>Physical Review B</i> , <b>2000</b> , 62, 8564-8567	3.9	430
48	Atomistic Finite Deformation Simulations: A Discussion on Length Scale Effects in Relation to Mechanical Stresses. <i>Journal of Engineering Materials and Technology, Transactions of the ASME</i> , <b>1999</b> , 121, 114-119	1.8	93
47	Many-Body Effects in fcc Metals: A Lennard-Jones Embedded-Atom Potential. <i>Physical Review Letters</i> , <b>1999</b> , 83, 2592-2595	7.4	67
46	Strain Tensors at the Atomic Scale. <i>Materials Research Society Symposia Proceedings</i> , <b>1999</b> , 578, 15		10
45	Atomistic Modeling of Void Growth and Coalescence in Ni+H. <i>Materials Research Society Symposia Proceedings</i> , <b>1999</b> , 578, 333		3
44	An atomistic study of the strength of an extended-dislocation barrier. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>1998</b> , 6, 9-18	2	24
43	Calculation of the behaviour of Si ad-dimers on Si(001). <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>1997</b> , 5, 149-158	2	26
42	Roles of dendrite tip undercooling and solid state diffusion in microsegregation of Fe/Nb welds. <i>Science and Technology of Welding and Joining</i> , <b>1997</b> , 2, 160-166	3.7	1
41	Molecular Dynamics Studies of Thin-Films of Sn On Cu. <i>Materials Research Society Symposia Proceedings</i> , <b>1997</b> , 492, 43		7
40	Trapping of hydrogen to lattice defects in nickel. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>1997</b> , 5, 651-652	2	89
39	Properties of a Single Asperity and the Interface between Molecular Dynamics and Continuum Mechanics: A Commentary □ <i>Langmuir</i> , <b>1996</b> , 12, 4535-4536	4	1
38	Trapping of hydrogen to lattice defects in nickel. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>1995</b> , 3, 289-307	2	274
37	Modified embedded atom potentials for HCP metals. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>1994</b> , 2, 147-163	2	304
36	Atomistic calculations of composite interfaces. <i>Modelling and Simulation in Materials Science and Engineering</i> , <b>1994</b> , 2, 505-518	2	135
35	Hydrogen interactions with defects in crystalline solids. <i>Reviews of Modern Physics</i> , <b>1992</b> , 64, 559-617	40.5	417

34	Modified embedded-atom potentials for cubic materials and impurities. <i>Physical Review B</i> , <b>1992</b> , 46, 2723-2742	3.3	1447
33	Solidification modeling and solid-state transformations in high-energy density stainless steel welds. <i>Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science</i> , <b>1991</b> , 22, 915-926		53
32	The Nature of Crack Tip Fields in Atomic Scale Models of Aluminum. <i>Materials Research Society Symposia Proceedings</i> , <b>1990</b> , 193, 283		
31	An atomic model of crack tip deformation in aluminum using an embedded atom potential. <i>Journal of Materials Research</i> , <b>1990</b> , 5, 313-324	2.5	73
30	Semiempirical modified embedded-atom potentials for silicon and germanium. <i>Physical Review B</i> , <b>1989</b> , 40, 6085-6100	3.3	375
29	Atomistic Simulation of Superdislocation Dissociation in Ni3Al <b>1989</b> , 401-410		16
28	Summary Abstract: Surface-limited permeation of deuterium through iron as a function of oxygen coverage. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , <b>1988</b> , 6, 1076-1077	2.9	1
27	Atomic-Scale Simulation in Materials Science. <i>MRS Bulletin</i> , <b>1988</b> , 13, 28-35	3.2	27
26	The Embedded Atom Method: Theory and Application. <i>Materials Research Society Symposia Proceedings</i> , <b>1988</b> , 141, 31		8
25	APPLICATION OF THE EMBEDDED ATOM METHOD TO THE FRACTURE OF INTERFACES. <i>Journal De Physique Colloque</i> , <b>1988</b> , 49, C5-483-C5-495		10
24	Hydrogen isotope retention and release from copper. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , <b>1987</b> , 5, 2319-2324	2.9	23
23	Application of the embedded-atom method to covalent materials: A semiempirical potential for silicon. <i>Physical Review Letters</i> , <b>1987</b> , 59, 2666-2669	7.4	404
22	The retention of deuterium and tritium in POCO AXF-5Q graphite. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , <b>1986</b> , 4, 1189-1192	2.9	81
21	Summary Abstract: The Tara neutral beamline hydrogen pumping system. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , <b>1986</b> , 4, 1759-1761	2.9	3
20	Embedded-atom-method functions for the fcc metals Cu, Ag, Au, Ni, Pd, Pt, and their alloys. <i>Physical Review B</i> , <b>1986</b> , 33, 7983-7991	3.3	3562
19	Trapping of hydrogen and helium at grain boundaries in nickel: An atomistic study. <i>Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science</i> , <b>1985</b> , 16, 1625-1631		45
18	Embedded-atom method: Derivation and application to impurities, surfaces, and other defects in metals. <i>Physical Review B</i> , <b>1984</b> , 29, 6443-6453	3.3	5299
17	A combined atomistic and monte carlo simulation of point defect-dislocation interactions. <i>Physica Status Solidi A</i> , <b>1983</b> , 75, 323-334		4

16	Kinetics of helium self-trapping in metals. <i>Physical Review B</i> , <b>1983</b> , 27, 2210-2217	3.3	34
15	Semiempirical, Quantum Mechanical Calculation of Hydrogen Embrittlement in Metals. <i>Physical Review Letters</i> , <b>1983</b> , 50, 1285-1288	7.4	2147
14	Design of first walls and beam dumps for Tandem Mirror Experiment Upgrade. <i>Journal of Vacuum Science and Technology</i> , <b>1982</b> , 20, 1288-1291		4
13	Self-trapping of helium in metals. <i>Physical Review B</i> , <b>1981</b> , 24, 5616-5624	3.3	309
12	Atomistic computer calculation of the dilatation caused by a $1/2 \langle 111 \rangle \{110\}$ edge dislocation in molybdenum. <i>Physica Status Solidi A</i> , <b>1981</b> , 67, 585-589		2
11	Explicit studies of the quantum theory of light interstitial diffusion. <i>Hyperfine Interactions</i> , <b>1979</b> , 6, 255-259		9
10	Pair potentials for fcc metals. <i>Physical Review B</i> , <b>1979</b> , 20, 3197-3204	3.3	170
9	The Diffusion of Hydrogen and its Isotopes in BCC Metals*. <i>Zeitschrift Fur Physikalische Chemie</i> , <b>1979</b> , 114, 231-238	3.1	31
8	Theoretical Study of the Trapping and Mobility of Hydrogen Near Vacancies, Dislocations, and Cracks in Nickel*. <i>Zeitschrift Fur Physikalische Chemie</i> , <b>1979</b> , 116, 19-29	3.1	24
7	Low-temperature helium release in nickel. <i>Journal of Applied Physics</i> , <b>1979</b> , 50, 6942-6947	2.5	82
6	Small-Polaronic Diffusion of Light Interstitials in bcc Metals. <i>Physical Review Letters</i> , <b>1979</b> , 42, 791-794	7.4	135
5	Volume changes in copper due to point defects. <i>Physical Review B</i> , <b>1978</b> , 17, 422-426	3.3	13
4	A statistical model of low temperature blister formation in helium-implemented metals. <i>Radiation Effects</i> , <b>1978</b> , 37, 93-98		12
3	Atomistics of helium bubble formation in a face-centered-cubic metal. <i>Physical Review B</i> , <b>1976</b> , 13, 2470-2478	3.3	116
2	Magnetic investigation of the effect of small additions of cobalt and manganese on the martensite reversal in an Fe-Ni alloy. <i>Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science</i> , <b>1972</b> , 3, 1407-1411		
1	Magnetic Investigation of the Effect of Small Additions of Co and Mn on the Martensite Reversal in Fe-Ni Alloys. <i>Journal of Applied Physics</i> , <b>1971</b> , 42, 1697-1697	2.5	1