michael Baskes

List of Publications by Year
in descending order

124 papers	22,801 citations	50276 46 h-index	20961 115 g-index
127 all docs	127 docs citations	127 times ranked	9117 citing authors

#	Article	IF	Citations
1	Development of 2NN MEAM potential for Feâ€“Al and atomistic investigation of surface and interface properties of the inhibition layer in galvanized Fe. Modelling and Simulation in Materials Science and Engineering, 2022, 30, 045001.	2.0	2
2	Molecular dynamics simulations of phospholipid bilayer mechanoporation under different strain statesâ€”a comparison between GROMACS and LAMMPS. Modelling and Simulation in Materials Science and Engineering, 2021, 29, 055015.	2.0	4
3	Modified embedded-atom method potential for high-temperature crystal-melt properties of Tiâ€“Ni alloys and its application to phase field simulation of solidification. Modelling and Simulation in Materials Science and Engineering, 2020, 28, 015006.	2.0	24
4	Coherent phase decomposition in the Pdâ€“H system. Journal of Materials Science, 2020, 55, 4864-4882.	3.7	7
5	Correlating damage progression to fragmentation at high strain rates using molecular dynamics. Modelling and Simulation in Materials Science and Engineering, 2020, 28, 025009.	2.0	2
6	Molecular dynamics investigation of grain boundaries and surfaces in U3Si2. Journal of Nuclear Materials, 2019, 514, 290-298.	2.7	21
7	Molecular dynamics simulations showing 1-palmitoyl-2-oleoyl-phosphatidylcholine (POPC) membrane mechanoporation damage under different strain paths. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1346-1359.	3.5	8
8	Mechanical instabilities in the modeling of phase transitions of titanium. Modelling and Simulation in Materials Science and Engineering, 2018, 26, 065002.	2.0	20
9	A multi-state modified embedded atom method potential for titanium. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 015010.	2.0	4
10	A modified Embedded-Atom Method interatomic potential for uranium-silicide. Journal of Nuclear Materials, 2017, 495, 267-276.	2.7	24
11	Commentary on â€˜modified embedded atom method potentials for hcp metalsâ€™ M I Baskes and R A Johnson (1994) Modelling Simul. Mater. Sci. Eng.â€”the early basis for modeling hcp materials using MEAM. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 071002.	2.0	6
12	A modified embedded-atom method interatomic potential for ionic systems:2NNMEAM+Qeq. Physical Review B, 2016, 93, .	3.2	19
13	Scaling Laws in the Ductile Fracture of Metallic Crystals. Journal of Applied Mechanics, Transactions ASME, 2015, 82, .	2.2	0
14	Hierarchical Bridging Between Ab Initio and Atomistic Level Computations: Calibrating the Modified Embedded Atom Method (MEAM) Potential (Part A). Jom, 2015, 67, 143-147.	1.9	13
15	Hierarchical Bridging Between Ab Initio and Atomistic Level Computations: Sensitivity and Uncertainty Analysis for the Modified Embedded-Atom Method (MEAM) Potential (Part B). Jom, 2015, 67, 148-153.	1.9	13
16	Phase-Field Crystal Model for Fe Connected to MEAM Molecular Dynamics Simulations. Jom, 2014, 66, 429-436.	1.9	31
17	Structural, elastic, and thermal properties of cementite (<mml:math) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 107 Td (xmlns:mml= calculated using a modified embedded atom method. Physical Review B, 2014, 89, .	3.2	81
18	An interatomic potential for saturated hydrocarbons based on the modified embedded-atom method. Physical Chemistry Chemical Physics, 2014, 16, 6233-6249.	2.8	41

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19	The embedded atom method ansatz: validation and violation. Modelling and Simulation in Materials Science and Engineering, 2014, 22, 025025.	2.0	3
20	Atomistic Ordering in Body Centered Cubic Uranium-Zirconium Alloy. Materials Research Society Symposia Proceedings, 2013, 1514, 27-35.	0.1	5
21	First principles calculations of the structure and elastic constants of Î±, Î² and Î³ uranium. Journal of Nuclear Materials, 2013, 433, 143-151.	2.7	91
22	Atomistic Investigations of Intrinsic and Extrinsic Point Defects in bcc Uranium. , 2013, , 231-247.		1
23	Modified embedded atom method potential for Al, Si, Mg, Cu, and Fe alloys. Physical Review B, 2012, 85, .	3.2	267
24	Atomistic properties of Î³ uranium. Journal of Physics Condensed Matter, 2012, 24, 075401.	1.8	34
25	The role of interface structure in spallation of a layered nanocomposite. Jom, 2011, 63, 74-77.	1.9	40
26	Modified embedded atom method study of the mechanical properties of carbon nanotube reinforced nickel composites. Physical Review B, 2010, 81, .	3.2	31
27	Semi-Empirical Potential Methods for Atomistic Simulations of Metals and Their Construction Procedures. Journal of Engineering Materials and Technology, Transactions of the ASME, 2009, 131, .	1.4	16
28	A deformation gradient tensor and strain tensors for atomistic simulations. Modelling and Simulation in Materials Science and Engineering, 2008, 16, 015001.	2.0	86
29	Bridge structure for the graphene/Ni(111) system: A first principles study. Physical Review B, 2008, 77, .	3.2	158
30	Influence of interfacial dislocations on hysteresis loops of ferroelectric films. Journal of Applied Physics, 2008, 104, .	2.5	41
31	Multistate modified embedded atom method. Physical Review B, 2007, 75, .	3.2	52
32	Atomistic simulations of shock induced microstructural evolution and spallation in single crystal nickel. Journal of Applied Physics, 2007, 101, 043504.	2.5	66
33	Phase-field modeling of microvoid evolution under elastic-plastic deformation. Applied Physics Letters, 2007, 90, 081921.	3.3	22
34	Modified embedded-atom method interatomic potentials for theMgâˆ'Alalloy system. Physical Review B, 2007, 75, .	3.2	60
35	Self-Irradiation Cascade Simulations in Plutonium Metal: Model Behavior at High Energy. Journal of Computer-Aided Materials Design, 2007, 14, 357-365.	0.7	12
36	Effect of Elastic Anisotropy and Inhomogeneity on Coring Structure Evolution in Pu-Ga Alloys â€“ Phase-field modeling. Journal of Computer-Aided Materials Design, 2007, 14, 389-402.	0.7	2

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37	Atomistic simulations of Ga atom ordering in Pu 5Âat. % Ga alloys. Journal of Computer-Aided Materials Design, 2007, 14, 379-388.	0.7	20
38	Atomistic model of helium bubbles in gallium-stabilized plutonium alloys. Physical Review B, 2006, 73, .	3.2	69
39	Modified embedded-atom method interatomic potentials for Ti and Zr. Physical Review B, 2006, 74, .	3.2	174
40	Spallation of single crystal nickel by void nucleation at shock induced grain junctions. Journal of Materials Science, 2006, 41, 7838-7842.	3.7	14
41	Dr Smith goes to Los Alamos. Resonance, 2006, 11, 8-25.	0.3	0
42	Kinetics of the Nucleation and Growth of Helium Bubbles in bcc Iron. Materials Research Society Symposia Proceedings, 2006, 929, 1.	0.1	1
43	The Role of Metallic Bonding in the Crystallographic Pitting of Magnesium. Journal of the Electrochemical Society, 2006, 153, B358.	2.9	39
44	Surface Structures of Cubo-Octahedral Ptâ^'Mo Catalyst Nanoparticles from Monte Carlo Simulations. Journal of Physical Chemistry B, 2005, 109, 11683-11692.	2.6	35
45	Compact and Dissociated Dislocations in Aluminum: Implications for Deformation. Physical Review Letters, 2005, 94, 125502.	7.8	60
46	MEAM molecular dynamics study of lead free solder for electronic packaging applications. Modelling and Simulation in Materials Science and Engineering, 2005, 13, 1279-1290.	2.0	22
47	Lattice vibrations inÎ´-plutonium: Molecular dynamics calculation. Physical Review B, 2005, 72, .	3.2	30
48	Monte Carlo simulations of segregation in Pt-Ni catalyst nanoparticles. Journal of Chemical Physics, 2005, 122, 024706.	3.0	116
49	Stress-induced platelet formation in silicon: A molecular dynamics study. Physical Review B, 2005, 72, .	3.2	29
50	Formation mechanism of wide stacking faults in nanocrystalline Al. Applied Physics Letters, 2004, 84, 3564-3566.	3.3	183
51	Nucleation and growth of deformation twins in nanocrystalline aluminum. Applied Physics Letters, 2004, 85, 5049-5051.	3.3	202
52	Non-classical nucleation in supercooled nickel. Modelling and Simulation in Materials Science and Engineering, 2004, 12, 1063-1068.	2.0	33
53	Monte Carlo simulations of segregation in Pt-Re catalyst nanoparticles. Journal of Chemical Physics, 2004, 121, 5410-5422.	3.0	62
54	An atomistic study of solid/liquid interfaces in binary systems. Jom, 2004, 56, 45-48.	1.9	11

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55	On the Lennardâ€“Jones EAM potential. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 2004, 460, 1649-1672.	2.1	14
56	Shock Hugoniot and Melt Curve for a Modified Embedded Atom Method Model of Gallium. AIP Conference Proceedings, 2004, , .	0.4	3
57	An atomistic study of solid/liquid interfaces and phase equilibrium in binary systems. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2003, 34, 435-439.	2.2	21
58	Using the modified embedded-atom method to calculate the properties of Pu-Ga alloys. Jom, 2003, 55, 41-50.	1.9	38
59	A multiscale analysis of fixed-end simple shear using molecular dynamics, crystal plasticity, and a macroscopic internal state variable theory. Modelling and Simulation in Materials Science and Engineering, 2003, 11, 265-286.	2.0	61
60	Nucleation of kink pairs on partial dislocations: A new model for solution hardening and softening. Philosophical Magazine, 2003, 83, 1329-1346.	1.6	37
61	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. Physical Review B, 2003, 68, .	3.2	446
62	Deformation mechanism in nanocrystalline Al: Partial dislocation slip. Applied Physics Letters, 2003, 83, 632-634.	3.3	382
63	Predicted transport properties of liquid plutonium. Physical Review B, 2003, 67, .	3.2	14
64	Phase Stability of Pu and Pu-Ga Alloys from Atomistic Calculations. AIP Conference Proceedings, 2003, , .	0.4	0
65	Accelerated Molecular Dynamics Study of Vacancies in Pu. AIP Conference Proceedings, 2003, , .	0.4	7
66	Torsion/Simple Shear of Single Crystal Copper. Journal of Engineering Materials and Technology, Transactions of the ASME, 2002, 124, 322-328.	1.4	25
67	Interpretations of Indentation Size Effects. Journal of Applied Mechanics, Transactions ASME, 2002, 69, 433-442.	2.2	243
68	Calculations of the Structure and Properties of Rapidly Quenched Ni/Zr Alloys. Materials Research Society Symposia Proceedings, 2002, 754, 1.	0.1	0
69	Molecular Dynamics Simulation of Brittle Fracture in Silicon. Physical Review Letters, 2002, 89, 085503.	7.8	136
70	Atomistic model of gallium. Physical Review B, 2002, 66, .	3.2	56
71	Properties of liquid nickel: A critical comparison of EAM and MEAM calculations. Physical Review B, 2001, 65, .	3.2	88
72	Stacking-fault energy and yield stress asymmetry in molybdenum disilicide. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 2001, 81, 1079-1097.	0.6	17

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73	Determining the range of forces in empirical many-body potentials using first-principles calculations. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 2001, 81, 991-1008.	0.6	26
74	Atomistic model of plutonium. Physical Review B, 2000, 62, 15532-15537.	3.2	87
75	Morphology and dynamics of 2D Sn-Cu alloys on (100) and (111) Cu surfaces. Modelling and Simulation in Materials Science and Engineering, 2000, 8, 335-344.	2.0	34
76	Second nearest-neighbor modified embedded-atom-method potential. Physical Review B, 2000, 62, 8564-8567.	3.2	533
77	Atomistic Finite Deformation Simulations: A Discussion on Length Scale Effects in Relation to Mechanical Stresses. Journal of Engineering Materials and Technology, Transactions of the ASME, 1999, 121, 114-119.	1.4	104
78	Many-Body Effects in fcc Metals: A Lennard-Jones Embedded-Atom Potential. Physical Review Letters, 1999, 83, 2592-2595.	7.8	77
79	Strain Tensors at the Atomic Scale. Materials Research Society Symposia Proceedings, 1999, 578, 15.	0.1	14
80	Atomistic Modeling of Void Growth and Coalescence in Ni+H. Materials Research Society Symposia Proceedings, 1999, 578, 333.	0.1	3
81	An atomistic study of the strength of an extended-dislocation barrier. Modelling and Simulation in Materials Science and Engineering, 1998, 6, 9-18.	2.0	28
82	Calculation of the behaviour of Si ad-dimers on Si(001). Modelling and Simulation in Materials Science and Engineering, 1997, 5, 149-158.	2.0	26
83	Roles of dendrite tip undercooling and solid state diffusion in microsegregation of Feâ€“Nb welds. Science and Technology of Welding and Joining, 1997, 2, 160-166.	3.1	2
84	Molecular Dynamics Studies of Thin-Films of Sn On Cu. Materials Research Society Symposia Proceedings, 1997, 492, 43.	0.1	8
85	Trapping of hydrogen to lattice defects in nickel. Modelling and Simulation in Materials Science and Engineering, 1997, 5, 651-652.	2.0	102
86	Properties of a Single Asperity and the Interface between Molecular Dynamics and Continuum Mechanics:Â A Commentaryâ€. Langmuir, 1996, 12, 4535-4536.	3.5	1
87	Trapping of hydrogen to lattice defects in nickel. Modelling and Simulation in Materials Science and Engineering, 1995, 3, 289-307.	2.0	336
88	Modified embedded atom potentials for HCP metals. Modelling and Simulation in Materials Science and Engineering, 1994, 2, 147-163.	2.0	343
89	Atomistic calculations of composite interfaces. Modelling and Simulation in Materials Science and Engineering, 1994, 2, 505-518.	2.0	159
90	Hydrogen interactions with defects in crystalline solids. Reviews of Modern Physics, 1992, 64, 559-617.	45.6	471

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91	Modified embedded-atom potentials for cubic materials and impurities. Physical Review B, 1992, 46, 2727-2742.	3.2	1,703
92	Solidification modeling and solid-state transformations in high-energy density stainless steel welds. Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science, 1991, 22, 915-926.	1.4	70
93	The Nature of Crack Tip Fields in Atomic Scale Models of Aluminum. Materials Research Society Symposia Proceedings, 1990, 193, 283.	0.1	0
94	An atomic model of crack tip deformation in aluminum using an embedded atom potential. Journal of Materials Research, 1990, 5, 313-324.	2.6	81
95	Semiempirical modified embedded-atom potentials for silicon and germanium. Physical Review B, 1989, 40, 6085-6100.	3.2	421
96	Summary Abstract: Surfaceâ€limited permeation of deuterium through iron as a function of oxygen coverage. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1988, 6, 1076-1077.	2.1	2
97	Atomic-Scale Simulation in Materials Science. MRS Bulletin, 1988, 13, 28-35.	3.5	28
98	The Embedded Atom Method: Theory and Application. Materials Research Society Symposia Proceedings, 1988, 141, 31.	0.1	8
99	APPLICATION OF THE EMBEDDED ATOM METHOD TO THE FRACTURE OF INTERFACES. Journal De Physique Colloque, 1988, 49, C5-483-C5-495.	0.2	10
100	Hydrogen isotope retention and release from copper. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1987, 5, 2319-2324.	2.1	24
101	Application of the Embedded-Atom Method to Covalent Materials: A Semiempirical Potential for Silicon. Physical Review Letters, 1987, 59, 2666-2669.	7.8	459
102	Embedded-atom-method functions for the fcc metals Cu, Ag, Au, Ni, Pd, Pt, and their alloys. Physical Review B, 1986, 33, 7983-7991.	3.2	4,002
103	The retention of deuterium and tritium in POCO AXFâ€5Q graphite. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1986, 4, 1189-1192.	2.1	88
104	Summary Abstract: The Tara neutral beamline hydrogen pumping system. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1986, 4, 1759-1761.	2.1	3
105	Trapping of hydrogen and helium at grain boundaries in nickel: An atomistic study. Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science, 1985, 16, 1625-1631.	1.4	48
106	Embedded-atom method: Derivation and application to impurities, surfaces, and other defects in metals. Physical Review B, 1984, 29, 6443-6453.	3.2	6,059
107	A combined atomistic and monte carlo simulation of point defectâ€“dislocation interactions. Physica Status Solidi A, 1983, 75, 323-334.	1.7	5
108	Kinetics of helium self-trapping in metals. Physical Review B, 1983, 27, 2210-2217.	3.2	34

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109	Semiempirical, Quantum Mechanical Calculation of Hydrogen Embrittlement in Metals. Physical Review Letters, 1983, 50, 1285-1288.	7.8	2,414
110	Design of first walls and beam dumps for Tandem Mirror Experiment Upgrade. Journal of Vacuum Science and Technology, 1982, 20, 1288-1291.	1.9	4
111	Self-trapping of helium in metals. Physical Review B, 1981, 24, 5616-5624.	3.2	340
112	Atomistic computer calculation of the dilatation caused by a 1/2 ã€ˆ111ã€‰ {110} edge dislocation in molybdenum. Physica Status Solidi A, 1981, 67, 585-589.	1.7	4
113	Lowâ€temperature helium release in nickel. Journal of Applied Physics, 1979, 50, 6942-6947.	2.5	86
114	Small-Polaronic Diffusion of Light Interstitials in bcc Metals. Physical Review Letters, 1979, 42, 791-794.	7.8	147
115	Explicit studies of the quantum theory of light interstitial diffusion. Hyperfine Interactions, 1979, 6, 255-259.	0.5	10
116	Pair potentials for fcc metals. Physical Review B, 1979, 20, 3197-3204.	3.2	171
117	The Diffusion of Hydrogen and its Isotopes in BCC Metals*. Zeitschrift Fur Physikalische Chemie, 1979, 114, 231-238.	2.8	33
118	Theoretical Study of the Trapping and Mobility of Hydrogen Near Vacancies, Dislocations, and Cracks in Nickel*. Zeitschrift Fur Physikalische Chemie, 1979, 116, 19-29.	2.8	27
119	Volume changes in copper due to point defects. Physical Review B, 1978, 17, 422-426.	3.2	14
120	A statistical model of low temperature blister formation in helium-implanted metals. Radiation Effects, 1978, 37, 93-98.	0.4	13
121	Atomistics of helium bubble formation in a face-centered-cubic metal. Physical Review B, 1976, 13, 2470-2478.	3.2	119
122	Magnetic investigation of the effect of small additions of cobalt and manganese on the martensite reversal in an Fe-Ni alloy. Metallurgical and Materials Transactions A - Physical Metallurgy and Materials Science, 1972, 3, 1407-1411.	1.4	0
123	Magnetic Investigation of the Effect of Small Additions of Co and Mn on the Martensite Reversal in Feâ€“Ni Alloys. Journal of Applied Physics, 1971, 42, 1697-1697.	2.5	1
124	Kinetics of the Migration and Clustering of Extrinsic Gas in bcc Metals. , 0, , 177-177-13.		0