S M Foiles

List of Publications by Year
in descending order

129 papers	13,515 citations	38720 50 h-index	20943 115 g-index
132 all docs	132 docs citations	132 times ranked	6556 citing authors

#	Article	IF	Citations
1	Embedded-atom-method functions for the fcc metals Cu, Ag, Au, Ni, Pd, Pt, and their alloys. Physical Review B, 1986, 33, 7983-7991.	1.1	4,002
2	The embedded-atom method: a review of theory and applications. Materials Science and Engineering Reports, 1993, 9, 251-310.	5.8	1,343
3	Survey of computed grain boundary properties in face-centered cubic metals: I. Grain boundary energy. Acta Materialia, 2009, 57, 3694-3703.	3.8	527
4	Calculation of the surface segregation of Ni-Cu alloys with the use of the embedded-atom method. Physical Review B, 1985, 32, 7685-7693.	1.1	500
5	Surface Step Effects on Nanoindentation. Physical Review Letters, 2001, 87, 165507.	2.9	429
6	Application of the embedded-atom method to liquid transition metals. Physical Review B, 1985, 32, 3409-3415.	1.1	398
7	Application of the embedded atom method to Ni₃Al. Journal of Materials Research, 1987, 2, 5-15.	1.2	354
8	Self-diffusion and impurity diffusion of fee metals using the five-frequency model and the Embedded Atom Method. Journal of Materials Research, 1989, 4, 102-112.	1.2	318
9	Survey of computed grain boundary properties in face-centered cubic metalsâ€”II: Grain boundary mobility. Acta Materialia, 2009, 57, 3704-3713.	3.8	310
10	Solutions of the reference-hypernetted-chain equation with minimized free energy. Physical Review A, 1983, 28, 2374-2379.	1.0	304
11	Computing the mobility of grain boundaries. Nature Materials, 2006, 5, 124-127.	13.3	222
12	How Grain Growth Stops: A Mechanism for Grain-Growth Stagnation in Pure Materials. Science, 2010, 328, 1138-1141.	6.0	211
13	Thermodynamic properties of fcc transition metals as calculated with the embedded-atom method. Physical Review B, 1989, 40, 5909-5915.	1.1	208
14	Evaluation of harmonic methods for calculating the free energy of defects in solids. Physical Review B, 1994, 49, 14930-14938.	1.1	173
15	Ordered surface phases of Au on Cu. Surface Science, 1987, 191, 329-338.	0.8	163
16	Order-Disorder Transition of Au and Pt (110) Surfaces: The Significance of Relaxations and Vibrations. Physical Review Letters, 1987, 59, 2756-2759.	2.9	126
17	Dislocation Mechanism for Island Diffusion on fcc (111) Surfaces. Physical Review Letters, 1995, 74, 2760-2763.	2.9	116
18	Comparing grain boundary energies in face-centered cubic metals: Al, Au, Cu and Ni. Scripta Materialia, 2010, 63, 905-908.	2.6	116

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19	Development of an embedded-atom potential for a bcc metal: Vanadium. Physical Review B, 1990, 41, 3316-3328.	1.1	112
20	Temperature dependence of grain boundary free energy and elastic constants. Scripta Materialia, 2010, 62, 231-234.	2.6	110
21	Comparing calculated and measured grain boundary energies in nickel. Acta Materialia, 2010, 58, 5063-5069.	3.8	101
22	Roadmap on multiscale materials modeling. Modelling and Simulation in Materials Science and Engineering, 2020, 28, 043001.	0.8	100
23	Phenomenology of shear-coupled grain boundary motion in symmetric tilt and general grain boundaries. Acta Materialia, 2013, 61, 1048-1060.	3.8	99
24	Theory of subsurface occupation, ordered structures, and order-disorder transitions for hydrogen on Pd(111). Physical Review B, 1987, 35, 2128-2136.	1.1	98
25	A crossover integral equation for the structure of simple liquids. Journal of Chemical Physics, 1984, 80, 4441-4447.	1.2	95
26	Embedded-atom-method study of structural, thermodynamic, and atomic-transport properties of liquid Ni-Al alloys. Physical Review B, 1999, 59, 14271-14281.	1.1	90
27	Peierls potential of screw dislocations in bcc transition metals: Predictions from density functional theory. Physical Review B, 2013, 87, .	1.1	89
28	Interatomic interactions for Mo and W based on the low-order moments of the density of states. Physical Review B, 1993, 48, 4287-4298.	1.1	87
29	Thin Film Compressive Stresses due to Adatom Insertion into Grain Boundaries. Physical Review Letters, 2007, 99, 036102.	2.9	82
30	An atomic model of crack tip deformation in aluminum using an embedded atom potential. Journal of Materials Research, 1990, 5, 313-324.	1.2	81
31	Structure of platinum adatom clusters on Pt(100): Experimental observations and embedded-atom-method calculations. Physical Review B, 1989, 40, 10639-10642.	1.1	75
32	Atomistic Underpinnings for Orientation Selection in Alloy Dendritic Growth. Physical Review Letters, 2007, 98, 125701.	2.9	75
33	Grain boundary segregation in immiscible nanocrystalline alloys. Acta Materialia, 2017, 126, 528-539.	3.8	73
34	Quantifying the influence of twin boundaries on the deformation of nanocrystalline copper using atomistic simulations. International Journal of Plasticity, 2015, 65, 191-205.	4.1	71
35	Grain boundary interface roughening transition and its effect on grain boundary mobility for non-faceting boundaries. Scripta Materialia, 2007, 57, 1161-1164.	2.6	70
36	Trends in Grain Boundary Mobility: Survey of Motion Mechanisms. Jom, 2014, 66, 114-120.	0.9	68

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37	Validating computed grain boundary energies in fcc metals using the grain boundary character distribution. Acta Materialia, 2011, 59, 5250-5256.	3.8	67
38	Calculation of the thermal expansion of metals using the embedded-atom method. Physical Review B, 1988, 38, 12643-12644.	1.1	66
39	Embedded-atom-method effective-pair-interaction study of the structural and thermodynamic properties of Cu-Ni, Cu-Ag, and Au-Ni solid solutions. Physical Review B, 1996, 53, 2389-2404.	1.1	66
40	Grain boundary phase transformations in PtAu and relevance to thermal stabilization of bulk nanocrystalline metals. Journal of Materials Science, 2018, 53, 2911-2927.	1.7	65
41	Calculation of grain-boundary segregation in Ni-Cu alloys. Physical Review B, 1989, 40, 11502-11506.	1.1	64
42	Near-Surface Buckling in Strained Metal Overlayer Systems. Physical Review Letters, 1995, 75, 4242-4245.	2.9	64
43	Variational theory of phase separation in binary liquid mixtures. Journal of Chemical Physics, 1981, 75, 3594-3598.	1.2	62
44	Elastic properties of grain boundaries in copper and their relationship to bulk elastic constants. Physical Review B, 1989, 40, 9479-9484.	1.1	62
45	Dislocation-Pairing Transitions in Hot Grain Boundaries. Physical Review Letters, 2011, 106, 046101.	2.9	60
46	Atomic structure of the (310) twin in niobium: Experimental determination and comparison with theoretical predictions. Physical Review Letters, 1993, 70, 449-452.	2.9	59
47	Misfit Dislocation Structure for Close-Packed Metal-Metal Interfaces. Physical Review Letters, 1995, 75, 882-885.	2.9	59
48	Stabilization of nanocrystalline alloys via grain boundary segregation: A diffuse interface model. Acta Materialia, 2015, 101, 159-171.	3.8	59
49	Atomistic studies of segregation and diffusion in Al-Cu grain boundaries. Applied Physics Letters, 1998, 72, 1578-1580.	1.5	58
50	Vibrational spectra in ordered and disorderedNi3Al. Physical Review B, 1997, 56, R5705-R5708.	1.1	52
51	Molecular dynamics simulations of rate-dependent grain growth during the surface indentation of nanocrystalline nickel. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2013, 571, 207-214.	2.6	51
52	Embedded-Atom and Related Methods for Modeling Metallic Systems. MRS Bulletin, 1996, 21, 24-28.	1.7	48
53	Simulation of surface segregation free energies. Physical Review B, 1994, 50, 12004-12014.	1.1	45
54	Absence of power-law behavior of the hypernetted chain equation. Physical Review A, 1981, 24, 424-428.	1.0	44

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55	Atomistic simulations of crystal-melt interfaces in a model binary alloy: Interfacial free energies, adsorption coefficients, and excess entropy. Physical Review B, 2009, 79, .	1.1	44
56	Kinetic isotope effects for hydrogen diffusion in bulk nickel and on nickel surfaces. Journal of Chemical Physics, 1990, 92, 775-791.	1.2	38
57	High-resolution transmission electron microscopy studies of dislocation cores in metals and intermetallic compounds. Ultramicroscopy, 1994, 56, 79-93.	0.8	38
58	Summary Abstract: A theoretical study of the orderâ€“disorder transitions for hydrogen on Pd(111). Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1985, 3, 1565-1566.	0.9	37
59	Multi-scale modeling of polycrystal plasticity: a workshop report. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 1998, 251, 1-22.	2.6	37
60	Accommodation of the lattice mismatch in a Ag/Ni heterophase boundary. Physical Review B, 1991, 43, 13833-13837.	1.1	36
61	Equilibrium adsorption at crystal-melt interfaces in Lennard-Jones alloys. Journal of Chemical Physics, 2006, 124, 164708.	1.2	36
62	The role of grain boundary character in solute segregation and thermal stability of nanocrystalline Ptâ€“Au. Nanoscale, 2021, 13, 3552-3563.	2.8	35
63	Atomistic simulations of stress and microstructure evolution during polycrystalline Ni film growth. Physical Review B, 2009, 79, .	1.1	32
64	Energy conserving orientational force for determining grain boundary mobility. Modelling and Simulation in Materials Science and Engineering, 2015, 23, 025007.	0.8	32
65	Long-range correlations in adsorbed layers. Physical Review B, 1982, 25, 1366-1369.	1.1	31
66	The role of the interface stiffness tensor on grain boundary dynamics. Acta Materialia, 2018, 158, 440-453.	3.8	31
67	Structure factor and direct correlation function of a fluid from finite range simulation data. Journal of Chemical Physics, 1984, 81, 6140-6145.	1.2	30
68	New nanoscale toughening mechanisms mitigate embrittlement in binary nanocrystalline alloys. Nanoscale, 2018, 10, 21231-21243.	2.8	27
69	Unraveling irradiation induced grain growth with in situ transmission electron microscopy and coordinated modeling. Applied Physics Letters, 2015, 107, .	1.5	26
70	Exploration of the mechanisms of temperature-dependent grain boundary mobility: search for the common origin of ultrafast grain boundary motion. Journal of Materials Science, 2016, 51, 6607-6623.	1.7	25
71	Contributions of the embedded-atom method to materials science and engineering. MRS Bulletin, 2012, 37, 485-491.	1.7	24
72	Properties of the liquid-vapor interface of fcc metals calculated using the embedded atom method. Journal of Materials Research, 1991, 6, 298-302.	1.2	23

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73	Detailed characterization of defect production in molecular dynamics simulations of cascades in Si. Nuclear Instruments & Methods in Physics Research B, 2007, 255, 101-104.	0.6	23
74	Quantitative HREM observation of the Î£11(113)/[1Â¯10] grainâ€boundary structure in aluminium and comparison with atomistic simulation. Journal of Microscopy, 1998, 190, 131-143.	0.8	22
75	Copper Segregation to the Â5 (310)/[001] Symmetric Tilt Grain Boundary in Aluminum. Journal of Materials Science, 2004, 12, 165-174.	1.2	19
76	Calculation of the Defect and Interface Properties of Ni3Al. Materials Research Society Symposia Proceedings, 1986, 81, 51.	0.1	18
77	High-resolution electron microscopy investigation of the (710) twin in Nb. Ultramicroscopy, 1993, 51, 247-263.	0.8	18
78	Strain-rate dependence of ramp-wave evolution and strength in tantalum. Physical Review B, 2016, 94, .	1.1	18
79	A diffuse interface model of grain boundary faceting. Journal of Applied Physics, 2016, 119, 235306.	1.1	17
80	Hydrogen segregation to inclined twin grain boundaries in nickel. Philosophical Magazine, 2016, 96, 2808-2828.	0.7	17
81	Summary Abstract: Calculations of the energetics and structure of Pt(110) using the embedded atom method. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1986, 4, 1412-1413.	0.9	14
82	The effect of synthetic driving force on the atomic mechanisms associated with grain boundary motion below the interface roughening temperature. Computational Materials Science, 2014, 86, 38-42.	1.4	14
83	Misoriented grain boundaries vicinal to the twin in nickel Part I: thermodynamics & temperature-dependent structure. Philosophical Magazine, 2016, 96, 1285-1304.	0.7	14
84	Revealing inconsistencies in X-ray width methods for nanomaterials. Nanoscale, 2019, 11, 22456-22466.	2.8	14
85	Perturbation theory of liquid-metal surfaces: The importance of the self-energy. Physical Review A, 1984, 30, 3136-3146.	1.0	13
86	Summary Abstract: Calculation of the surface segregation of Pdâ€“Cu, Pdâ€“Ag, and Pdâ€“Au alloys. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1987, 5, 889-891.	0.9	13
87	Simulation of Equilibrium Segregation in Alloys Using the Embedded Atom Method. Materials Research Society Symposia Proceedings, 1985, 63, 61.	0.1	10
88	Solute-Atom Segregation at Internal Interfaces. MRS Bulletin, 1990, 15, 51-57.	1.7	10
89	Calculation of the Surface Segregation of Pd-Cu, Pd-Ag, and Pd-Au Alloys. Materials Research Society Symposia Proceedings, 1986, 83, 175.	0.1	9
90	Electronic structure of grain boundaries. Physical Review B, 1989, 40, 9993-9996.	1.1	9

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91	Application of the Embedded Atom Method to Interfaces in Metals. Materials Science Forum, 1989, 46, 187-198.	0.3	9
92	Mo(001) seventh-order reconstruction: Ground-state structure and reconstruction mechanism. Physical Review B, 1993, 48, 11287-11290.	1.1	9
93	Misoriented grain boundaries vicinal to the (111)âŸ¨11Â¯0âŸ© twin in Nickel part II: thermodynamics of hydrogen segregation. Philosophical Magazine, 2016, 96, 1463-1484.	0.7	9
94	The Embedded Atom Method: Theory and Application. Materials Research Society Symposia Proceedings, 1988, 141, 31.	0.1	8
95	Hrtem Observation and EAM Calculation of Dislocation Cores in Nial. Materials Research Society Symposia Proceedings, 1992, 288, 257.	0.1	8
96	First-principles survey of the structure, formation energies, and transition levels of As-interstitial defects in InGaAs. Physical Review B, 2015, 92, .	1.1	7
97	Multi-objective optimization of interatomic potentials with application to MgO. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 074007.	0.8	7
98	Atomistic Studies of Interfacial Structure and Properties. Materials Research Society Symposia Proceedings, 1988, 122, 343.	0.1	6
99	Comment on â€œToward realistic molecular dynamics simulations of grain boundary mobilityâ€•by Zhou and Mohles. Scripta Materialia, 2012, 66, 714-716.	2.6	6
100	Fatigue-driven acceleration of abnormal grain growth in nanocrystalline wires. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 025008.	0.8	6
101	Determination of recombination radius in Si for binary collision approximation codes. Nuclear Instruments & Methods in Physics Research B, 2016, 371, 111-115.	0.6	5
102	Summary Abstract: Computer simulation of the surface segregation in binary alloys using the embedded atom method. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1986, 4, 761-762.	0.9	4
103	An Atomistic Study of the Equilibrium Segregation of Hydrogen to Tilt Boundaries in Nickel. Materials Research Society Symposia Proceedings, 1991, 229, 179.	0.1	4
104	Interatomic Interactions for BCC Metals Based on the Low Order Moments of the Density of States. Materials Research Society Symposia Proceedings, 1992, 278, 339.	0.1	4
105	Atomistic Simulations of Surfaces and Interfaces. , 1992, , 89-122.		4
106	The rigid-body displacement observed at the âˆ‘ = 5, (310)-[001] symmetric tilt grain boundary in central transition bcc metals. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 2002, 82, 1573-1594.	0.7	3
107	Molecular Dynamics Simulation of Grain Growth in Nanocrystalline Ni. Materials Science Forum, 0, 715-716, 599-604.	0.3	3
108	Theoretical Studies of Helium in Metals. NATO ASI Series Series B: Physics, 1991, , 3-16.	0.2	3

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109	Grain Boundary Dislocation Structure and Motion in an Aluminum Î£=3 [011] Bicrystal. Materials Research Society Symposia Proceedings, 1996, 466, 125.	0.1	2
110	Effect of Surface Steps on Dislocation Structure During Nanoindentation. Materials Research Society Symposia Proceedings, 2000, 649, 881.	0.1	2
111	Self-Diffusion and Impurity Diffusion of FCC Metals Using the Embedded Atom Method. , 1989, , 419-424.		2
112	Elastic Properties of Grain Boundaries in Copper. Materials Research Society Symposia Proceedings, 1989, 153, 369.	0.1	1
113	Atomistic Structure and Composition of a Ag/Ni Interphase Boundary. Materials Research Society Symposia Proceedings, 1990, 187, 287.	0.1	1
114	Tilt Boundaries In BCC Metals:Comparison of Results Using Different Interatomic Interactions. Materials Research Society Symposia Proceedings, 1990, 209, 65.	0.1	1
115	An Atomistic Study of Hydrogen Effects on the Fracture of Tilt Boundaries in Nickel.. Materials Research Society Symposia Proceedings, 1991, 238, 381.	0.1	1
116	Temperature-Dependent Structure of a<101> Superdislocations in Ni3Al. Materials Research Society Symposia Proceedings, 1994, 364, 731.	0.1	1
117	Grain Growth Stagnation Caused by the Grain Boundary Roughening Transition. Materials Science Forum, 2012, 715-716, 415-415.	0.3	1
118	Simulation and modeling of the electronic structure of GaAs damage clusters. Journal of Applied Physics, 2013, 113, 093706.	1.1	1
119	Interface-Driven Phenomena in Solids: Thermodynamics, Kinetics and Chemistry. Jom, 2016, 68, 1594-1595.	0.9	1
120	Preface for focus issue on uncertainty quantification in materials modeling. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 080301.	0.8	1
121	Calculations of Structural Phases of Transition Metal Surfaces Using the Embedded Atom Method. Springer Series in Surface Sciences, 1988, , 125-131.	0.3	1
122	Calculation of the Structure of Au Grain Boundaries Using the Embedded Atom Method. Materials Research Society Symposia Proceedings, 1988, 138, 471.	0.1	0
123	Calculation of the Atomic Structure of Grain Boundaries in Metals and Alloys. Materials Research Society Symposia Proceedings, 1990, 193, 247.	0.1	0
124	The Structure and Properties of Boundaries in Bicrystals of Boron-Doped Ni3(Al,l at% Ta). Materials Research Society Symposia Proceedings, 1990, 213, 423.	0.1	0
125	Hrem Investigation of the Structure of the Î£5(210)/[001] Symmetric Tilt Grain Boundaries in Nb.. Materials Research Society Symposia Proceedings, 1991, 229, 191.	0.1	0
126	Electronic Effects on Grain Boundary Structure in Bcc Metals. Materials Research Society Symposia Proceedings, 1999, 589, 347.	0.1	0

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127	Substitutional Impurity Segregation to the Î£ 5 (310)/[001] Stgb in Cu Doped Aluminum and Ag Doped Copper. Microscopy and Microanalysis, 2001, 7, 246-247.	0.2	0
128	Grain Boundary Structure and Its Effect on Plasticity. Microscopy and Microanalysis, 2004, 10, 12-13.	0.2	0
129	Survey of Grain Boundary Energies in Four Elemental Metals. Materials Science Forum, 0, 715-716, 179-179.	0.3	0