S M Foiles

List of Publications by Year in Descending Order

129 papers	11,874 citations	48 h-index	108 g-index
132 ext. papers	12,576 ext. citations	4.4 avg, IF	6.3 L-index

#	Paper	IF	Citations
129	The role of grain boundary character in solute segregation and thermal stability of nanocrystalline Pt-Au. *Nanoscale*, **2021**, 13, 3552-3563	7.7	15
128	Roadmap on multiscale materials modeling. *Modelling and Simulation in Materials Science and Engineering*, **2020**, 28, 043001	2	40
127	Multi-objective optimization of interatomic potentials with application to MgO. *Modelling and Simulation in Materials Science and Engineering*, **2019**, 27, 074007	2	5
126	Preface for focus issue on uncertainty quantification in materials modeling. *Modelling and Simulation in Materials Science and Engineering*, **2019**, 27, 080301	2	1
125	Revealing inconsistencies in X-ray width methods for nanomaterials. *Nanoscale*, **2019**, 11, 22456-22466	7.7	7
124	Fatigue-driven acceleration of abnormal grain growth in nanocrystalline wires. *Modelling and Simulation in Materials Science and Engineering*, **2019**, 27, 025008	2	5
123	The role of the interface stiffness tensor on grain boundary dynamics. *Acta Materialia*, **2018**, 158, 440-453	8.4	18
122	Grain boundary phase transformations in PtAu and relevance to thermal stabilization of bulk nanocrystalline metals. *Journal of Materials Science*, **2018**, 53, 2911-2927	4.3	43
121	New nanoscale toughening mechanisms mitigate embrittlement in binary nanocrystalline alloys. *Nanoscale*, **2018**, 10, 21231-21243	7.7	15
120	Grain boundary segregation in immiscible nanocrystalline alloys. *Acta Materialia*, **2017**, 126, 528-539	8.4	55
119	Strain-rate dependence of ramp-wave evolution and strength in tantalum. *Physical Review B*, **2016**, 94,	3.3	14
118	Interface-Driven Phenomena in Solids: Thermodynamics, Kinetics and Chemistry. *Jom*, **2016**, 68, 1594-1595	2.1	1
117	Determination of recombination radius in Si for binary collision approximation codes. *Nuclear Instruments & Methods in Physics Research B*, **2016**, 371, 111-115	1.2	5
116	Misoriented grain boundaries vicinal to the twin in nickel Part I: thermodynamics & temperature-dependent structure. *Philosophical Magazine*, **2016**, 96, 1285-1304	1.6	13
115	Misoriented grain boundaries vicinal to the (111)<11$\bar{2}$0> twin in Nickel part II: thermodynamics of hydrogen segregation. *Philosophical Magazine*, **2016**, 96, 1463-1484	1.6	7
114	A diffuse interface model of grain boundary faceting. *Journal of Applied Physics*, **2016**, 119, 235306	2.5	12
113	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	4.3	20

112	Hydrogen segregation to inclined twin grain boundaries in nickel. *Philosophical Magazine*, **2016**, 96, 2808-2828	1.8	12
111	Energy conserving orientational force for determining grain boundary mobility. *Modelling and Simulation in Materials Science and Engineering*, **2015**, 23, 025007	2	26
110	Stabilization of nanocrystalline alloys via grain boundary segregation: A diffuse interface model. *Acta Materialia*, **2015**, 101, 159-171	8.4	44
109	Quantifying the influence of twin boundaries on the deformation of nanocrystalline copper using atomistic simulations. *International Journal of Plasticity*, **2015**, 65, 191-205	7.6	58
108	First-principles survey of the structure, formation energies, and transition levels of As-interstitial defects in InGaAs. *Physical Review B*, **2015**, 92,	3.3	6
107	Unraveling irradiation induced grain growth with in situ transmission electron microscopy and coordinated modeling. *Applied Physics Letters*, **2015**, 107, 191901	3.4	23
106	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	3.2	14
105	Trends in Grain Boundary Mobility: Survey of Motion Mechanisms. *Jom*, **2014**, 66, 114-120	2.1	49
104	Phenomenology of shear-coupled grain boundary motion in symmetric tilt and general grain boundaries. *Acta Materialia*, **2013**, 61, 1048-1060	8.4	83
103	Peierls potential of screw dislocations in bcc transition metals: Predictions from density functional theory. *Physical Review B*, **2013**, 87,	3.3	73
102	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	5.3	43
101	Simulation and modeling of the electronic structure of GaAs damage clusters. *Journal of Applied Physics*, **2013**, 113, 093706	2.5	1
100	Comment on "Toward realistic molecular dynamics simulations of grain boundary mobility" by Zhou and Mohles. *Scripta Materialia*, **2012**, 66, 714-716	5.6	6
99	Survey of Grain Boundary Energies in Four Elemental Metals. *Materials Science Forum*, **2012**, 715-716, 179-179	0.4	
98	Grain Growth Stagnation Caused by the Grain Boundary Roughening Transition. *Materials Science Forum*, **2012**, 715-716, 415-415	0.4	1
97	Molecular Dynamics Simulation of Grain Growth in Nanocrystalline Ni. *Materials Science Forum*, **2012**, 715-716, 599-604	0.4	3
96	Contributions of the embedded-atom method to materials science and engineering. *MRS Bulletin*, **2012**, 37, 485-491	3.2	23
95	Validating computed grain boundary energies in fcc metals using the grain boundary character distribution. *Acta Materialia*, **2011**, 59, 5250-5256	8.4	53

94	Dislocation-pairing transitions in hot grain boundaries. *Physical Review Letters*, **2011**, 106, 046101	7.4	54
93	How grain growth stops: a mechanism for grain-growth stagnation in pure materials. *Science*, **2010**, 328, 1138-41	33.3	180
92	Temperature dependence of grain boundary free energy and elastic constants. *Scripta Materialia*, **2010**, 62, 231-234	5.6	75
91	Comparing grain boundary energies in face-centered cubic metals: Al, Au, Cu and Ni. *Scripta Materialia*, **2010**, 63, 905-908	5.6	91
90	Comparing calculated and measured grain boundary energies in nickel. *Acta Materialia*, **2010**, 58, 5063-5069	3.4	88
89	Atomistic simulations of stress and microstructure evolution during polycrystalline Ni film growth. *Physical Review B*, **2009**, 79,	3.3	30
88	Atomistic simulations of crystal-melt interfaces in a model binary alloy: Interfacial free energies, adsorption coefficients, and excess entropy. *Physical Review B*, **2009**, 79,	3.3	38
87	Survey of computed grain boundary properties in face-centered cubic metals: I. Grain boundary energy. *Acta Materialia*, **2009**, 57, 3694-3703	8.4	416
86	Survey of computed grain boundary properties in face-centered cubic metals□: Grain boundary mobility. *Acta Materialia*, **2009**, 57, 3704-3713	8.4	249
85	Detailed characterization of defect production in molecular dynamics simulations of cascades in Si. *Nuclear Instruments & Methods in Physics Research B*, **2007**, 255, 101-104	1.2	19
84	Grain boundary interface roughening transition and its effect on grain boundary mobility for non-faceting boundaries. *Scripta Materialia*, **2007**, 57, 1161-1164	5.6	62
83	Thin film compressive stresses due to adatom insertion into grain boundaries. *Physical Review Letters*, **2007**, 99, 036102	7.4	74
82	Atomistic underpinnings for orientation selection in alloy dendritic growth. *Physical Review Letters*, **2007**, 98, 125701	7.4	70
81	Equilibrium adsorption at crystal-melt interfaces in Lennard-Jones alloys. *Journal of Chemical Physics*, **2006**, 124, 164708	3.9	32
80	Computing the mobility of grain boundaries. *Nature Materials*, **2006**, 5, 124-7	27	197
79	Copper Segregation to the □ (310)/[001] Symmetric Tilt Grain Boundary in Aluminum. *Journal of Materials Science*, **2004**, 12, 165-174		16
78	Grain Boundary Structure and Its Effect on Plasticity. *Microscopy and Microanalysis*, **2004**, 10, 12-13	0.5	
77	The rigid-body displacement observed at the □= 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		3

76	Surface step effects on nanoindentation. *Physical Review Letters*, **2001**, 87, 165507	7.4	382
75	Substitutional Impurity Segregation to the Σ5 (310)/[001] Stgb in Cu Doped Aluminum and Ag Doped Copper. *Microscopy and Microanalysis*, **2001**, 7, 246-247	0.5	
74	Effect of Surface Steps on Dislocation Structure During Nanoindentation. *Materials Research Society Symposia Proceedings*, **2000**, 649, 881		1
73	Embedded-atom-method study of structural, thermodynamic, and atomic-transport properties of liquid Ni-Al alloys. *Physical Review B*, **1999**, 59, 14271-14281	3.3	81
72	Electronic Effects on Grain Boundary Structure in BCC Metals. *Materials Research Society Symposia Proceedings*, **1999**, 589, 347		
71	Multi-scale modeling of polycrystal plasticity: a workshop report. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **1998**, 251, 1-22	5.3	32
70	Quantitative HREM observation of the Σ11(113)/[1̄10] grain-boundary structure in aluminium and comparison with atomistic simulation. *Journal of Microscopy*, **1998**, 190, 131-143	1.9	21
69	Atomistic studies of segregation and diffusion in Al-Cu grain boundaries. *Applied Physics Letters*, **1998**, 72, 1578-1580	3.4	52
68	Vibrational spectra in ordered and disordered Ni3Al. *Physical Review B*, **1997**, 56, R5705-R5708	3.3	49
67	Grain Boundary Dislocation Structure and Motion in an Aluminum Σ3 [011] Bicrystal. *Materials Research Society Symposia Proceedings*, **1996**, 466, 125		2
66	Embedded-Atom and Related Methods for Modeling Metallic Systems. *MRS Bulletin*, **1996**, 21, 24-28	3.2	42
65	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	3.3	58
64	Misfit dislocation structure for close-packed metal-metal interfaces. *Physical Review Letters*, **1995**, 75, 882-885	7.4	57
63	Near-Surface Buckling in Strained Metal Overlayer Systems. *Physical Review Letters*, **1995**, 75, 4242-4245	7.4	63
62	Dislocation Mechanism for Island Diffusion on fcc (111) Surfaces. *Physical Review Letters*, **1995**, 74, 2760-2763	7.4	112
61	Simulation of surface segregation free energies. *Physical Review B*, **1994**, 50, 12004-12014	3.3	40
60	High-resolution transmission electron microscopy studies of dislocation cores in metals and intermetallic compounds. *Ultramicroscopy*, **1994**, 56, 79-93	3.1	31
59	Evaluation of harmonic methods for calculating the free energy of defects in solids. *Physical Review B*, **1994**, 49, 14930-14938	3.3	157

58	Temperature-Dependent Structure of a Superdislocations in Ni3Al. *Materials Research Society Symposia Proceedings*, **1994**, 364, 731		1
57	The embedded-atom method: a review of theory and applications. *Materials Science and Engineering Reports*, **1993**, 9, 251-310		1177
56	Mo(001) seventh-order reconstruction: Ground-state structure and reconstruction mechanism. *Physical Review B*, **1993**, 48, 11287-11290	3.3	7
55	Atomic structure of the (310) twin in niobium: Experimental determination and comparison with theoretical predictions. *Physical Review Letters*, **1993**, 70, 449-452	7.4	55
54	Interatomic interactions for Mo and W based on the low-order moments of the density of states. *Physical Review B*, **1993**, 48, 4287-4298	3.3	72
53	High-resolution electron microscopy investigation of the (710) twin in Nb. *Ultramicroscopy*, **1993**, 51, 247-263	3.1	16
52	Interatomic Interactions for BCC Metals Based on the Low Order Moments of the Density of States. *Materials Research Society Symposia Proceedings*, **1992**, 278, 339		4
51	Hrtem Observation and EAM Calculation of Dislocation Cores in NiAl. *Materials Research Society Symposia Proceedings*, **1992**, 288, 257		6
50	Atomistic Simulations of Surfaces and Interfaces **1992**, 89-122		3
49	An Atomistic Study of the Equilibrium Segregation of Hydrogen to Tilt Boundaries in Nickel. *Materials Research Society Symposia Proceedings*, **1991**, 229, 179		2
48	HREM Investigation of the Structure of the Σ5(210)/[001] Symmetric Tilt Grain Boundaries in Nb. *Materials Research Society Symposia Proceedings*, **1991**, 229, 191		
47	An Atomistic Study of Hydrogen Effects on the Fracture of Tilt Boundaries in Nickel.. *Materials Research Society Symposia Proceedings*, **1991**, 238, 381		1
46	Properties of the liquid-vapor interface of fcc metals calculated using the embedded atom method. *Journal of Materials Research*, **1991**, 6, 298-302	2.5	23
45	Application of the Embedded Atom Method to Interfaces in Metals. *Materials Science Forum*, **1991**, 46, 187-198	0.4	9
44	Accommodation of the lattice mismatch in a Ag/Ni heterophase boundary. *Physical Review B*, **1991**, 43, 13833-13837	3.3	33
43	Theoretical Studies of Helium in Metals. *NATO ASI Series Series B: Physics*, **1991**, 3-16		3
42	Atomistic Structure and Composition of a Ag/Ni Interphase Boundary. *Materials Research Society Symposia Proceedings*, **1990**, 187, 287		0
41	Calculation of the Atomic Structure of Grain Boundaries in Metals and Alloys*. *Materials Research Society Symposia Proceedings*, **1990**, 193, 247		

40	Tilt Boundaries In BCC Metals:Comparison of Results Using Different Interatomic Interactions. *Materials Research Society Symposia Proceedings*, **1990**, 209, 65		1
39	The Structure and Properties of Boundaries in Bicrystals of Boron-Doped Ni3(Al, 1 at% Ta). *Materials Research Society Symposia Proceedings*, **1990**, 213, 423		
38	Kinetic isotope effects for hydrogen diffusion in bulk nickel and on nickel surfaces. *Journal of Chemical Physics*, **1990**, 92, 775-791	3.9	36
37	Development of an embedded-atom potential for a bcc metal: Vanadium. *Physical Review B*, **1990**, 41, 3316-3328	3.3	109
36	Solute-Atom Segregation at Internal Interfaces. *MRS Bulletin*, **1990**, 15, 51-57	3.2	9
35	An atomic model of crack tip deformation in aluminum using an embedded atom potential. *Journal of Materials Research*, **1990**, 5, 313-324	2.5	73
34	Structure of platinum adatom clusters on Pt(100): Experimental observations and embedded-atom-method calculations. *Physical Review B*, **1989**, 40, 10639-10642	3.3	72
33	Elastic properties of grain boundaries in copper and their relationship to bulk elastic constants. *Physical Review B*, **1989**, 40, 9479-9484	3.3	54
32	Electronic structure of grain boundaries. *Physical Review B*, **1989**, 40, 9993-9996	3.3	9
31	Self-diffusion and impurity diffusion of fcc metals using the five-frequency model and the Embedded Atom Method. *Journal of Materials Research*, **1989**, 4, 102-112	2.5	283
30	Calculation of grain-boundary segregation in Ni-Cu alloys. *Physical Review B*, **1989**, 40, 11502-11506	3.3	53
29	Thermodynamic properties of fcc transition metals as calculated with the embedded-atom method. *Physical Review B*, **1989**, 40, 5909-5915	3.3	195
28	Elastic Properties of Grain Boundaries in Copper. *Materials Research Society Symposia Proceedings*, **1989**, 153, 369		
27	Self-Diffusion and Impurity Diffusion of FCC Metals Using the Embedded Atom Method **1989**, 419-424		1
26	Calculation of the thermal expansion of metals using the embedded-atom method. *Physical Review B*, **1988**, 38, 12643-12644	3.3	65
25	Atomistic Studies of Interfacial Structure and Properties. *Materials Research Society Symposia Proceedings*, **1988**, 122, 343		6
24	Calculation of the Structure of Au Grain Boundaries Using the Embedded Atom Method. *Materials Research Society Symposia Proceedings*, **1988**, 138, 471		
23	The Embedded Atom Method: Theory and Application. *Materials Research Society Symposia Proceedings*, **1988**, 141, 31		8

22	Calculations of Structural Phases of Transition Metal Surfaces Using the Embedded Atom Method. *Springer Series in Surface Sciences*, **1988**, 125-131	0.4	1
21	Application of the embedded atom method to Ni3Al. *Journal of Materials Research*, **1987**, 2, 5-15	2.5	335
20	Summary Abstract: Calculation of the surface segregation of Pd□Cu, Pd□Ag, and Pd□Au alloys. *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **1987**, 5, 889-891	2.9	13
19	Order-disorder transition of Au and Pt(110) surfaces: The significance of relaxations and vibrations. *Physical Review Letters*, **1987**, 59, 2756-2759	7.4	114
18	Ordered surface phases of Au on Cu. *Surface Science*, **1987**, 191, 329-338	1.8	160
17	Theory of subsurface occupation, ordered structures, and order-disorder transitions for hydrogen on Pd(111). *Physical Review B*, **1987**, 35, 2128-2136	3.3	89
16	Calculation of the Defect and Interface Properties of Ni3Al. *Materials Research Society Symposia Proceedings*, **1986**, 81, 51		17
15	Calculation of the Surface Segregation of Pd-Cu, Pd-Ag, and Pd-Au Alloys. *Materials Research Society Symposia Proceedings*, **1986**, 83, 175		8
14	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	2.9	4
13	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	2.9	13
12	Embedded-atom-method functions for the fcc metals Cu, Ag, Au, Ni, Pd, Pt, and their alloys. *Physical Review B*, **1986**, 33, 7983-7991	3.3	3562
11	Simulation of Equilibrium Segregation in Alloys Using the Embedded Atom Method. *Materials Research Society Symposia Proceedings*, **1985**, 63, 61		9
10	Summary Abstract: A theoretical study of the order□disorder transitions for hydrogen on Pd(111). *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **1985**, 3, 1565-1566	2.9	36
9	Application of the embedded-atom method to liquid transition metals. *Physical Review B*, **1985**, 32, 3409-3415	3.3	368
8	Calculation of the surface segregation of Ni-Cu alloys with the use of the embedded-atom method. *Physical Review B*, **1985**, 32, 7685-7693	3.3	463
7	Perturbation theory of liquid-metal surfaces: The importance of the self-energy. *Physical Review A*, **1984**, 30, 3136-3146	2.6	13
6	A crossover integral equation for the structure of simple liquids. *Journal of Chemical Physics*, **1984**, 80, 4441-4447	3.9	91
5	Structure factor and direct correlation function of a fluid from finite range simulation data. *Journal of Chemical Physics*, **1984**, 81, 6140-6145	3.9	27

4	Solutions of the reference-hypernetted-chain equation with minimized free energy. *Physical Review A*, **1983**, 28, 2374-2379	2.6	290
3	Long-range correlations in adsorbed layers. *Physical Review B*, **1982**, 25, 1366-1369	3.3	31
2	Absence of power-law behavior of the hypernetted chain equation. *Physical Review A*, **1981**, 24, 424-428	2.6	44
1	Variational theory of phase separation in binary liquid mixtures. *Journal of Chemical Physics*, **1981**, 75, 3594-3598	3.9	60