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129
papers

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132
ext. papers

12,576
ext. citations

4.4
avg, IF

6.3
L-index

#	Paper	IF	Citations
129	Embedded-atom-method functions for the fcc metals Cu, Ag, Au, Ni, Pd, Pt, and their alloys. <i>Physical Review B</i> , 1986 , 33, 7983-7991	3.3	3562
128	The embedded-atom method: a review of theory and applications. <i>Materials Science and Engineering Reports</i> , 1993 , 9, 251-310		1177
127	Calculation of the surface segregation of Ni-Cu alloys with the use of the embedded-atom method. <i>Physical Review B</i> , 1985 , 32, 7685-7693	3.3	463
126	Survey of computed grain boundary properties in face-centered cubic metals: I. Grain boundary energy. <i>Acta Materialia</i> , 2009 , 57, 3694-3703	8.4	416
125	Surface step effects on nanoindentation. <i>Physical Review Letters</i> , 2001 , 87, 165507	7.4	382
124	Application of the embedded-atom method to liquid transition metals. <i>Physical Review B</i> , 1985 , 32, 3409-3415	3.3	368
123	Application of the embedded atom method to Ni ₃ Al. <i>Journal of Materials Research</i> , 1987 , 2, 5-15	2.5	335
122	Solutions of the reference-hypernetted-chain equation with minimized free energy. <i>Physical Review A</i> , 1983 , 28, 2374-2379	2.6	290
121	Self-diffusion and impurity diffusion of fcc metals using the five-frequency model and the Embedded Atom Method. <i>Journal of Materials Research</i> , 1989 , 4, 102-112	2.5	283
120	Survey of computed grain boundary properties in face-centered cubic metalsII: Grain boundary mobility. <i>Acta Materialia</i> , 2009 , 57, 3704-3713	8.4	249
119	Computing the mobility of grain boundaries. <i>Nature Materials</i> , 2006 , 5, 124-7	27	197
118	Thermodynamic properties of fcc transition metals as calculated with the embedded-atom method. <i>Physical Review B</i> , 1989 , 40, 5909-5915	3.3	195
117	How grain growth stops: a mechanism for grain-growth stagnation in pure materials. <i>Science</i> , 2010 , 328, 1138-41	33.3	180
116	Ordered surface phases of Au on Cu. <i>Surface Science</i> , 1987 , 191, 329-338	1.8	160
115	Evaluation of harmonic methods for calculating the free energy of defects in solids. <i>Physical Review B</i> , 1994 , 49, 14930-14938	3.3	157
114	Order-disorder transition of Au and Pt(110) surfaces: The significance of relaxations and vibrations. <i>Physical Review Letters</i> , 1987 , 59, 2756-2759	7.4	114
113	Dislocation Mechanism for Island Diffusion on fcc (111) Surfaces. <i>Physical Review Letters</i> , 1995 , 74, 2760-2763	7.4	112

112	Development of an embedded-atom potential for a bcc metal: Vanadium. <i>Physical Review B</i> , 1990 , 41, 3316-3328	3.3	109
111	Comparing grain boundary energies in face-centered cubic metals: Al, Au, Cu and Ni. <i>Scripta Materialia</i> , 2010 , 63, 905-908	5.6	91
110	A crossover integral equation for the structure of simple liquids. <i>Journal of Chemical Physics</i> , 1984 , 80, 4441-4447	3.9	91
109	Theory of subsurface occupation, ordered structures, and order-disorder transitions for hydrogen on Pd(111). <i>Physical Review B</i> , 1987 , 35, 2128-2136	3.3	89
108	Comparing calculated and measured grain boundary energies in nickel. <i>Acta Materialia</i> , 2010 , 58, 5063-5069	5.6	88
107	Phenomenology of shear-coupled grain boundary motion in symmetric tilt and general grain boundaries. <i>Acta Materialia</i> , 2013 , 61, 1048-1060	8.4	83
106	Embedded-atom-method study of structural, thermodynamic, and atomic-transport properties of liquid Ni-Al alloys. <i>Physical Review B</i> , 1999 , 59, 14271-14281	3.3	81
105	Temperature dependence of grain boundary free energy and elastic constants. <i>Scripta Materialia</i> , 2010 , 62, 231-234	5.6	75
104	Thin film compressive stresses due to adatom insertion into grain boundaries. <i>Physical Review Letters</i> , 2007 , 99, 036102	7.4	74
103	Peierls potential of screw dislocations in bcc transition metals: Predictions from density functional theory. <i>Physical Review B</i> , 2013 , 87,	3.3	73
102	An atomic model of crack tip deformation in aluminum using an embedded atom potential. <i>Journal of Materials Research</i> , 1990 , 5, 313-324	2.5	73
101	Interatomic interactions for Mo and W based on the low-order moments of the density of states. <i>Physical Review B</i> , 1993 , 48, 4287-4298	3.3	72
100	Structure of platinum adatom clusters on Pt(100): Experimental observations and embedded-atom-method calculations. <i>Physical Review B</i> , 1989 , 40, 10639-10642	3.3	72
99	Atomistic underpinnings for orientation selection in alloy dendritic growth. <i>Physical Review Letters</i> , 2007 , 98, 125701	7.4	70
98	Calculation of the thermal expansion of metals using the embedded-atom method. <i>Physical Review B</i> , 1988 , 38, 12643-12644	3.3	65
97	Near-Surface Buckling in Strained Metal Overlayer Systems. <i>Physical Review Letters</i> , 1995 , 75, 4242-4245	7.4	63
96	Grain boundary interface roughening transition and its effect on grain boundary mobility for non-faceting boundaries. <i>Scripta Materialia</i> , 2007 , 57, 1161-1164	5.6	62
95	Variational theory of phase separation in binary liquid mixtures. <i>Journal of Chemical Physics</i> , 1981 , 75, 3594-3598	3.9	60

94	Quantifying the influence of twin boundaries on the deformation of nanocrystalline copper using atomistic simulations. <i>International Journal of Plasticity</i> , 2015 , 65, 191-205	7.6	58
93	Embedded-atom-method effective-pair-interaction study of the structural and thermodynamic properties of Cu-Ni, Cu-Ag, and Au-Ni solid solutions. <i>Physical Review B</i> , 1996 , 53, 2389-2404	3.3	58
92	Misfit dislocation structure for close-packed metal-metal interfaces. <i>Physical Review Letters</i> , 1995 , 75, 882-885	7.4	57
91	Grain boundary segregation in immiscible nanocrystalline alloys. <i>Acta Materialia</i> , 2017 , 126, 528-539	8.4	55
90	Atomic structure of the (310) twin in niobium: Experimental determination and comparison with theoretical predictions. <i>Physical Review Letters</i> , 1993 , 70, 449-452	7.4	55
89	Dislocation-pairing transitions in hot grain boundaries. <i>Physical Review Letters</i> , 2011 , 106, 046101	7.4	54
88	Elastic properties of grain boundaries in copper and their relationship to bulk elastic constants. <i>Physical Review B</i> , 1989 , 40, 9479-9484	3.3	54
87	Validating computed grain boundary energies in fcc metals using the grain boundary character distribution. <i>Acta Materialia</i> , 2011 , 59, 5250-5256	8.4	53
86	Calculation of grain-boundary segregation in Ni-Cu alloys. <i>Physical Review B</i> , 1989 , 40, 11502-11506	3.3	53
85	Atomistic studies of segregation and diffusion in Al-Cu grain boundaries. <i>Applied Physics Letters</i> , 1998 , 72, 1578-1580	3.4	52
84	Trends in Grain Boundary Mobility: Survey of Motion Mechanisms. <i>Jom</i> , 2014 , 66, 114-120	2.1	49
83	Vibrational spectra in ordered and disordered Ni ₃ Al. <i>Physical Review B</i> , 1997 , 56, R5705-R5708	3.3	49
82	Stabilization of nanocrystalline alloys via grain boundary segregation: A diffuse interface model. <i>Acta Materialia</i> , 2015 , 101, 159-171	8.4	44
81	Absence of power-law behavior of the hypernetted chain equation. <i>Physical Review A</i> , 1981 , 24, 424-428	2.6	44
80	Molecular dynamics simulations of rate-dependent grain growth during the surface indentation of nanocrystalline nickel. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2013 , 571, 207-214	5.3	43
79	Grain boundary phase transformations in PtAu and relevance to thermal stabilization of bulk nanocrystalline metals. <i>Journal of Materials Science</i> , 2018 , 53, 2911-2927	4.3	43
78	Embedded-Atom and Related Methods for Modeling Metallic Systems. <i>MRS Bulletin</i> , 1996 , 21, 24-28	3.2	42
77	Roadmap on multiscale materials modeling. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2020 , 28, 043001	2	40

76	Simulation of surface segregation free energies. <i>Physical Review B</i> , 1994 , 50, 12004-12014	3.3	40
75	Atomistic simulations of crystal-melt interfaces in a model binary alloy: Interfacial free energies, adsorption coefficients, and excess entropy. <i>Physical Review B</i> , 2009 , 79,	3.3	38
74	Kinetic isotope effects for hydrogen diffusion in bulk nickel and on nickel surfaces. <i>Journal of Chemical Physics</i> , 1990 , 92, 775-791	3.9	36
73	Summary Abstract: A theoretical study of the order-disorder transitions for hydrogen on Pd(111). <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 1985 , 3, 1565-1566	2.9	36
72	Accommodation of the lattice mismatch in a Ag/Ni heterophase boundary. <i>Physical Review B</i> , 1991 , 43, 13833-13837	3.3	33
71	Multi-scale modeling of polycrystal plasticity: a workshop report. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 1998 , 251, 1-22	5.3	32
70	Equilibrium adsorption at crystal-melt interfaces in Lennard-Jones alloys. <i>Journal of Chemical Physics</i> , 2006 , 124, 164708	3.9	32
69	High-resolution transmission electron microscopy studies of dislocation cores in metals and intermetallic compounds. <i>Ultramicroscopy</i> , 1994 , 56, 79-93	3.1	31
68	Long-range correlations in adsorbed layers. <i>Physical Review B</i> , 1982 , 25, 1366-1369	3.3	31
67	Atomistic simulations of stress and microstructure evolution during polycrystalline Ni film growth. <i>Physical Review B</i> , 2009 , 79,	3.3	30
66	Structure factor and direct correlation function of a fluid from finite range simulation data. <i>Journal of Chemical Physics</i> , 1984 , 81, 6140-6145	3.9	27
65	Energy conserving orientational force for determining grain boundary mobility. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2015 , 23, 025007	2	26
64	Unraveling irradiation induced grain growth with in situ transmission electron microscopy and coordinated modeling. <i>Applied Physics Letters</i> , 2015 , 107, 191901	3.4	23
63	Contributions of the embedded-atom method to materials science and engineering. <i>MRS Bulletin</i> , 2012 , 37, 485-491	3.2	23
62	Properties of the liquid-vapor interface of fcc metals calculated using the embedded atom method. <i>Journal of Materials Research</i> , 1991 , 6, 298-302	2.5	23
61	Quantitative HREM observation of the $\sqrt{3}\times\sqrt{3}$ grain-boundary structure in aluminium and comparison with atomistic simulation. <i>Journal of Microscopy</i> , 1998 , 190, 131-143	1.9	21
60	Exploration of the mechanisms of temperature-dependent grain boundary mobility: search for the common origin of ultrafast grain boundary motion. <i>Journal of Materials Science</i> , 2016 , 51, 6607-6623	4.3	20
59	Detailed characterization of defect production in molecular dynamics simulations of cascades in Si. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2007 , 255, 101-104	1.2	19

58	The role of the interface stiffness tensor on grain boundary dynamics. <i>Acta Materialia</i> , 2018 , 158, 440-453	4	18
57	Calculation of the Defect and Interface Properties of Ni ₃ Al. <i>Materials Research Society Symposia Proceedings</i> , 1986 , 81, 51		17
56	Copper Segregation to the Σ (310)/[001] Symmetric Tilt Grain Boundary in Aluminum. <i>Journal of Materials Science</i> , 2004 , 12, 165-174		16
55	High-resolution electron microscopy investigation of the (710) twin in Nb. <i>Ultramicroscopy</i> , 1993 , 51, 247-263	3.1	16
54	The role of grain boundary character in solute segregation and thermal stability of nanocrystalline Pt-Au. <i>Nanoscale</i> , 2021 , 13, 3552-3563	7.7	15
53	New nanoscale toughening mechanisms mitigate embrittlement in binary nanocrystalline alloys. <i>Nanoscale</i> , 2018 , 10, 21231-21243	7.7	15
52	Strain-rate dependence of ramp-wave evolution and strength in tantalum. <i>Physical Review B</i> , 2016 , 94,	3.3	14
51	The effect of synthetic driving force on the atomic mechanisms associated with grain boundary motion below the interface roughening temperature. <i>Computational Materials Science</i> , 2014 , 86, 38-42	3.2	14
50	Misoriented grain boundaries vicinal to the twin in nickel Part I: thermodynamics & temperature-dependent structure. <i>Philosophical Magazine</i> , 2016 , 96, 1285-1304	1.6	13
49	Summary Abstract: Calculations of the energetics and structure of Pt(110) using the embedded atom method. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 1986 , 4, 1412-1413	2.9	13
48	Summary Abstract: Calculation of the surface segregation of Pd ₃ Cu, Pd ₃ Ag, and Pd ₃ Au alloys. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 1987 , 5, 889-891	2.9	13
47	Perturbation theory of liquid-metal surfaces: The importance of the self-energy. <i>Physical Review A</i> , 1984 , 30, 3136-3146	2.6	13
46	A diffuse interface model of grain boundary faceting. <i>Journal of Applied Physics</i> , 2016 , 119, 235306	2.5	12
45	Hydrogen segregation to inclined twin grain boundaries in nickel. <i>Philosophical Magazine</i> , 2016 , 96, 2808-2828	1.2	12
44	Application of the Embedded Atom Method to Interfaces in Metals. <i>Materials Science Forum</i> , 1991 , 46, 187-198	0.4	9
43	Electronic structure of grain boundaries. <i>Physical Review B</i> , 1989 , 40, 9993-9996	3.3	9
42	Solute-Atom Segregation at Internal Interfaces. <i>MRS Bulletin</i> , 1990 , 15, 51-57	3.2	9
41	Simulation of Equilibrium Segregation in Alloys Using the Embedded Atom Method. <i>Materials Research Society Symposia Proceedings</i> , 1985 , 63, 61		9

40	Calculation of the Surface Segregation of Pd-Cu, Pd-Ag, and Pd-Au Alloys. <i>Materials Research Society Symposia Proceedings</i> , 1986 , 83, 175		8
39	The Embedded Atom Method: Theory and Application. <i>Materials Research Society Symposia Proceedings</i> , 1988 , 141, 31		8
38	Misoriented grain boundaries vicinal to the (111)<110> twin in Nickel part II: thermodynamics of hydrogen segregation. <i>Philosophical Magazine</i> , 2016 , 96, 1463-1484	1.6	7
37	Mo(001) seventh-order reconstruction: Ground-state structure and reconstruction mechanism. <i>Physical Review B</i> , 1993 , 48, 11287-11290	3.3	7
36	Revealing inconsistencies in X-ray width methods for nanomaterials. <i>Nanoscale</i> , 2019 , 11, 22456-22466	7.7	7
35	Comment on "Toward realistic molecular dynamics simulations of grain boundary mobility" by Zhou and Mohles. <i>Scripta Materialia</i> , 2012 , 66, 714-716	5.6	6
34	First-principles survey of the structure, formation energies, and transition levels of As-interstitial defects in InGaAs. <i>Physical Review B</i> , 2015 , 92,	3.3	6
33	Hrtem Observation and EAM Calculation of Dislocation Cores in NiAl. <i>Materials Research Society Symposia Proceedings</i> , 1992 , 288, 257		6
32	Atomistic Studies of Interfacial Structure and Properties. <i>Materials Research Society Symposia Proceedings</i> , 1988 , 122, 343		6
31	Multi-objective optimization of interatomic potentials with application to MgO. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2019 , 27, 074007	2	5
30	Determination of recombination radius in Si for binary collision approximation codes. <i>Nuclear Instruments & Methods in Physics Research B</i> , 2016 , 371, 111-115	1.2	5
29	Fatigue-driven acceleration of abnormal grain growth in nanocrystalline wires. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2019 , 27, 025008	2	5
28	Interatomic Interactions for BCC Metals Based on the Low Order Moments of the Density of States. <i>Materials Research Society Symposia Proceedings</i> , 1992 , 278, 339		4
27	Summary Abstract: Computer simulation of the surface segregation in binary alloys using the embedded atom method. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 1986 , 4, 761-762	2.9	4
26	Molecular Dynamics Simulation of Grain Growth in Nanocrystalline Ni. <i>Materials Science Forum</i> , 2012 , 715-716, 599-604	0.4	3
25	The rigid-body displacement observed at the $\frac{1}{2}$ 5, (310)-[001] symmetric tilt grain boundary in central transition bcc metals. <i>Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties</i> , 2002 , 82, 1573-1594		3
24	Theoretical Studies of Helium in Metals. <i>NATO ASI Series Series B: Physics</i> , 1991 , 3-16		3
23	Atomistic Simulations of Surfaces and Interfaces 1992 , 89-122		3

22	Grain Boundary Dislocation Structure and Motion in an Aluminum Σ 3 [011] Bicrystal. <i>Materials Research Society Symposia Proceedings</i> , 1996 , 466, 125		2
21	An Atomistic Study of the Equilibrium Segregation of Hydrogen to Tilt Boundaries in Nickel. <i>Materials Research Society Symposia Proceedings</i> , 1991 , 229, 179		2
20	Interface-Driven Phenomena in Solids: Thermodynamics, Kinetics and Chemistry. <i>Jom</i> , 2016 , 68, 1594-1595		1
19	Preface for focus issue on uncertainty quantification in materials modeling. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2019 , 27, 080301	2	1
18	Simulation and modeling of the electronic structure of GaAs damage clusters. <i>Journal of Applied Physics</i> , 2013 , 113, 093706	2.5	1
17	Grain Growth Stagnation Caused by the Grain Boundary Roughening Transition. <i>Materials Science Forum</i> , 2012 , 715-716, 415-415	0.4	1
16	Effect of Surface Steps on Dislocation Structure During Nanoindentation. <i>Materials Research Society Symposia Proceedings</i> , 2000 , 649, 881		1
15	Temperature-Dependent Structure of a Superdislocations in Ni ₃ Al. <i>Materials Research Society Symposia Proceedings</i> , 1994 , 364, 731		1
14	An Atomistic Study of Hydrogen Effects on the Fracture of Tilt Boundaries in Nickel.. <i>Materials Research Society Symposia Proceedings</i> , 1991 , 238, 381		1
13	Tilt Boundaries In BCC Metals:Comparison of Results Using Different Interatomic Interactions. <i>Materials Research Society Symposia Proceedings</i> , 1990 , 209, 65		1
12	Calculations of Structural Phases of Transition Metal Surfaces Using the Embedded Atom Method. <i>Springer Series in Surface Sciences</i> , 1988 , 125-131	0.4	1
11	Self-Diffusion and Impurity Diffusion of FCC Metals Using the Embedded Atom Method 1989 , 419-424		1
10	Atomistic Structure and Composition of a Ag/Ni Interphase Boundary. <i>Materials Research Society Symposia Proceedings</i> , 1990 , 187, 287		0
9	Survey of Grain Boundary Energies in Four Elemental Metals. <i>Materials Science Forum</i> , 2012 , 715-716, 179-179	0.4	
8	Grain Boundary Structure and Its Effect on Plasticity. <i>Microscopy and Microanalysis</i> , 2004 , 10, 12-13	0.5	
7	Substitutional Impurity Segregation to the Σ (310)/[001] Stgb in Cu Doped Aluminum and Ag Doped Copper. <i>Microscopy and Microanalysis</i> , 2001 , 7, 246-247	0.5	
6	Electronic Effects on Grain Boundary Structure in BCC Metals. <i>Materials Research Society Symposia Proceedings</i> , 1999 , 589, 347		
5	HREM Investigation of the Structure of the Σ (210)/[001] Symmetric Tilt Grain Boundaries in Nb. <i>Materials Research Society Symposia Proceedings</i> , 1991 , 229, 191		

- 4 Elastic Properties of Grain Boundaries in Copper. *Materials Research Society Symposia Proceedings*, **1989**, 153, 369
- 3 Calculation of the Atomic Structure of Grain Boundaries in Metals and Alloys*. *Materials Research Society Symposia Proceedings*, **1990**, 193, 247
- 2 The Structure and Properties of Boundaries in Bicrystals of Boron-Doped Ni₃(Al, 1 at% Ta). *Materials Research Society Symposia Proceedings*, **1990**, 213, 423
- 1 Calculation of the Structure of Au Grain Boundaries Using the Embedded Atom Method. *Materials Research Society Symposia Proceedings*, **1988**, 138, 471