Yuri Mishin

List of Publications by Citations

135 papers	11,097 citations	46 h-index	104 g-index
140 ext. papers	12,303 ext. citations	5.8 avg, IF	6.75 L-index

#	Paper	IF	Citations
135	Structural stability and lattice defects in copper: Ab initio, tight-binding, and embedded-atom calculations. *Physical Review B*, **2001**, 63,	3.3	1500
134	Interatomic potentials for monoatomic metals from experimental data and ab initio calculations. *Physical Review B*, **1999**, 59, 3393-3407	3.3	1055
133	Coupling grain boundary motion to shear deformation. *Acta Materialia*, **2006**, 54, 4953-4975	8.4	591
132	Diffusion in the TiAl system. *Acta Materialia*, **2000**, 48, 589-623	8.4	485
131	Interatomic potentials for atomistic simulations of the Ti-Al system. *Physical Review B*, **2003**, 68,	3.3	413
130	Atomistic modeling of interfaces and their impact on microstructure and properties. *Acta Materialia*, **2010**, 58, 1117-1151	8.4	379
129	An embedded-atom potential for the CuAg system. *Modelling and Simulation in Materials Science and Engineering*, **2006**, 14, 817-833	2	365
128	Atomistic modeling of the and -phases of the NiAl system. *Acta Materialia*, **2004**, 52, 1451-1467	8.4	351
127	Development of an interatomic potential for the Ni-Al system. *Philosophical Magazine*, **2009**, 89, 3245-3267	2.2	261
126	Embedded-atom potential for B2NiAl. *Physical Review B*, **2002**, 65,	3.3	251
125	Structural phase transformations in metallic grain boundaries. *Nature Communications*, **2013**, 4, 1899	17.4	238
124	Phase stability in the FeNi system: Investigation by first-principles calculations and atomistic simulations. *Acta Materialia*, **2005**, 53, 4029-4041	8.4	217
123	Grain boundary diffusion: recent progress and future research. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **1999**, 260, 55-71	5.3	196
122	Diffusion mechanisms in Cu grain boundaries. *Physical Review B*, **2000**, 62, 3658-3673	3.3	162
121	Self-diffusion in TiAl: an experimental study and atomistic calculations. *Intermetallics*, **1999**, 7, 389-404	3.5	157
120	Atomistic Modeling of Point Defects and Diffusion in Copper Grain Boundaries. *Journal of Materials Science*, **2003**, 11, 131-148		156
119	Effect of interface phase transformations on diffusion and segregation in high-angle grain boundaries. *Physical Review Letters*, **2013**, 110, 255502	7.4	142

118	Embedded-atom potential for Fe and its application to self-diffusion on Fe(100). *Surface Science*, **2006**, 600, 1793-1803	1.8	141
117	Duality of dislocation content of grain boundaries. *Philosophical Magazine*, **2006**, 86, 3965-3980	1.6	136
116	Intrinsic self-diffusion and substitutional Al diffusion in Ti. *Acta Materialia*, **1997**, 45, 4181-4191	8.4	134
115	Stabilization and strengthening of nanocrystalline copper by alloying with tantalum. *Acta Materialia* , **2012**, 60, 2158-2168	8.4	125
114	Grain size stabilization of nanocrystalline copper at high temperatures by alloying with tantalum. *Journal of Alloys and Compounds*, **2013**, 573, 142-150	5.7	117
113	Characterization and visualization of the lattice misfit associated with dislocation cores. *Acta Materialia*, **2005**, 53, 1313-1321	8.4	116
112	Grain boundary migration and grain rotation studied by molecular dynamics. *Acta Materialia*, **2012**, 60, 2407-2424	8.4	115
111	Dynamics of grain boundary motion coupled to shear deformation: An analytical model and its verification by molecular dynamics. *Physical Review B*, **2008**, 78,	3.3	112
110	Atomic mechanisms of grain boundary diffusion: Low versus high temperatures. *Journal of Materials Science*, **2005**, 40, 3155-3161	4.3	102
109	Coupled motion of asymmetrical tilt grain boundaries: Molecular dynamics and phase field crystal simulations. *Acta Materialia*, **2012**, 60, 6528-6546	8.4	101
108	Segregation-induced phase transformations in grain boundaries. *Physical Review B*, **2015**, 92,	3.3	100
107	Interatomic potential for the Al-Cu system. *Physical Review B*, **2011**, 83,	3.3	99
106	Grain boundary diffusion: fundamentals to recent developments. *International Materials Reviews*, **1997**, 42, 155-178	16.1	92
105	Calculation of point-defect entropy in metals. *Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties*, **2001**, 81, 2591-2612		91
104	Thermodynamics of grain boundary premelting in alloys. I. Phase-field modeling. *Acta Materialia*, **2009**, 57, 3771-3785	8.4	88
103	Physically-informed artificial neural networks for atomistic modeling of materials. *Nature Communications*, **2019**, 10, 2339	17.4	86
102	Stick-slip behavior of grain boundaries studied by accelerated molecular dynamics. *Physical Review B*, **2007**, 75,	3.3	86
101	Temperature dependence of the surface free energy and surface stress: An atomistic calculation for Cu(110). *Physical Review B*, **2009**, 79,	3.3	82

100	Atomistic simulation of point defects and diffusion in B2 NiAl. *Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties*, **1997**, 75, 169-185		82
99	Interaction of Point Defects with Grain Boundaries in fcc Metals. *Journal of Materials Science*, **2003**, 11, 425-437		77
98	Evaluation of diffusion mechanisms in NiAl by embedded-atom and first-principles calculations. *Physical Review B*, **2003**, 67,	3.3	66
97	Angular-dependent interatomic potential for the Cu–Ta system and its application to structural stability of nano-crystalline alloys. *Acta Materialia*, **2015**, 100, 377-391	8.4	59
96	Angular-dependent interatomic potential for tantalum. *Acta Materialia*, **2006**, 54, 5013-5026	8.4	58
95	Embedded-atom potential for hcp and fcc cobalt. *Physical Review B*, **2012**, 86,	3.3	56
94	Thermodynamics of grain boundary premelting in alloys. II. Atomistic simulation. *Acta Materialia*, **2009**, 57, 3786-3794	8.4	56
93	Molecular dynamics modeling of self-diffusion along a triple junction. *Physical Review B*, **2009**, 79,	3.3	55
92	Interatomic potential for the ternary Ni–Al–Co system and application to atomistic modeling of the B2–L10martensitic transformation. *Modelling and Simulation in Materials Science and Engineering*, **2015**, 23, 065006	2	50
91	Relationship between equilibrium fluctuations and shear-coupled motion of grain boundaries. *Physical Review Letters*, **2012**, 109, 095501	7.4	50
90	A molecular dynamics study of self-diffusion in the cores of screw and edge dislocations in aluminum. *Acta Materialia*, **2009**, 57, 5531-5542	8.4	48
89	Dissociation and faceting of asymmetrical tilt grain boundaries: Molecular dynamics simulations of copper. *Physical Review B*, **2007**, 76,	3.3	46
88	Correlation between grain boundary energy and geometry in Ni-rich NiAl. *Acta Materialia*, **2005**, 53, 3795-3805	8.4	46
87	Microstructural evolution in a nanocrystalline Cu-Ta alloy: A combined in-situ TEM and atomistic study. *Materials and Design*, **2017**, 113, 178-185	8.1	45
86	Atomistic simulation of point defects and diffusion in B2 NiAl. *Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties*, **1997**, 75, 187-199		44
85	Solid-liquid interface free energy in binary systems: theory and atomistic calculations for the (110) Cu-Ag interface. *Journal of Chemical Physics*, **2009**, 131, 054702	3.9	43
84	First-principles study of thermodynamical and mechanical stabilities of thin copper film on tantalum. *Physical Review B*, **2007**, 76,	3.3	43
83	Thermodynamics of coherent interfaces under mechanical stresses. I. Theory. *Physical Review B*, **2012**, 85,	3.3	42

82	Diffusion in fine-grained materials: Theoretical aspects and experimental possibilities. *Scripta Materialia*, **1995**, 6, 859-862		42
81	Nickel nanoparticles set a new record of strength. *Nature Communications*, **2018**, 9, 4102	17.4	42
80	Interatomic potential for the Cu-Ta system and its application to surface wetting and dewetting. *Physical Review B*, **2008**, 77,	3.3	40
79	Thermodynamics of coherent interfaces under mechanical stresses. II. Application to atomistic simulation of grain boundaries. *Physical Review B*, **2012**, 85,	3.3	37
78	Calculation of the□□ interface free energy in the Ni□Al system by the capillary fluctuation method. *Modelling and Simulation in Materials Science and Engineering*, **2014**, 22, 045001	2	36
77	Effect of Ta Solute Concentration on the Microstructural Evolution in Immiscible Cu-Ta Alloys. *Jom*, **2015**, 67, 2802-2809	2.1	36
76	Thermodynamic theory of equilibrium fluctuations. *Annals of Physics*, **2015**, 363, 48-97	2.5	35
75	Thermodynamic and kinetic aspects of interfacial decohesion. *Acta Materialia*, **2002**, 50, 3609-3622	8.4	35
74	Atomistic simulation of [001] symmetrical tilt grain boundaries in NiAl. *Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties*, **1998**, 78, 29-56		32
73	Interatomic Potentials for Al and Ni From Experimental Data and AB Initio Calculations. *Materials Research Society Symposia Proceedings*, **1998**, 538, 535		32
72	Phase transformations at interfaces: Observations from atomistic modeling. *Current Opinion in Solid State and Materials Science*, **2016**, 20, 308-315	12	30
71	Phases, phase equilibria, and phase rules in low-dimensional systems. *Journal of Chemical Physics*, **2015**, 143, 044706	3.9	30
70	Zener Pinning of Grain Boundaries and Structural Stability of Immiscible Alloys. *Jom*, **2016**, 68, 1596-1604	2.1	29
69	Effect of surface stress on Ni segregation in (110) NiAl thin films. *Physical Review B*, **2004**, 69,	3.3	29
68	Point defects in NiAl: The effect of lattice vibrations. *Physical Review B*, **2003**, 68,	3.3	29
67	Representation of dislocation cores using Nye tensor distributions. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2005**, 400-401, 18-21	5.3	27
66	Optimized interatomic potential for silicon and its application to thermal stability of silicene. *Physical Review B*, **2017**, 95,	3.3	26
65	Atomistic study of grain-boundary segregation and grain-boundary diffusion in Al-Mg alloys. *Acta Materialia*, **2020**, 201, 596-603	8.4	26

64	Atomistic modeling of capillary-driven grain boundary motion in Cu-Ta alloys. *Acta Materialia*, **2018**, 148, 311-319	8.4	25
63	Calculation of diffusion coefficients and correlation factors in grain-boundary diffusion. *Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties*, **1995**, 72, 1589-1607		25
62	Capillary-driven grain boundary motion and grain rotation in a tricrystal: A molecular dynamics study. *Acta Materialia*, **2014**, 65, 19-31	8.4	24
61	Orientation dependence of the solid–liquid interface stress: atomistic calculations for copper. *Modelling and Simulation in Materials Science and Engineering*, **2010**, 18, 074003	2	24
60	Monte Carlo simulation of grain boundary segregation and decohesion in NiAl. *Acta Materialia*, **2002**, 50, 4303-4313	8.4	23
59	Multiscale modeling of sensory properties of CoNiAl shape memory particles embedded in an Al metal matrix. *Journal of Materials Science*, **2016**, 51, 1204-1216	4.3	22
58	Irreversible thermodynamics of creep in crystalline solids. *Physical Review B*, **2013**, 88,	3.3	22
57	Thermodynamics of Cottrell atmospheres tested by atomistic simulations. *Acta Materialia*, **2016**, 117, 197-206	8.4	21
56	Machine-learning interatomic potentials for materials science. *Acta Materialia*, **2021**, 214, 116980	8.4	21
55	Monte Carlo modeling of low-index surfaces in stoichiometric and Ni-rich NiAl. *Physical Review B*, **2003**, 67,	3.3	20
54	Temperature fluctuations in canonical systems: Insights from molecular dynamics simulations. *Physical Review B*, **2016**, 94,	3.3	20
53	Effect of nonhydrostatic stresses on solid-fluid equilibrium. II. Interface thermodynamics. *Physical Review B*, **2010**, 82,	3.3	19
52	Disjoining potential and grain boundary premelting in binary alloys. *Physical Review B*, **2016**, 93,	3.3	18
51	Molecular dynamics simulation of the martensitic phase transformation in NiAl alloys. *Journal of Physics Condensed Matter*, **2010**, 22, 395403	1.8	18
50	Interatomic Potentials for Metals **2005**, 459-478		18
49	Structure and thermal decomposition of a nanocrystalline mechanically alloyed supersaturated CuTa solid solution. *MRS Communications*, **2015**, 5, 333-339	2.7	17
48	Liquid nucleation at superheated grain boundaries. *Physical Review Letters*, **2011**, 106, 155702	7.4	16
47	Effect of nonhydrostatic stresses on solid-fluid equilibrium. I. Bulk thermodynamics. *Physical Review B*, **2010**, 82,	3.3	16

46	Angular-dependent interatomic potential for the aluminum-hydrogen system. *Physical Review B*, **2010**, 82,	3.3	16
45	Atomistic simulation of hillock growth. *Acta Materialia*, **2010**, 58, 5471-5480	8.4	16
44	Segregation and structural transformations at Σ3 grain boundaries in NiAl: A Monte-Carlo study. *Acta Materialia*, **2005**, 53, 2149-2156	8.4	16
43	Nanotechnology enabled design of a structural material with extreme strength as well as thermal and electrical properties. *Materials Today*, **2019**, 31, 10-20	21.8	15
42	Hydrogen effect on shearing and cleavage of Al: A first-principles study. *Physical Review B*, **2011**, 84,	3.3	15
41	Stable nanocolloidal structures in metallic systems. *Physical Review Letters*, **2010**, 104, 055701	7.4	15
40	Solute drag and dynamic phase transformations in moving grain boundaries. *Acta Materialia*, **2019**, 179, 383-395	8.4	14
39	Recrystallization initiated by low-temperature grain boundary motion coupled to stress. *International Journal of Materials Research*, **2009**, 100, 510-515	0.5	14
38	A methodology to aid in the design of naval steels: Linking first principles calculations to mesoscale modeling. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2007**, 452-453, 558-568	5.3	14
37	Angular-dependent interatomic potential for the binary NiCr system. *Modelling and Simulation in Materials Science and Engineering*, **2018**, 26, 085008	2	14
36	Grain Boundary Diffusion in Metals **2005**, 337-366		14
35	Extra variable in grain boundary description. *Physical Review Materials*, **2017**, 1,	3.2	13
34	Unraveling the dislocation core structure at a van der Waals gap in bismuth telluride. *Nature Communications*, **2019**, 10, 1820	17.4	12
33	An Atomistic View of Grain Boundary Diffusion. *Defect and Diffusion Forum*, **2015**, 363, 1-11	0.7	12
32	Direct atomistic modeling of solute drag by moving grain boundaries. *Acta Materialia*, **2020**, 198, 111-128	8.4	12
31	Monte Carlo simulation of correlation effects in a random bcc alloy. *Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties*, **1997**, 75, 201-219		11
30	The pre-wetting transition at antiphase boundaries: an atomistic modeling study of Ni3Al. *Journal of Materials Science*, **2008**, 43, 3873-3880	4.3	10
29	Grain boundary diffusion metals versus non-stoichiometric compounds. *Ionics*, **2001**, 7, 247-263	2.7	9

28	Atomistic Computer Simulation of Diffusion **2005**, 113-171		8
27	Model of diffusion coarsening of the raft structure in single crystals of nickel-base superalloys. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing* , **1993**, 171, 163-168	5.3	7
26	An experimental and modeling investigation of tensile creep resistance of a stable nanocrystalline alloy. *Acta Materialia*, **2020**, 199, 141-154	8.4	7
25	Calculation of open and closed system elastic coefficients for multicomponent solids. *Physical Review B*, **2015**, 91,	3.3	6
24	Thermodynamic model of hydride formation and dissolution in spherical particles. *Acta Materialia*, **2010**, 58, 4968-4977	8.4	6
23	Atomistic simulation of [001] symmetrical tilt grain boundaries in NiAl		5
22	Thermal conductivity and its relation to atomic structure for symmetrical tilt grain boundaries in silicon. *Physical Review Materials*, **2020**, 4,	3.2	5
21	Development of a general-purpose machine-learning interatomic potential for aluminum by the physically informed neural network method. *Physical Review Materials*, **2020**, 4,	3.2	4
20	Energy spectrum of a Langevin oscillator. *Physical Review E*, **2016**, 94, 062151	2.4	4
19	Stress-driven grain refinement in a microstructurally stable nanocrystalline binary alloy. *Scripta Materialia*, **2021**, 191, 185-190	5.6	4
18	Plastic Deformation by Grain Boundary Motion: Experiments and Simulations201-233		4
17	Interatomic Potentials for Metals **2005**, 459		4
16	Relationship between grain boundary segregation and grain boundary diffusion in Cu-Ag alloys. *Physical Review Materials*, **2020**, 4,	3.2	3
15	Sharp interface model of creep deformation in crystalline solids. *Physical Review B*, **2015**, 92,	3.3	2
14	A Molecular Dynamics Study of Self-Diffusion in the Core of a Screw Dislocation in Al. *Defect and Diffusion Forum*, **2007**, 266, 49-62	0.7	2
13	Thermodynamics and Kinetics of Interfacial Decohesion. *Materials Research Society Symposia Proceedings*, **1999**, 586, 27		2
12	Atomistic Simulation of Grain Boundary Structure and Diffusion in B2 NiAl. *Materials Research Society Symposia Proceedings*, **1996**, 458, 21		2
11	Theory of Oxygen Tracer Diffusion Along Grain Boundaries and in the Bulk in Two-Stage Oxidation Experiments. Part III: Monte-Carlo Simulations. *Journal De Physique III*, **1997**, 7, 1797-1811		2

List of Publications

10	The impact of alloying on defect-free nanoparticles exhibiting softer but tougher behavior. *Nature Communications*, **2021**, 12, 2515	17.4	2
9	Accommodation of Grain Boundary Coherency Strain by Interfacial Disconnections. *Microscopy and Microanalysis*, **2006**, 12, 888-889	0.5	1
8	Effect of vacancy creation and annihilation on grain boundary motion. *Acta Materialia*, **2020**, 185,	8.4	1
7	Interface migration by phase transformations. *Nature Materials*, **2021**, 20, 911-912	27	1
6	Size and shape effects on the strength of platinum nanoparticles. *Journal of Materials Science*, **2021** , 56, 18300-18312	4.3	1
5	The Role of Grain Boundary Diffusion in the Solute Drag Effect. *Nanomaterials*, **2021**, 11,	5.4	1
4	Development of a physically-informed neural network interatomic potential for tantalum. *Computational Materials Science*, **2022**, 205, 111180	3.2	0
3	Temperature dependence of the pre-wetting transition at the (1 1 1) anti-phase boundary in Ni3Al: an atomistic study. *Modelling and Simulation in Materials Science and Engineering*, **2010**, 18, 074004	2	
2	Atomistic Computer Simulation of Diffusion **2005**, 113-171		
1	Dynamic Embrittlement: Quasi-Static Interfacial Decohesion. *Materials Research Society Symposia Proceedings*, **1999**, 586, 303		