Mikhail I Mendelev

List of Publications by Year
in descending order

105 papers	6,522 citations	81900 39 h-index	64796 79 g-index
105 all docs	105 docs citations	105 times ranked	3483 citing authors

#	Article	IF	Citations
1	Development of new interatomic potentials appropriate for crystalline and liquid iron. Philosophical Magazine, 2003, 83, 3977-3994.	1.6	1,113
2	Development of an interatomic potential for phosphorus impurities in Â-iron. Journal of Physics Condensed Matter, 2004, 16, S2629-S2642.	1.8	502
3	Analysis of semi-empirical interatomic potentials appropriate for simulation of crystalline and liquid Al and Cu. Philosophical Magazine, 2008, 88, 1723-1750.	1.6	374
4	Development of suitable interatomic potentials for simulation of liquid and amorphous Cuâ€“Zr alloys. Philosophical Magazine, 2009, 89, 967-987.	1.6	357
5	Crystal-melt interfacial free energies in hcp metals: A molecular dynamics study of Mg. Physical Review B, 2006, 73, .	3.2	334
6	Using atomistic computer simulations to analyze x-ray diffraction data from metallic glasses. Journal of Applied Physics, 2007, 102, .	2.5	300
7	Development of an interatomic potential for the simulation of phase transformations in zirconium. Philosophical Magazine Letters, 2007, 87, 349-359.	1.2	281
8	Development of interatomic potentials appropriate for simulation of liquid and glass properties of NiZr₂ alloy. Philosophical Magazine, 2012, 92, 4454-4469.	1.6	128
9	Development of an interatomic potential for the simulation of defects, plasticity, and phase transformations in titanium. Journal of Chemical Physics, 2016, 145, 154102.	3.0	122
10	Development of interatomic potentials appropriate for simulation of solidâ€“liquid interface properties in Alâ€“Mg alloys. Philosophical Magazine, 2009, 89, 3269-3285.	1.6	120
11	Computer simulation of the elastically driven migration of a flat grain boundary. Acta Materialia, 2004, 52, 2569-2576.	7.9	115
12	Effect of Fe Segregation on the Migration of a Non-Symmetric Î£5 Tilt Grain Boundary in Al. Journal of Materials Research, 2005, 20, 208-218.	2.6	114
13	Molecular dynamics study of self-diffusion in bcc Fe. Physical Review B, 2009, 80, .	3.2	106
14	Determination of the crystal-melt interface kinetic coefficient from molecular dynamics simulations. Modelling and Simulation in Materials Science and Engineering, 2010, 18, 015004.	2.0	94
15	Molecular-dynamics study of solidâ€“liquid interface migration in fcc metals. Modelling and Simulation in Materials Science and Engineering, 2010, 18, 074002.	2.0	93
16	Crystal-melt interfacial free energies in metals: fcc versus bcc. Physical Review B, 2004, 69, .	3.2	92
17	Impurity effects on grain boundary migration. Modelling and Simulation in Materials Science and Engineering, 2002, 10, R79-R109.	2.0	74
18	Spatially Resolved Distribution Function and the Medium-Range Order in Metallic Liquid and Glass. Scientific Reports, 2011, 1, 194.	3.3	69

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19	Experimental and molecular dynamics simulation study of structure of liquid and amorphous Ni62Nb38 alloy. Journal of Chemical Physics, 2016, 145, 204505.	3.0	69
20	Molecular dynamics simulation of diffusion in supercooled Cuâ€“Zr alloys. Philosophical Magazine, 2009, 89, 109-126.	1.6	67
21	Computer simulation and experimental study of elastic properties of amorphous Cu-Zr alloys. Journal of Applied Physics, 2007, 102, .	2.5	64
22	Quantitative Parameter-Free Prediction of Simulated Crystal-Nucleation Times. Physical Review Letters, 2006, 96, 245701.	7.8	63
23	Simulation of the interaction between Fe impurities and point defects in V. Physical Review B, 2007, 76, .	3.2	63
24	Development of a semi-empirical potential suitable for molecular dynamics simulation of vitrification in Cu-Zr alloys. Journal of Chemical Physics, 2019, 151, 214502.	3.0	63
25	Anisotropy of the solidâ€“liquid interface properties of the Niâ€“Zr B33 phase from molecular dynamics simulation. Philosophical Magazine, 2015, 95, 224-241.	1.6	62
26	Development of interatomic potentials appropriate for simulation of devitrification of Al₉₀Sm₁₀alloy. Modelling and Simulation in Materials Science and Engineering, 2015, 23, 045013.	2.0	61
27	Molecular dynamics study of self-diffusion in Zr. Philosophical Magazine, 2010, 90, 637-654.	1.6	59
28	The interactions of self-interstitials with twin boundaries. Philosophical Magazine, 2013, 93, 1268-1278.	1.6	58
29	Effects of stable and unstable stacking fault energy on dislocation nucleation in nano-crystalline metals. Modelling and Simulation in Materials Science and Engineering, 2016, 24, 085017.	2.0	55
30	â€˜Crystal Genesâ€™ in Metallic Liquids and Glasses. Scientific Reports, 2016, 6, 23734.	3.3	52
31	Effects of sub-Tg annealing on Cu64.5Zr35.5 glasses: A molecular dynamics study. Applied Physics Letters, 2014, 104, .	3.3	51
32	Effect of stacking fault energy on mechanism of plastic deformation in nanotwinned FCC metals. Modelling and Simulation in Materials Science and Engineering, 2015, 23, 055003.	2.0	49
33	A regular solution model for impurity drag on a migrating grain boundary. Acta Materialia, 2001, 49, 589-597.	7.9	48
34	Experimental and computer simulation determination of the structural changes occurring through the liquidâ€“glass transition in Cuâ€“Zr alloys. Philosophical Magazine, 2010, 90, 3795-3815.	1.6	48
35	Cooling rate dependence of medium-range order development in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">C</mml:mi><mml:msub><mml:mi mathvariant="normal">u</mml:mi><mml:mrow><mml:mn mathvariant="bold">64</mml:mn><mml:mo>.</mml:mo><mml:mn mathvariant="bold">5</mml:mn></mml:mrow></mml:msub><mml:mi mathvariant="normal">Z</mml:mi>	3.2	47
36	Effects of solutes on dislocation nucleation from grain boundaries. International Journal of Plasticity, 2017, 90, 146-155.	8.8	47

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37	Asperity contacts at the nanoscale: Comparison of Ru and Au. Journal of Applied Physics, 2008, 104, .	2.5	46
38	Comparison of molecular dynamics simulation methods for the study of grain boundary migration. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 045017.	2.0	46
39	Overcoming the Time Limitation in Molecular Dynamics Simulation of Crystal Nucleation: A Persistent-Embryo Approach. Physical Review Letters, 2018, 120, 085703.	7.8	46
40	A unified relation for the solid-liquid interface free energy of pure FCC, BCC, and HCP metals. Journal of Chemical Physics, 2016, 144, 144707.	3.0	37
41	Mobility of ?5 tilt grain boundaries: Inclination dependence. Scripta Materialia, 2005, 52, 1193-1198.	5.2	36
42	Grain shape, grain boundary mobility and the Herring relation. Acta Materialia, 2004, 52, 285-292.	7.9	34
43	Interface mobility and the liquid-glass transition in a one-component system described by an embedded atom method potential. Physical Review B, 2006, 74, .	3.2	34
44	Determination of alloy interatomic potentials from liquid-state diffraction data. Physical Review B, 2002, 66, .	3.2	32
45	Molecular dynamics investigation of dynamical heterogeneity and local structure in the supercooled liquid and glass states of Al. Physical Review B, 2008, 77, .	3.2	32
46	Grain boundary self-diffusion in Ni: Effect of boundary inclination. Journal of Materials Research, 2005, 20, 1146-1153.	2.6	28
47	Diffusion in a Cu-Zr metallic glass studied by microsecond-scale molecular dynamics simulations. Physical Review B, 2015, 91, .	3.2	28
48	Grain-boundary migration in the presence of diffusing impurities: Simulations and analytical models. Philosophical Magazine A: Physics of Condensed Matter, Structure, Defects and Mechanical Properties, 2001, 81, 2243-2269.	0.6	27
49	Solid-liquid interface free energies of pure bcc metals and B2 phases. Journal of Chemical Physics, 2015, 142, 134705.	3.0	27
50	A comparison of crystalâ€“melt interfacial free energies using different Al potentials. Journal of Non-Crystalline Solids, 2007, 353, 3565-3569.	3.1	25
51	Development of a semi-empirical potential for simulation of Ni solute segregation into grain boundaries in Ag. Modelling and Simulation in Materials Science and Engineering, 2018, 26, 075004.	2.0	25
52	Deformation behavior of an amorphous Cu64.5Zr35.5 alloy: A combined computer simulation and experimental study. Journal of Applied Physics, 2008, 104, .	2.5	24
53	Composition-dependent stability of the medium-range order responsible for metallic glass formation. Acta Materialia, 2014, 81, 337-344.	7.9	24
54	Effects of Ag and Zr solutes on dislocation emission from Î£11(332)[110] symmetric tilt grain boundaries in Cu: Bigger is not always better. International Journal of Plasticity, 2018, 109, 79-87.	8.8	23

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55	Strong correlations of dynamical and structural heterogeneities with localized soft modes in a Cu-Zr metallic glass. Applied Physics Letters, 2014, 105, 151910.	3.3	22
56	Discovery of a metastable Al20Sm4 phase. Applied Physics Letters, 2015, 106, .	3.3	18
57	Structural ordering at solid-liquid interfaces in Al-Sm system: A molecular-dynamics study. Materials Letters, 2017, 186, 26-29.	2.6	18
58	Reliability of methods of computer simulation of structure of amorphous alloys. Journal of Applied Physics, 2010, 107, .	2.5	17
59	Theoretical calculation of the melting curve of Cu-Zr binary alloys. Physical Review E, 2014, 90, 052403.	2.1	17
60	Appearance of metastable B2 phase during solidification of Ni₅₀Zr₅₀alloy: electrostatic levitation and molecular dynamics simulation studies. Journal of Physics Condensed Matter, 2015, 27, 085004.	1.8	17
61	Effects of Schmid factor and slip nucleation on deformation mechanism in columnar-grained nanotwinned Ag and Cu. Journal of Applied Physics, 2015, 117, .	2.5	17
62	Temperature dependence of the solid-liquid interface free energy of Ni and Al from molecular dynamics simulation of nucleation. Journal of Chemical Physics, 2018, 149, 174501.	3.0	17
63	Solute effects on interfacial dislocation emission in nanomaterials: Nucleation site competition and neutralization. Scripta Materialia, 2018, 154, 12-15.	5.2	17
64	Molecular dynamics simulation of the solid-liquid interface migration in terbium. Journal of Chemical Physics, 2018, 148, 214705.	3.0	17
65	Nucleation of stoichiometric compounds from liquid: Role of the kinetic factor. Physical Review Materials, 2018, 2, .	2.4	17
66	Molecular dynamics simulation of solidification and devitrification in a one-component system. Modelling and Simulation in Materials Science and Engineering, 2012, 20, 045014.	2.0	16
67	Dependence of solidâ€“liquid interface free energy on liquid structure. Modelling and Simulation in Materials Science and Engineering, 2014, 22, 065004.	2.0	16
68	Kink model for extended defect migration in the presence of diffusing impurities: theory and simulation. Acta Materialia, 2001, 49, 2843-2852.	7.9	15
69	Molecular dynamics study of vacancy migration in Al. Materials Letters, 2007, 61, 2911-2914.	2.6	15
70	Equilibrium structure of multilayer van der Waals films and nanotubes. Physical Review B, 2002, 65, .	3.2	14
71	Structural hierarchy as a key to complex phase selection in Al-Sm. Physical Review Materials, 2017, 1, .	2.4	14
72	Two-step nucleation of the Earthâ€™s inner core. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	14

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73	Interface Mobility Under Different Driving Forces. Journal of Materials Research, 2002, 17, 234-245.	2.6	13
74	Impact of deformation on the atomic structures and dynamics of a Cu-Zr metallic glass: A molecular dynamics study. Physical Review B, 2014, 90, .	3.2	13
75	Discovery of a meta-stable Alâ€“Sm phase with unknown stoichiometry using a genetic algorithm. Scripta Materialia, 2014, 81, 32-35.	5.2	13
76	Effects of grain boundary disorder on dislocation emission. Materials Letters, 2019, 237, 303-305.	2.6	13
77	An iterative procedure for the creation of computer models of non-crystalline materials from diffraction data. Journal of Non-Crystalline Solids, 1998, 223, 230-240.	3.1	12
78	Co-Segregation Effects on Boundary Migration. Journal of Materials Science, 2002, 10, 191-199.	1.2	12
79	In SituObservation of Antisite Defect Formation during Crystal Growth. Physical Review Letters, 2010, 105, 245501.	7.8	12
80	Prediction of cooling rate dependent ordering in metallic glass transition using a two-state model. Computational Materials Science, 2010, 49, 615-618.	3.0	12
81	Structure of liquid Al and Al₆₇Mg₃₃alloy: comparison between experiment and simulation. Philosophical Magazine, 2014, 94, 1876-1892.	1.6	12
82	Kink model for extended defect migration: theory and simulations. Acta Materialia, 2000, 48, 3711-3717.	7.9	11
83	Solid-liquid phase diagrams for binary metallic alloys: Adjustable interatomic potentials. Physical Review B, 2007, 75, .	3.2	11
84	Effects of dopants on the glass forming ability in Al-based metallic alloy. Physical Review Materials, 2019, 3, .	2.4	10
85	Determination of grain boundary stiffness from molecular dynamics simulation. Applied Physics Letters, 2006, 88, 121927.	3.3	9
86	Cross Diffusion-Stresses Effects. Defect and Diffusion Forum, 2007, 264, 79-89.	0.4	7
87	Soluteâ€“solute correlations responsible for the prepeak in structure factors of undercooled Al-rich liquids: a molecular dynamics study. Journal of Physics Condensed Matter, 2015, 27, 205701.	1.8	7
88	Creation of two-component liquid alloys computer models from data of two diffraction experiments. Physica B: Condensed Matter, 1999, 262, 40-48.	2.7	6
89	Strain dependence of peak widths of reciprocal- and real-space distribution functions of metallic glasses fromin situx-ray scattering and molecular dynamics simulations. Physical Review B, 2009, 80, .	3.2	6
90	Competitive B2 and B33 Nucleation during Solidification of Ni50Zr50 Alloy: Molecular Dynamics Simulation and Classical Nucleation Theory. Journal of Physical Chemistry C, 2019, 123, 6685-6692.	3.1	6

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91	Computer Simulation of Fe Diffusion in Liquid Al and along Al Grain Boundaries. Defect and Diffusion Forum, 0, 309-310, 223-230.	0.4	5
92	Molecular dynamics simulation of phase competition in terbium. Journal of Chemical Physics, 2018, 149, 244501.	3.0	5
93	Effect of samarium doping on the nucleation of fcc-aluminum in undercooled liquids. Scripta Materialia, 2018, 154, 202-206.	5.2	5
94	Domain Wall Migration in 3-d in the Presence of Diffusing Impurities. Journal of Materials Science, 2002, 10, 91-98.	1.2	4
95	Anomalous diffusion in dilute solid solutions. Acta Materialia, 2007, 55, 5289-5296.	7.9	4
96	Effects of solutes on the thermal stability of nanotwinned materials. Philosophical Magazine, 2014, 94, 2875-2885.	1.6	4
97	Modification of dislocation emission sources at symmetric tilt grain boundaries in Ag by Cu solute atoms. Materials Letters, 2018, 223, 243-245.	2.6	4
98	Effect of Atomic Complexes Formation in Grain Boundaries on Grain Boundary Diffusion. Defect and Diffusion Forum, 0, 383, 103-111.	0.4	4
99	Observation of Î·-Al41Sm5 reveals motif-aware structural evolution in Al-Sm alloys. Scientific Reports, 2019, 9, 6692.	3.3	4
100	Molecular Dynamics Study of Mechanism of Solidâ€“Liquid Interface Migration and Defect Formation in Al3Sm Alloy. Jom, 2021, 73, 2312-2319.	1.9	4
101	Computer simulation of the structure of MZr₂liquid and amorphous alloys. Philosophical Magazine, 2012, 92, 4098-4112.	1.6	3
102	The influence of spatial and temporal averaging on interpretation of HRTEM images of solidâ€“liquid interfaces. Ultramicroscopy, 2013, 124, 40-45.	1.9	3
103	Partial structure correlations in amorphous Ni83La17. Journal of Non-Crystalline Solids, 1998, 240, 35-42.	3.1	1
104	Determining strain in amorphous alloys: Uncertainties with analyzing structural changes during deformation. Journal of Applied Physics, 2009, 105, 023509.	2.5	1
105	10.1063/1.5026922.1. , 2018, , .		0