Irina V Belova

List of Publications by Citations

125	892	17	23
papers	citations	h-index	g-index
127	994	1.7	4.34
ext. papers	ext. citations	avg, IF	L-index

#	Paper	IF	Citations
125	Molecular dynamics simulation of the alloying reaction in Al-coated Ni nanoparticle. *Computational Materials Science*, **2010**, 47, 712-720	3.2	50
124	Electronic, optical and bonding properties of CaCO3 calcite. *Solid State Communications*, **2009**, 149, 1201-1203	1.6	43
123	Electronic and optical properties of anatase TiO2 nanotubes. *Computational Materials Science*, **2010**, 48, 854-858	3.2	35
122	Energy cost of heat activating serpentinites for CO2 storage by mineralisation. *International Journal of Greenhouse Gas Control*, **2013**, 17, 225-239	4.2	34
121	Effect of Heat Treatment on the Compressive Behavior of Zinc Alloy ZA27 Syntactic Foam. *Materials*, **2019**, 12,	3.5	30
120	Lattice Monte Carlo and Experimental Analyses of the Thermal Conductivity of Random-Shaped Cellular Aluminum. *Advanced Engineering Materials*, **2009**, 11, 843-847	3.5	26
119	Molecular dynamics simulation and theoretical analysis of carbon diffusion in cementite. *Acta Materialia*, **2009**, 57, 846-853	8.4	24
118	Reaction of a Ni-coated Al nanoparticle to form B2-NiAl: A molecular dynamics study. *Philosophical Magazine Letters*, **2009**, 89, 815-830	1	24
117	Molecular dynamics simulation of alloying in a Ti-coated Al nanoparticle. *Intermetallics*, **2012**, 22, 193-202	3.5	22
116	Molecular dynamics determination of the time□temperature□transformation diagram for crystallization of an undercooled liquid Ni50Al50 alloy. *Acta Materialia*, **2011**, 59, 6412-6419	8.4	21
115	Analysis of the Effective Diffusivity in Nanocrystalline Materials. *Journal of Metastable and Nanocrystalline Materials*, **2004**, 19, 25-34	0.2	20
114	Analysis of diffusion in high entropy alloys. *Materials Chemistry and Physics*, **2018**, 210, 301-308	4.4	19
113	Influence of particle arrangement on the compression of functionally graded metal syntactic foams. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2019**, 764, 138242	5.3	19
112	Molecular dynamics simulation of the thermophysical properties of an undercooled liquid Ni50Al50 alloy. *Computational Materials Science*, **2010**, 50, 465-473	3.2	19
111	Interdiffusion and surface-sandwich ordering in initial Ni-core-Pd-shell nanoparticle. *Physical Chemistry Chemical Physics*, **2009**, 11, 3233-40	3.6	19
110	Mechanical and Microstructural Characterization of an AZ91?Activated Carbon Syntactic Foam. *Materials*, **2018**, 12,	3.5	18
109	Molecular dynamics study of reaction pathways in an Al-coated Ni nanoparticle. *Intermetallics*, **2011**, 19, 934-941	3.5	18

108	Molecular dynamics simulation of alloying in an Al-coated Ti nanoparticle. *Computational Materials Science*, **2013**, 79, 316-325	3.2	17
107	Thermotransport in binary system: case study on Ni50Al50 melt. *Philosophical Magazine*, **2014**, 94, 3574-3602	1.6	17
106	Molecular dynamics study of density, surface energy and self-diffusion in a liquid Ni50Al50 alloy. *Computational Materials Science*, **2010**, 50, 331-337	3.2	16
105	Molecular dynamics simulation of diffusion in a (110) B2-NiAl film. *Intermetallics*, **2011**, 19, 848-854	3.5	15
104	Molecular dynamics simulation of surface segregation in a (110) B2-NiAl thin film. *Physical Chemistry Chemical Physics*, **2011**, 13, 1214-21	3.6	15
103	Molecular dynamics prediction of phonon-mediated thermal conductivity of f.c.c. Cu. *Philosophical Magazine*, **2014**, 94, 731-751	1.6	14
102	Thermal Conductivity Enhancement of Compact Heat Sinks Using Cellular Metals. *Defect and Diffusion Forum*, **2008**, 273-276, 222-226	0.7	12
101	The Lattice Monte Carlo Method for Solving Phenomenological Mass and Thermal Diffusion Problems. *Defect and Diffusion Forum*, **2008**, 279, 13-22	0.7	12
100	Influence of the interatomic potential on thermotransport in binary liquid alloys: case study on NiAl. *Philosophical Magazine*, **2016**, 96, 3054-3074	1.6	11
99	Molecular dynamics study of phonon-mediated thermal transport in a Ni50Al50 melt: case analysis of the influence of the process on the kinetics of solidification. *Philosophical Magazine*, **2015**, 95, 90-111	1.6	10
98	Finite Difference Solution of the Diffusion Equation and Calculation of the Interdiffusion Coefficient using the Sauer-Freise and Hall Methods in Binary Systems. *Procedia Engineering*, **2015**, 105, 570-575		10
97	Formation of a Hollow Binary Alloy Nanosphere: A Kinetic Monte Carlo Study. *Journal of Nano Research*, **2009**, 7, 11-17	1	10
96	Dynamic compression of functionally-graded metal syntactic foams. *Composite Structures*, **2021**, 261, 113308	5.3	10
95	Decomposition model for phonon thermal conductivity of a monatomic lattice. *Philosophical Magazine*, **2014**, 94, 3992-4014	1.6	9
94	Stability of Hollow Nanospheres: A Molecular Dynamics Study. *Solid State Phenomena*, **2007**, 129, 125-130	0.4	9
93	Bridging Different Length and Time Scales in Diffusion Problems Using a Lattice Monte Carlo Method. *Solid State Phenomena*, **2007**, 129, 1-10	0.4	8
92	Calculation of the Effective Thermal Conductivity in Composites Using Finite Element and Monte Carlo Methods. *Materials Science Forum*, **2007**, 553, 51-56	0.4	8
91	Fatigue characterization of functionally graded ZA27 alloy syntactic foams. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2020**, 798, 140255	5.3	8

90	Mass and thermal transport in liquid Cu-Ag alloys. *Philosophical Magazine*, **2019**, 99, 468-491	1.6	8
89	Simultaneous Measurement of Isotope-Free Tracer Diffusion Coefficients and Interdiffusion Coefficients in the Cu-Ni System. *Journal of Phase Equilibria and Diffusion*, **2018**, 39, 862-869	1	8
88	Interdiffusion in Intermetallics. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2013**, 44, 4417-4421	2.3	7
87	The Synthesis, Stability and Shrinkage of Hollow Nanoparticles: An Overview. *Journal of Nano Research*, **2009**, 7, 19-26	1	7
86	Collective and Tracer Diffusion via a Defect Cluster in LSGM. *Defect and Diffusion Forum*, **2007**, 263, 81-86	0.7	7
85	Atomistic Modeling of Diffusion in the TiAl Compound. *Defect and Diffusion Forum*, **2005**, 237-240, 271-276	0.7	7
84	Interdiffusion and thermotransport in NiAl liquid alloys. *Philosophical Magazine*, **2018**, 98, 2221-2246	1.6	7
83	Prediction of the lattice thermal conductivity of zircon and the cubic and monoclinic phases of zirconia by molecular dynamics simulation. *Computational Materials Science*, **2020**, 176, 109522	3.2	6
82	Lattice-Based Walks and the Monte Carlo Method for Addressing Mass, Thermal and Elasticity Problems. *Defect and Diffusion Forum*, **2009**, 283-286, 13-23	0.7	6
81	Calculations of the Effective Thermal Conductivity in a Model of Syntactic Metallic Hollow Sphere Structures Using a Lattice Monte Carlo Method. *Defect and Diffusion Forum*, **2008**, 273-276, 216-221	0.7	6
80	Chemical Diffusion in Ni3Al. *Defect and Diffusion Forum*, **2001**, 194-199, 541-546	0.7	6
79	The Thermal Conductivity of Magnesite, Dolomite and Calcite as Determined by Molecular Dynamics Simulation **2018**, 19, 18-34		6
78	Comments on Experimental assessment of the thermodynamic factor for diffusion in CoCrFeNi and CoCrFeMnNi high entropy alloys *Scripta Materialia*, **2019**, 172, 110-112	5.6	5
77	A structural model for surface-enhanced stabilization in some metallic glass formers. *Philosophical Magazine Letters*, **2013**, 93, 50-57	1	5
76	Theoretical Study of the Heat of Transport in a Liquid Ni50Al50 Alloy: Green-Kubo Approach **2014**, 2, 159-189		5
75	Diffusion correlation effects of molybdenum and silicon in molybdenum disilicide. *Philosophical Magazine*, **2011**, 91, 3727-3743	1.6	5
74	Theoretical Analysis and Atomistic Modelling of Diffusion and Stability of Pure Element Hollow Nanospheres and Nanotubes. *Defect and Diffusion Forum*, **2008**, 277, 21-26	0.7	5
73	The Six-Jump Cycle Diffusion Mechanism in Non-Stoichiometric B2 Intermetallics: the Vacancy-Wind Factor. *Defect and Diffusion Forum*, **2003**, 213-215, 95-106	0.7	5

72	Tracer Correlation, Collective Correlation and Vacancy Wind Factors in Intermetallics Taking the B2 Structures. *Defect and Diffusion Forum*, **2000**, 179-180, 1-16	0.7	5
71	Determination of the lattice thermal conductivity of the TiO2 polymorphs rutile and anatase by molecular dynamics simulation. *Computational Condensed Matter*, **2018**, 17, e00342	1.7	5
70	Investigation of Interdiffusion in High Entropy Alloys: Application of the Random Alloy Model **2019**, 22, 94-108		4
69	Phonon-mediated heat dissipation in a monatomic lattice: case study on Ni. *Philosophical Magazine*, **2015**, 95, 3640-3673	1.6	4
68	Vibrational contribution to thermal transport in liquid cooper: Equilibrium molecular dynamics study. *Computational Materials Science*, **2015**, 96, 229-236	3.2	4
67	Insight into lattice thermal impedance via equilibrium molecular dynamics: case study on Al. *Philosophical Magazine*, **2016**, 96, 596-619	1.6	4
66	Thermal Conductivity Computations of Sintered Hollow Sphere Structures. *Metals*, **2012**, 2, 113-121	2.3	4
65	Phonon Thermal Conductivity of F.C.C. Cu by Molecular Dynamics Simulation. *Defect and Diffusion Forum*, **2013**, 336, 169-184	0.7	4
64	Solving Complex Thermal and Mass Transport Problems with the Lattice Monte Carlo Method. *Materials Science Forum*, **2010**, 654-656, 1476-1481	0.4	4
63	A Lattice Monte Carlo Analysis of Thermal Transport in Phase Change Materials. *Defect and Diffusion Forum*, **2010**, 297-301, 154-161	0.7	4
62	Numerical Characterization of Anisotropic Heat Sink Composites. *Materials Science Forum*, **2010**, 654-656, 1500-1503	0.4	4
61	Investigation of Harrison Type-A, B and Intermediate AB Kinetics Regimes in Grain Boundary Diffusion. *Defect and Diffusion Forum*, **2009**, 283-286, 697-704	0.7	4
60	Modelling of the Formation of Pd-Ni Alloy Nanoparticles by Interdiffusion. *Defect and Diffusion Forum*, **2008**, 277, 207-212	0.7	4
59	Stability and Shrinkage by Diffusion in Hollow Nanotubes. *Defect and Diffusion Forum*, **2007**, 266, 39-47	0.7	4
58	A Simple Iterative Method for Analysing Experimental Tracer Diffusivities in Concentrated Binary Alloys. *Defect and Diffusion Forum*, **2003**, 224-225, 127-0	0.7	4
57	Random-Walk Calculations in Intermetallic Compounds. *Defect and Diffusion Forum*, **2005**, 237-240, 291-302	0.7	4
56	Time Dependence of the Segregation of Diffusing Solute in Nanocrystalline Materials. *Materials Research Society Symposia Proceedings*, **2002**, 731, 541		4
55	Molecular Dynamics Prediction of the Influence of Composition on Thermotransport in Ni-Al Melts **2017**, 12, 93-110		3

54	First-principles calculations of a corrugated anatase TiO2 surface. *Computational Materials Science*, **2012**, 51, 78-82	3.2	3
53	The Harrison Diffusion Kinetics Regimes in Grain Boundary Diffusion: Lattice Monte Carlo Modelling of the Effect of Segregation. *Defect and Diffusion Forum*, **2011**, 309-310, 9-18	0.7	3
52	Exploration of the Transition from Harrison Type-A Kinetics to Type-B Kinetics Regimes in Grain Boundary Diffusion. *Defect and Diffusion Forum*, **2008**, 273-276, 425-430	0.7	3
51	Phenomenological Aspects of Grain Boundary Diffusion. *Defect and Diffusion Forum*, **2006**, 258-260, 483-490	0.7	3
50	Monte Carlo Modelling of the Effective Diffusivity in Composite Material. *Defect and Diffusion Forum*, **2007**, 261-262, 103-108	0.7	3
49	A Self-Consistent Theory of Atomic Transport in the B2 Ordered Alloy: The Sum Rule. *Defect and Diffusion Forum*, **2001**, 194-199, 547-552	0.7	3
48	Activation volume dominated diffusivity of Ni50Al50 melt under extreme conditions. *Computational Materials Science*, **2020**, 171, 109263	3.2	3
47	Computer simulation of thermodynamic factors in Ni-Al and Cu-Ag liquid alloys. *Computational Materials Science*, **2019**, 166, 124-135	3.2	2
46	Two-fluid nature of phonon heat conduction in a monatomic lattice. *Philosophical Magazine*, **2015**, 95, 2571-2595	1.6	2
45	Interdiffusion Analysis in Ternary Systems to Process Composition Profiles and Obtain Constant Interdiffusion Coefficients Using One Compact Diffusion Couple. *Journal of Phase Equilibria and Diffusion*, **2019**, 40, 522-531	1	2
44	Composition Effect on Shrinkage of Hollow Binary Alloy Nanospheres. *Defect and Diffusion Forum*, **2009**, 289-292, 665-672	0.7	2
43	Visualization of the Vacancy-Wind Effect Occurring in Chemical Diffusion and Ionic Conductivity in Solids. *Defect and Diffusion Forum*, **2008**, 273-276, 431-444	0.7	2
42	Atomic Mechanism of Carbon Diffusion in Cementite. *Defect and Diffusion Forum*, **2008**, 277, 101-106	0.7	2
41	Thermal Properties of Composite Materials and Porous Media: Lattice-Based Monte Carlo Approaches73-95		2
40	Diffusion in the Presence of Grain Boundaries: a Variable Length Scale Simulation Method. *Materials Research Society Symposia Proceedings*, **2001**, 677, 7201		2
39	Measurement of Interdiffusion and Tracer Diffusion Coefficients in FCC Co-Cr-Fe-Ni Multi-Principal Element Alloy. *Journal of Phase Equilibria and Diffusion*,1	1	2
38	Impurity Diffusion Coefficients of Al and Zn in Mg Determined from Solid-to-Solid Diffusion Couples505-509		2
37	Molecular Dynamics Determination of the Lattice Thermal Conductivity of the Cubic Phase of Hafnium Dioxide **2020**, 27, 177-185		1

36	The Nature of the Vacancy-Wind Effect Occurring in Diffusion via Six-Jump-Cycles in B2 Intermetallics. *Defect and Diffusion Forum*, **2010**, 297-301, 1218-1225	0.7	1
35	Parametric Analysis of the Classification of Harrison Kinetics Regimes in Grain Boundary Diffusion. *Defect and Diffusion Forum*, **2010**, 297-301, 1226-1231	0.7	1
34	Carbon Diffusion in Cementite: A Molecular Dynamics Study. *Defect and Diffusion Forum*, **2009**, 283-286, 24-29	0.7	1
33	Surface-Sandwich Segregation Phenomena in Bimetallic Ag-Ni and Pd-Ni Nanoparticles: A Molecular Dynamics Study. *Defect and Diffusion Forum*, **2009**, 289-292, 657-664	0.7	1
32	Vacancy-Wind Factors and Collective Correlation Factors in Nonstoichiometric B2 Intermetallic Compounds. *Defect and Diffusion Forum*, **2006**, 251-252, 69-78	0.7	1
31	The sum-rule relation among phenomenological transport coefficients and its consequences in the analysis of collective diffusion problems. *Physical Chemistry Chemical Physics*, **2004**, 006, 3620-3624	3.6	1
30	Calculation of Tracer and Chemical Diffusion Coefficients in the Intermetallic Compound AgMg. *Defect and Diffusion Forum*, **2003**, 224-225, 45-52	0.7	1
29	Collective Correlation Factors in Random Non-Stoichiometric Inermetallic Compounds. *Defect and Diffusion Forum*, **2005**, 247-248, 1-8	0.7	1
28	Tracer Diffusion by Six-Jump-Cycles in Nonstoichiometric B2 Intermetallic Compounds. *Defect and Diffusion Forum*, **2005**, 247-248, 9-20	0.7	1
27	An overview of thermotransport in fluorite-related ionic oxides. *Zeitschrift Fur Physikalische Chemie*, **2021**,	3.1	1
26	Novel Interdiffusion Analysis in Multicomponent Alloys - Part 2: Application to Quaternary, Quinary and Higher Alloys29, 179-203		1
25	Exact phenomenological theory for thermotransport in a solid binary alloy. *Philosophical Magazine Letters*, **2021**, 101, 123-131	1	1
24	The Diffusion Isotope Effect and Diffusion Mechanism in Liquid Cu-Ag and Cu-Ni Alloys. *Defect and Diffusion Forum*,413, 136-145	0.7	1
23	Pores shrinkage and growth in polycrystalline hollow nanoparticles and nanotubes. *Scripta Materialia*, **2020**, 180, 93-96	5.6	0
22	Interdiffusion Data in Multicomponent Alloys as a Source of Quantitative Fundamental Diffusion Information. *Defect and Diffusion Forum*, **2007**, 263, 1-10	0.7	0
21	The Vacancy-Wind Factor and the Manning Factor Occurring in Interdiffusion and Ionic Conductivity in Solids **2019**, 22, 170-183		
20	Compressive Properties of Corevo Foam under Uni-Axial Loading Based on Experimental and Numerical Analysis. *Applied Mechanics and Materials*, **2014**, 597, 121-126	0.3	
19	Recent Advances in the Prediction of the Thermal Properties of Metallic Hollow Sphere Structures **2010**, 73-110		

18	Theoretical Studies of Diffusion Kinetics in Austenite. *Defect and Diffusion Forum*, **2008**, 273-276, 455-460	0.7
17	Diffusion Kinetics Analysis of Cation Diffusion in YSZ and LSGM. *Defect and Diffusion Forum*, **2008**, 273-276, 445-454	0.7
16	Finite Element Modelling of Oxygen Diffusion and Segregation at Interfaces in Ag-MgO Composites: Parametric Studies. *Defect and Diffusion Forum*, **2008**, 273-276, 461-466	0.7
15	In-Diffusion and Out-Diffusion of Oxygen from a Composite Containing Random Traps. *Solid State Phenomena*, **2008**, 139, 35-40	0.4
14	Contribution to the Theory of Demixing of Yttrium in Yttria-Stabilized-Zirconia in an Electric Field. *Advances in Science and Technology*, **2006**, 46, 42-47	0.1
13	Analysis of Interdiffusion and Intrinsic Diffusion in Multicomponent Alloys to Obtain Information about Diffusion Mechanisms. *Defect and Diffusion Forum*, **2006**, 258-260, 237-246	0.7
12	Cation Diffusion and Demixing in Yttria Stabilized Zirconia: Comparison of Assumptions of Constant Electric Field and Constant Current. *Defect and Diffusion Forum*, **2006**, 258-260, 247-252	0.7
11	Six-Jump-Cycle Mechanism for Collective Correlations in Nonstoichiometric Intermetallic Compounds. *Defect and Diffusion Forum*, **2006**, 251-252, 59-68	0.7
10	Sum-Rule Relations among Phenomenological Coefficients: Application to Segregation and Chemical Diffusion in Multicomponent Alloys and Mixed Ceramic Oxides. *Defect and Diffusion Forum*, **2006**, 249, 17-26	0.7
9	Extraction of Diffusion Correlation Information from Tracer, Interdiffusion and Ionic Conductivity Data. *Advances in Science and Technology*, **2006**, 46, 54-62	0.1
8	Calculation of Phenomenological Coefficients by Monte Carlo Computer Simulation Methods. *Defect and Diffusion Forum*, **2006**, 249, 27-34	0.7
7	Molecular Dynamics Study of Carbon Diffusion in Austenite. *Defect and Diffusion Forum*, **2006**, 258-260, 253-258	0.7
6	Non-Random Interaction of Vacancies with Atoms during Interdiffusion and Ionic Conductivity in Materials. *Defect and Diffusion Forum*, **2007**, 266, 119-130	0.7
5	Modelling of Oxygen Diffusion and Segregation at Interfaces in Ag-MgO Composites. *Defect and Diffusion Forum*, **2007**, 266, 29-38	0.7
4	A Formalism to Describe Demixing of Mixed Oxides of Large and Small Grain Size in an Electric Field. *Materials Research Society Symposia Proceedings*, **2004**, 822, S6.14.1	
3	Expressions for the effective diffusivity in materials with interphase boundaries. *Materials Research Society Symposia Proceedings*, **2004**, 819, N3.14.1	
2	Tracer Diffusion in Nonstoichiometric Intermetallic Compounds with Random Mixing on Each Sublattice. *Defect and Diffusion Forum*, **2005**, 247-248, 21-28	0.7
1	Relationships between chemical and tracer diffusion coefficients in strongly ionic crystals. *International Journal of Materials Research*, **2022**, 95, 870-875	0.5