

Irina V Belova

List of Publications by Year in descending order

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124
papers

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citations

393982

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g-index

127
all docs

127
docs citations

127
times ranked

844
citing authors

#	ARTICLE	IF	CITATIONS
1	Electronic, optical and bonding properties of CaCO ₃ calcite. Solid State Communications, 2009, 149, 1201-1203.	0.9	58
2	Molecular dynamics simulation of the alloying reaction in Al-coated Ni nanoparticle. Computational Materials Science, 2010, 47, 712-720.	1.4	56
3	Effect of Heat Treatment on the Compressive Behavior of Zinc Alloy ZA27 Syntactic Foam. Materials, 2019, 12, 792.	1.3	41
4	Electronic and optical properties of anatase TiO ₂ nanotubes. Computational Materials Science, 2010, 48, 854-858.	1.4	40
5	Energy cost of heat activating serpentinites for CO ₂ storage by mineralisation. International Journal of Greenhouse Gas Control, 2013, 17, 225-239.	2.3	40
6	Mechanical and Microstructural Characterization of an AZ91MP Activated Carbon Syntactic Foam. Materials, 2019, 12, 3.	1.3	36
7	Analysis of diffusion in high entropy alloys. Materials Chemistry and Physics, 2018, 210, 301-308.	2.0	32
8	Molecular dynamics simulation and theoretical analysis of carbon diffusion in cementite. Acta Materialia, 2009, 57, 846-853.	3.8	30
9	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.	2.6	30
10	Dynamic compression of functionally-graded metal syntactic foams. Composite Structures, 2021, 261, 113308.	3.1	30
11	Lattice Monte Carlo and Experimental Analyses of the Thermal Conductivity of Randomly Shaped Cellular Aluminum. Advanced Engineering Materials, 2009, 11, 843-847.	1.6	29
12	Reaction of a Ni-coated Al nanoparticle to form B ₂ -NiAl: A molecular dynamics study. Philosophical Magazine Letters, 2009, 89, 815-830.	0.5	26
13	Molecular dynamics simulation of alloying in a Ti-coated Al nanoparticle. Intermetallics, 2012, 22, 193-202.	1.8	24
14	Molecular dynamics determination of the time-temperature transformation diagram for crystallization of an undercooled liquid Ni ₅₀ Al ₅₀ alloy. Acta Materialia, 2011, 59, 6412-6419.	3.8	23
15	Analysis of the Effective Diffusivity in Nanocrystalline Materials. Journal of Metastable and Nanocrystalline Materials, 2004, 19, 25-34.	0.1	21
16	Molecular dynamics simulation of the thermophysical properties of an undercooled liquid Ni ₅₀ Al ₅₀ alloy. Computational Materials Science, 2010, 50, 465-473.	1.4	21
17	Interdiffusion and surface-sandwich ordering in initial Ni-core-Pd-shell nanoparticle. Physical Chemistry Chemical Physics, 2009, 11, 3233.	1.3	20
18	Molecular dynamics study of reaction pathways in an Al-coated Ni nanoparticle. Intermetallics, 2011, 19, 934-941.	1.8	19

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19	Molecular dynamics simulation of alloying in an Al-coated Ti nanoparticle. Computational Materials Science, 2013, 79, 316-325.	1.4	19
20	Thermotransport in binary system: case study on Ni ₅₀ Al ₅₀ melt. Philosophical Magazine, 2014, 94, 3574-3602.	0.7	19
21	Molecular dynamics prediction of phonon-mediated thermal conductivity of f.c.c. Cu. Philosophical Magazine, 2014, 94, 731-751.	0.7	18
22	Molecular dynamics study of density, surface energy and self-diffusion in a liquid Ni ₅₀ Al ₅₀ alloy. Computational Materials Science, 2010, 50, 331-337.	1.4	16
23	Molecular dynamics simulation of surface segregation in a (110) B ₂ -NiAl thin film. Physical Chemistry Chemical Physics, 2011, 13, 1214-1221.	1.3	16
24	Molecular dynamics simulation of diffusion in a (110) B ₂ -NiAl film. Intermetallics, 2011, 19, 848-854.	1.8	16
25	Finite Difference Solution of the Diffusion Equation and Calculation of the Interdiffusion Coefficient using the Sauer-Freize and Hall Methods in Binary Systems. Procedia Engineering, 2015, 105, 570-575.	1.2	15
26	Thermal Conductivity Enhancement of Compact Heat Sinks Using Cellular Metals. Defect and Diffusion Forum, 0, 273-276, 222-226.	0.4	14
27	The Lattice Monte Carlo Method for Solving Phenomenological Mass and Thermal Diffusion Problems. Defect and Diffusion Forum, 0, 279, 13-22.	0.4	14
28	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.	0.5	14
29	Molecular dynamics study of phonon-mediated thermal transport in a Ni ₅₀ Al ₅₀ melt: case analysis of the influence of the process on the kinetics of solidification. Philosophical Magazine, 2015, 95, 90-111.	0.7	12
30	Influence of the interatomic potential on thermotransport in binary liquid alloys: case study on NiAl. Philosophical Magazine, 2016, 96, 3054-3074.	0.7	12
31	Fatigue characterization of functionally graded ZA27 alloy syntactic foams. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2020, 798, 140255.	2.6	12
32	Formation of a Hollow Binary Alloy Nanosphere: A Kinetic Monte Carlo Study. Journal of Nano Research, 0, 7, 11-17.	0.8	11
33	Interdiffusion and thermotransport in NiAl liquid alloys. Philosophical Magazine, 2018, 98, 2221-2246.	0.7	11
34	Calculation of the Effective Thermal Conductivity in Composites Using Finite Element and Monte Carlo Methods. Materials Science Forum, 2007, 553, 51-56.	0.3	10
35	Mass and thermal transport in liquid Cu-Ag alloys. Philosophical Magazine, 2019, 99, 468-491.	0.7	10
36	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.	1.4	10

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37	Stability of Hollow Nanospheres: A Molecular Dynamics Study. Solid State Phenomena, 0, 129, 125-130.	0.3	9
38	The Synthesis, Stability and Shrinkage of Hollow Nanoparticles: An Overview. Journal of Nano Research, 2009, 7, 19-26.	0.8	9
39	Decomposition model for phonon thermal conductivity of a monatomic lattice. Philosophical Magazine, 2014, 94, 3992-4014.	0.7	9
40	Bridging Different Length and Time Scales in Diffusion Problems Using a Lattice Monte Carlo Method. Solid State Phenomena, 2007, 129, 1-10.	0.3	8
41	Collective and Tracer Diffusion via a Defect Cluster in LSGM. Defect and Diffusion Forum, 2007, 263, 81-86.	0.4	8
42	Determination of the lattice thermal conductivity of the TiO ₂ polymorphs rutile and anatase by molecular dynamics simulation. Computational Condensed Matter, 2018, 17, e00342.	0.9	8
43	Measurement of Interdiffusion and Tracer Diffusion Coefficients in FCC Co-Cr-Fe-Ni Multi-Principal Element Alloy. Journal of Phase Equilibria and Diffusion, 2021, 42, 696-707.	0.5	8
44	Atomistic Modeling of Diffusion in the TiAl Compound. Defect and Diffusion Forum, 2005, 237-240, 271-276.	0.4	7
45	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, 0, 273-276, 216-221.	0.4	7
46	Interdiffusion in Intermetallics. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2013, 44, 4417-4421.	1.1	7
47	The Thermal Conductivity of Magnesite, Dolomite and Calcite as Determined by Molecular Dynamics Simulation. , 0, 19, 18-34.		7
48	Comments on "Experimental assessment of the thermodynamic factor for diffusion in CoCrFeNi and CoCrFeMnNi high entropy alloys". Scripta Materialia, 2019, 172, 110-112.	2.6	7
49	Chemical Diffusion in Ni ₃ Al. Defect and Diffusion Forum, 2001, 194-199, 541-546.	0.4	6
50	Thermal Properties of Composite Materials and Porous Media: Lattice-Based Monte Carlo Approaches. , 0, , 73-95.		6
51	Lattice-Based Walks and the Monte Carlo Method for Addressing Mass, Thermal and Elasticity Problems. Defect and Diffusion Forum, 0, 283-286, 13-23.	0.4	6
52	Diffusion correlation effects of molybdenum and silicon in molybdenum disilicide. Philosophical Magazine, 2011, 91, 3727-3743.	0.7	6
53	Thermal Conductivity Computations of Sintered Hollow Sphere Structures. Metals, 2012, 2, 113-121.	1.0	6
54	Theoretical Study of the Heat of Transport in a Liquid Ni ₅₀ Al ₅₀ Alloy: Green-Kubo Approach. , 0, 2, 159-189.		6

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55	Investigation of Interdiffusion in High Entropy Alloys: Application of the Random Alloy Model. , 0, 22, 94-108.		6
56	Tracer Correlation, Collective Correlation and Vacancy Wind Factors in Intermetallics Taking the B2 Structures. Defect and Diffusion Forum, 2000, 179-180, 1-16.	0.4	5
57	Time Dependence of the Segregation of Diffusing Solute in Nanocrystalline Materials. Materials Research Society Symposia Proceedings, 2002, 731, 541.	0.1	5
58	The Six-Jump Cycle Diffusion Mechanism in Non-Stoichiometric B2 Intermetallics: the Vacancy-Wind Factor. Defect and Diffusion Forum, 2003, 213-215, 95-106.	0.4	5
59	Theoretical Analysis and Atomistic Modelling of Diffusion and Stability of Pure Element Hollow Nanospheres and Nanotubes. Defect and Diffusion Forum, 0, 277, 21-26.	0.4	5
60	Investigation of Harrison Type-A, B and Intermediate AB Kinetics Regimes in Grain Boundary Diffusion. Defect and Diffusion Forum, 2009, 283-286, 697-704.	0.4	5
61	Solving Complex Thermal and Mass Transport Problems with the Lattice Monte Carlo Method. Materials Science Forum, 2010, 654-656, 1476-1481.	0.3	5
62	The Harrison Diffusion Kinetics Regimes in Grain Boundary Diffusion: Lattice Monte Carlo Modelling of the Effect of Segregation. Defect and Diffusion Forum, 0, 309-310, 9-18.	0.4	5
63	A structural model for surface-enhanced stabilization in some metallic glass formers. Philosophical Magazine Letters, 2013, 93, 50-57.	0.5	5
64	Phonon Thermal Conductivity of F.C.C. Cu by Molecular Dynamics Simulation. Defect and Diffusion Forum, 0, 336, 169-184.	0.4	5
65	Phonon-mediated heat dissipation in a monatomic lattice: case study on Ni. Philosophical Magazine, 2015, 95, 3640-3673.	0.7	5
66	Activation volume dominated diffusivity of Ni50Al50 melt under extreme conditions. Computational Materials Science, 2020, 171, 109263.	1.4	5
67	Novel Interdiffusion Analysis in Multicomponent Alloys - Part 2: Application to Quaternary, Quinary and Higher Alloys. , 0, 29, 179-203.		5
68	A Self-Consistent Theory of Atomic Transport in the B2 Ordered Alloy: The Sum Rule. Defect and Diffusion Forum, 2001, 194-199, 547-552.	0.4	4
69	A Simple Iterative Method for Analysing Experimental Tracer Diffusivities in Concentrated Binary Alloys. Defect and Diffusion Forum, 2004, 224-225, 127-0.	0.4	4
70	Random-Walk Calculations in Intermetallic Compounds. Defect and Diffusion Forum, 2005, 237-240, 291-302.	0.4	4
71	Stability and Shrinkage by Diffusion in Hollow Nanotubes. Defect and Diffusion Forum, 2007, 266, 39-47.	0.4	4
72	Modelling of the Formation of Pd-Ni Alloy Nanoparticles by Interdiffusion. Defect and Diffusion Forum, 0, 277, 207-212.	0.4	4

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73	A Lattice Monte Carlo Analysis of Thermal Transport in Phase Change Materials. Defect and Diffusion Forum, 0, 297-301, 154-161.	0.4	4
74	Numerical Characterization of Anisotropic Heat Sink Composites. Materials Science Forum, 0, 654-656, 1500-1503.	0.3	4
75	Vibrational contribution to thermal transport in liquid copper: Equilibrium molecular dynamics study. Computational Materials Science, 2015, 96, 229-236.	1.4	4
76	Insight into lattice thermal impedance via equilibrium molecular dynamics: case study on Al. Philosophical Magazine, 2016, 96, 596-619.	0.7	4
77	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.	0.5	4
78	Phenomenological Aspects of Grain Boundary Diffusion. Defect and Diffusion Forum, 2006, 258-260, 483-490.	0.4	3
79	Monte Carlo Modelling of the Effective Diffusivity in Composite Material. Defect and Diffusion Forum, 2007, 261-262, 103-108.	0.4	3
80	Exploration of the Transition from Harrison Type-A Kinetics to Type-B Kinetics Regimes in Grain Boundary Diffusion. Defect and Diffusion Forum, 0, 273-276, 425-430.	0.4	3
81	First-principles calculations of a corrugated anatase TiO ₂ surface. Computational Materials Science, 2012, 51, 78-82.	1.4	3
82	Molecular Dynamics Prediction of the Influence of Composition on Thermotransport in Ni-Al Melts. , 0, 12, 93-110.		3
83	Computer simulation of thermodynamic factors in Ni-Al and Cu-Ag liquid alloys. Computational Materials Science, 2019, 166, 124-135.	1.4	3
84	An overview of thermotransport in fluorite-related ionic oxides. Zeitschrift Fur Physikalische Chemie, 2022, 236, 1103-1124.	1.4	3
85	Diffusion in the Presence of Grain Boundaries: a Variable Length Scale Simulation Method. Materials Research Society Symposia Proceedings, 2001, 677, 7201.	0.1	2
86	Visualization of the Vacancy-Wind Effect Occurring in Chemical Diffusion and Ionic Conductivity in Solids. Defect and Diffusion Forum, 2008, 273-276, 431-444.	0.4	2
87	Atomic Mechanism of Carbon Diffusion in Cementite. Defect and Diffusion Forum, 0, 277, 101-106.	0.4	2
88	Carbon Diffusion in Cementite: A Molecular Dynamics Study. Defect and Diffusion Forum, 2009, 283-286, 24-29.	0.4	2
89	Composition Effect on Shrinkage of Hollow Binary Alloy Nanospheres. Defect and Diffusion Forum, 0, 289-292, 665-672.	0.4	2
90	Parametric Analysis of the Classification of Harrison Kinetics Regimes in Grain Boundary Diffusion. Defect and Diffusion Forum, 2010, 297-301, 1226-1231.	0.4	2

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91	Two-fluid nature of phonon heat conduction in a monatomic lattice. Philosophical Magazine, 2015, 95, 2571-2595.	0.7	2
92	Molecular Dynamics Determination of the Lattice Thermal Conductivity of the Cubic Phase of Hafnium Dioxide. , 0, 27, 177-185.		2
93	Exact phenomenological theory for thermotransport in a solid binary alloy. Philosophical Magazine Letters, 2021, 101, 123-131.	0.5	2
94	Calculation of Tracer and Chemical Diffusion Coefficients in the Intermetallic Compound $\hat{\text{I}}^2\text{-AgMg}$. Defect and Diffusion Forum, 2003, 224-225, 45-52.	0.4	1
95	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.	1.3	1
96	Collective Correlation Factors in Random Non-Stoichiometric Intermetallic Compounds. Defect and Diffusion Forum, 2005, 247-248, 1-8.	0.4	1
97	Tracer Diffusion by Six-Jump-Cycles in Nonstoichiometric B2 Intermetallic Compounds. Defect and Diffusion Forum, 2005, 247-248, 9-20.	0.4	1
98	Vacancy-Wind Factors and Collective Correlation Factors in Nonstoichiometric B2 Intermetallic Compounds. Defect and Diffusion Forum, 2006, 251-252, 69-78.	0.4	1
99	Molecular Dynamics Study of Carbon Diffusion in Austenite. Defect and Diffusion Forum, 2006, 258-260, 253-258.	0.4	1
100	Interdiffusion Data in Multicomponent Alloys as a Source of Quantitative Fundamental Diffusion Information. Defect and Diffusion Forum, 2007, 263, 1-10.	0.4	1
101	Surface-Sandwich Segregation Phenomena in Bimetallic Ag-Ni and Pd-Ni Nanoparticles: A Molecular Dynamics Study. Defect and Diffusion Forum, 0, 289-292, 657-664.	0.4	1
102	The Nature of the Vacancy-Wind Effect Occurring in Diffusion via Six-Jump-Cycles in B2 Intermetallics. Defect and Diffusion Forum, 0, 297-301, 1218-1225.	0.4	1
103	Compressive Properties of Core-Shell Foam under Uni-Axial Loading Based on Experimental and Numerical Analysis. Applied Mechanics and Materials, 2014, 597, 121-126.	0.2	1
104	The Vacancy-Wind Factor and the Manning Factor Occurring in Interdiffusion and Ionic Conductivity in Solids. , 0, 22, 170-183.		1
105	Pores shrinkage and growth in polycrystalline hollow nanoparticles and nanotubes. Scripta Materialia, 2020, 180, 93-96.	2.6	1
106	The Lattice Monte Carlo Method for Solving Phenomenological Mass and Thermal Diffusion Problems. Defect and Diffusion Forum, 0, , 13-22.	0.4	1
107	The Diffusion Isotope Effect and Diffusion Mechanism in Liquid Cu-Ag and Cu-Ni Alloys. Defect and Diffusion Forum, 0, 413, 136-145.	0.4	1
108	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.	0.1	0

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109	Expressions for the effective diffusivity in materials with interphase boundaries. Materials Research Society Symposia Proceedings, 2004, 819, N3.14.1.	0.1	0
110	Tracer Diffusion in Nonstoichiometric Intermetallic Compounds with Random Mixing on Each Sublattice. Defect and Diffusion Forum, 2005, 247-248, 21-28.	0.4	0
111	Contribution to the Theory of Demixing of Yttrium in Ytria-Stabilized-Zirconia in an Electric Field. Advances in Science and Technology, 2006, 46, 42.	0.2	0
112	Analysis of Interdiffusion and Intrinsic Diffusion in Multicomponent Alloys to Obtain Information about Diffusion Mechanisms. Defect and Diffusion Forum, 2006, 258-260, 237-246.	0.4	0
113	Cation Diffusion and Demixing in Ytria Stabilized Zirconia: Comparison of Assumptions of Constant Electric Field and Constant Current. Defect and Diffusion Forum, 2006, 258-260, 247-252.	0.4	0
114	Six-Jump-Cycle Mechanism for Collective Correlations in Nonstoichiometric Intermetallic Compounds. Defect and Diffusion Forum, 2006, 251-252, 59-68.	0.4	0
115	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.	0.4	0
116	Extraction of Diffusion Correlation Information from Tracer, Interdiffusion and Ionic Conductivity Data. Advances in Science and Technology, 2006, 46, 54.	0.2	0
117	Calculation of Phenomenological Coefficients by Monte Carlo Computer Simulation Methods. Defect and Diffusion Forum, 2006, 249, 27-34.	0.4	0
118	Non-Random Interaction of Vacancies with Atoms during Interdiffusion and Ionic Conductivity in Materials. Defect and Diffusion Forum, 2007, 266, 119-130.	0.4	0
119	Modelling of Oxygen Diffusion and Segregation at Interfaces in Ag-MgO Composites. Defect and Diffusion Forum, 2007, 266, 29-38.	0.4	0
120	Theoretical Studies of Diffusion Kinetics in Austenite. Defect and Diffusion Forum, 2008, 273-276, 455-460.	0.4	0
121	Diffusion Kinetics Analysis of Cation Diffusion in YSZ and LSGM. Defect and Diffusion Forum, 0, 273-276, 445-454.	0.4	0
122	Finite Element Modelling of Oxygen Diffusion and Segregation at Interfaces in Ag-MgO Composites: Parametric Studies. Defect and Diffusion Forum, 0, 273-276, 461-466.	0.4	0
123	In-Diffusion and Out-Diffusion of Oxygen from a Composite Containing Random Traps. Solid State Phenomena, 0, 139, 35-40.	0.3	0
124	Relationships between chemical and tracer diffusion coefficients in strongly ionic crystals. International Journal of Materials Research, 2022, 95, 870-875.	0.1	0