Vsevolod Razumovskiy

List of Publications by Year
in descending order

60	1,418	279701	360920
papers	citations	23 h-index	35 g-index

62	62	62	1029
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Influence of alloying on thermodynamic properties of AlCoCrFeNiTi high entropy alloys from DFT calculations. Computational Materials Science, 2022, 202, 110952.	1.4	9
2	Solute drag assessment of grain boundary migration in Au. Acta Materialia, 2022, 224, 117473.	3.8	16
3	The effect of solute atoms on the bulk and grain boundary cohesion in Ni: Implications for hydrogen embrittlement. Materialia, 2022, 21, 101293.	1.3	10
4	Selected Topics on Integrated Computational Material, Process, and Product Engineering. BHM-Zeitschrift Fuer Rohstoffe Geotechnik Metallurgie Werkstoffe Maschinen-Und Anlagentechnik, 2022, 167, 10-14.	0.4	1
5	Solubility and segregation of B in paramagnetic fcc Fe. Physical Review Materials, 2022, 6, .	0.9	4
6	Hydrogen assisted intergranular cracking of alloy 725: The effect of boron and copper alloying. Corrosion Science, 2022, 203, 110331.	3.0	8
7	Atomic Interactions and Orderâ€“Disorder Transition in FCC-Type FeCoNiAl1-xTix High-Entropy Alloys. Materials, 2022, 15, 3992.	1.3	2
8	Effect of alloying elements on hydrogen enhanced decohesion in bcc iron. Computational Materials Science, 2021, 188, 110215.	1.4	25
9	Surface and segregation energies of Ag based alloys with Ni, Co and Fe: Direct experimental measurement and DFT study. Acta Materialia, 2021, 205, 116565.	3.8	17
10	Hydrogen segregation near a crack tip in nickel. Scripta Materialia, 2021, 194, 113697.	2.6	18
11	An In Situ Synchrotron Dilatometry and Atomistic Study of Martensite and Carbide Formation during Partitioning and Tempering. Materials, 2021, 14, 3849.	1.3	0
12	Modern Powder Metallurgy: Chemical Composition Design for Improved Heat Resistant Alloys. Metals, 2021, 11, 1215.	1.0	1
13	An atomistic view on Oxygen, antisites and vacancies in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si165.svg"><mml:mrow><mml:mi>Î³</mml:mi></mml:mrow></mml:math>-TiAl phase. Computational Materials Science, 2021, 197, 110655.	1.4	5
14	Grain boundary segregation in Ni-base alloys: A combined atom probe tomography and first principles study. Acta Materialia, 2021, 221, 117354.	3.8	37
15	Hydrogen-enhanced intergranular failure of sulfur-doped nickel grain boundary: In situ electrochemical micro-cantilever bending vs.ÂDFT. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2020, 794, 139967.	2.6	27
16	Verification of the generalised chemical potential for stress-driven hydrogen diffusion in nickel. Philosophical Magazine Letters, 2020, 100, 513-523.	0.5	16
17	Hydrogen Trapping in bcc Iron. Materials, 2020, 13, 2288.	1.3	42
18	Segregation of Refractory Metals at Grain Boundaries in High-Temperature Alloys. Russian Metallurgy (Metally), 2020, 2020, 1292-1299.	0.1	4

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19	Thermodynamic and mechanical stability of Ni3X-type intermetallic compounds. Intermetallics, 2019, 114, 106604.	1.8	33
20	Hydrogen-enhanced decohesion mechanism of the special <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si55.svg"><mml:mrow><mml:mi mathvariant="normal">Î£</mml:mi></mml:mrow></mml:math>5(0 1 2)[1 0 0] grain boundary in Ni with Mo and C solutes. Computational Materials Science, 2019, 167, 100-110.	1.4	37
21	Ab Initio Study of Elastic and Mechanical Properties in FeCrMn Alloys. Materials, 2019, 12, 1129.	1.3	8
22	A synergistic reinforcement of Re and W for ideal shear strengths of Î³â€²-Ni3Al phases. Journal of Physics and Chemistry of Solids, 2019, 131, 34-43.	1.9	18
23	Effect of carbon on elastic properties and microstructure of maraging steel: First-principles and phase-field study. Computational Materials Science, 2019, 162, 1-11.	1.4	5
24	Kinetics of interaction of impurity interstitials with dislocations revisited. Progress in Materials Science, 2019, 101, 172-206.	16.0	34
25	Solute segregation in Cu: DFT vs. Experiment. Acta Materialia, 2018, 147, 122-132.	3.8	45
26	Point defects at the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:mtext>Î£</mml:mtext><mml:mn>5</mml:mn></mml:mrow></mml:math>(012)[100] grain boundary in TiN and the early stages of Cu diffusion: An ab initio study. Acta Materialia, 2018, 144, 496-504.	3.8	20
27	New Cr-Ni-Base Alloy for High-Temperature Applications Designed on the Basis of First Principles Calculations. Advances in Condensed Matter Physics, 2018, 2018, 1-8.	0.4	13
28	Impact of correlative defects induced by double Re-addition on the ideal shear strength of Î³â€²-Ni3Al phases. Computational Materials Science, 2018, 152, 408-416.	1.4	19
29	Thermal expansion coefficient of WRe alloys from first principles. Physical Review B, 2017, 96, .	1.1	17
30	Effect of Đ° Number of Transition Metals on the Cohesive Properties of Cr-Ni-Base Alloys. Materials Science Forum, 2016, 879, 1998-2002.	0.3	1
31	Ab initiostudy of Cu impurity diffusion in bulk TiN. Physical Review B, 2016, 94, .	1.1	14
32	Effective interactions and atomic ordering in Ni-rich Ni-Re alloys. Physical Review B, 2016, 94, .	1.1	19
33	Effect of thermal lattice expansion on the stacking fault energies of fcc Fe and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Fe</mml:mi><mml:mn>x</mml:mn></mml:msub></mml:mrow></mml:math>Mn_{1−x} alloys. Physical Review B, 2016, 93, .	1.1	20
34	Ab initio description of segregation and cohesion of grain boundaries in Wâ€“25 at.% Re alloys. Acta Materialia, 2015, 88, 180-189.	3.8	87
35	Formation and interaction of point defects in group IVb transition metal carbides and nitrides. Computational Materials Science, 2015, 104, 147-154.	1.4	36
36	A first-principles study of cementite (Fe3C) and its alloyed counterparts: Structural properties, stability, and electronic structure. Computational Materials Science, 2015, 110, 169-181.	1.4	34

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37	First-principles-aided design of a new Ni-base superalloy: Influence of transition metal alloying elements on grain boundary and bulk cohesion. Acta Materialia, 2015, 82, 369-377.	3.8	119
38	Ab initio Calculations as a Tool for Predicting Materials Properties. BHM-Zeitschrift Fuer Rohstoffe Geotechnik Metallurgie Werkstoffe Maschinen-Und Anlagentechnik, 2014, 159, 367-370.	0.4	3
39	Core polarity of screw dislocations in Feâ€“Co alloys. Philosophical Magazine Letters, 2014, 94, 334-341.	0.5	17
40	Effect of carbon vacancies on thermodynamic properties of TiCâ€“ZrC mixed carbides. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2014, 46, 87-91.	0.7	28
41	Self diffusion anomaly in ferromagnetic metals: A density-functional-theory investigation of magnetically ordered and disordered Fe and Co. Acta Materialia, 2014, 70, 130-136.	3.8	39
42	Vacancy-cluster mechanism of metal-atom diffusion in substoichiometric carbides. Physical Review B, 2013, 87, .	1.1	31
43	Role of magnetism in Cu precipitation in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>-Fe. Physical Review B, 2013, 88, .	1.1	31
44	Temperature dependence of stacking-fault and anti-phase boundary energies in Al Sc fromab initiocalculations. Philosophical Magazine, 2013, 93, 3423-3441.	0.7	5
45	First-principles based thermodynamic model of phase equilibria in bcc Fe-Cr alloys. Physical Review B, 2012, 86, .	1.1	48
46	Spin-wave method for the total energy of paramagnetic state. Physical Review B, 2012, 85, .	1.1	57
47	Multi-length scale modeling of martensitic transformations in stainless steels. Acta Materialia, 2012, 60, 6508-6517.	3.8	31
48	Effect of Temperature on the Elastic Anisotropy of Pure Fe and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Fe</mml:mi><mml:mn>0.9</mml:mn></mml:msub><mml:msub><mml:mi>Cr</mml:mi><mml:mn Alloy. Physical Review Letters, 2011, 107, 205504.	2.9	60
49	The effect of alloying elements on grain boundary and bulk cohesion in aluminum alloys: An ab initio study. Scripta Materialia, 2011, 65, 926-929.	2.6	56
50	Effect of alloying elements and impurities on interface properties in aluminum alloys. Physics of the Solid State, 2011, 53, 2189-2193.	0.2	12
51	First-principles study of elastic properties of Cr- and Fe-rich Fe-Cr alloys. Physical Review B, 2011, 84, .	1.1	49
52	The Influence of Alloying Elements on Grain Boundary and Bulk Cohesion in Aluminum Alloys: Ab Initio Study. Advanced Materials Research, 2011, 409, 417-422.	0.3	1
53	New generation of Ni-based superalloys designed on the basis of first-principles calculations. Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing, 2008, 497, 18-24.	2.6	38
54	Theoretical analysis of the alloying system and design of new nickel-base superalloys. Doklady Physics, 2008, 53, 438-441.	0.2	11

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55	Ab initio calculations of elastic properties of Ptâ€“Sc alloys. Intermetallics, 2008, 16, 982-986.	1.8	23
56	New Pt-based Superalloy System Designed from First Principles. Materials Research Society Symposia Proceedings, 2008, 1128, 52801.	0.1	0
57	Analysis of the Alloying System in Ni-Base Superalloys Based on <i>Ab Initio</i> Study of Impurity Segregation to Ni Grain Boundary. Advanced Materials Research, 0, 278, 192-197.	0.3	18
58	Effect of the Particle Size of Î³â€™ Phase on the Mechanical Properties of Ni Base Superalloy. Advanced Materials Research, 0, 278, 96-101.	0.3	8
59	<i>Ab Initio</i> Calculations of Kinetic Properties in ZrC and TiC Carbides. Solid State Phenomena, 0, 172-174, 990-995.	0.3	12
60	Effect of Alloying Elements and Impurity (N) on Bulk and Grain Boundary Cohesion in Cr-Base Alloys. Advanced Materials Research, 0, 1119, 569-574.	0.3	1