

Mohsen Asle Zaeem

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

124
papers

2,532
citations

29
h-index

45
g-index

134
ext. papers

3,259
ext. citations

4.8
avg, IF

6.12
L-index

#	Paper	IF	Citations
124	From fundamental to CO and COCl gas sensing properties of pristine and defective SiBN monolayers.. <i>Physical Chemistry Chemical Physics</i> , 2022 ,	3.6	1
123	A temperature-dependent atomistic-informed phase-field model to study dendritic growth. <i>Journal of Crystal Growth</i> , 2022 , 579, 126461	1.6	1
122	Modified embedded-atom method interatomic potentials for Al-Cu, Al-Fe and Al-Ni binary alloys: From room temperature to melting point. <i>Computational Materials Science</i> , 2022 , 201, 110902	3.2	7
121	Interactive Effects of Interfacial Energy Anisotropy and Solute Transport on Solidification Patterns of Al-Cu Alloys. <i>Acta Materialia</i> , 2022 , 117859	8.4	2
120	Formation energies, electronic properties and elemental diffusion of Cu _x Ir _{1-x} Nb (GRCop) alloys. <i>Physica B: Condensed Matter</i> , 2022 , 413909	2.8	0
119	Unveiling the effect of vacancy defects on structural, mechanical, electronic and diffusion properties of copper (I) iodide. <i>Scripta Materialia</i> , 2022 , 213, 114634	5.6	1
118	Ca ₂ C MXene monolayer as a superior anode for metal-ion batteries. <i>2D Materials</i> , 2021 , 8, 035015	5.9	8
117	Effects of applied load on formation and reorientation of zirconium hydrides: A multiphase field modeling study. <i>Computational Materials Science</i> , 2021 , 192, 110367	3.2	2
116	Quantitative prediction of rapid solidification by integrated atomistic and phase-field modeling. <i>Acta Materialia</i> , 2021 , 211, 116885	8.4	4
115	Superelasticity and shape memory effect in zirconia nanoparticles. <i>Extreme Mechanics Letters</i> , 2021 , 46, 101301	3.9	0
114	Nanotwin-induced strengthening in silicon: A molecular dynamics study. <i>International Journal of Mechanical Sciences</i> , 2021 , 189, 105990	5.5	5
113	Phase-field modeling of crack propagation in polycrystalline materials. <i>Computational Materials Science</i> , 2021 , 186, 110057	3.2	10
112	Transformation-induced fracture toughening in CuAlBe shape memory alloys: A phase-field study. <i>International Journal of Mechanical Sciences</i> , 2021 , 192, 106144	5.5	4
111	Unveiling the role of atomic defects on the electronic, mechanical and elemental diffusion properties in CuS. <i>Scripta Materialia</i> , 2021 , 192, 94-99	5.6	7
110	Quantitative phase-field modeling of solute trapping in rapid solidification. <i>Acta Materialia</i> , 2021 , 205, 116562	8.4	11
109	Solution processed Ni ₂ Co layered double hydroxides for high performance electrochemical sensors. <i>Applied Surface Science</i> , 2021 , 541, 148270	6.7	5
108	Phosgene Gas Sensing of Ti ₂ CT ₂ (T = F□O□OH)MXenes. <i>Advanced Theory and Simulations</i> , 2021 , 4, 2000250	3.5	8

107	Design of NiTi-based shape memory microcomposites with enhanced elastocaloric performance by a fully thermomechanical coupled phase-field model. <i>Materials and Design</i> , 2021 , 207, 109898	8.1	5
106	Liquid ordering induced heterogeneities in homogeneous nucleation during solidification of pure metals. <i>Journal of Materials Science and Technology</i> , 2021 ,	9.1	3
105	Effects of cleavage plane and material strength on fracture of polycrystalline brittle materials: A phase-field modeling study. <i>Computational Materials Science</i> , 2021 , 197, 110642	3.2	3
104	Superior sensing performance of two-dimensional ruthenium carbide (2D-RuC) in detection of NO, NO ₂ and NH ₃ gas molecules. <i>Applied Surface Science</i> , 2021 , 563, 150232	6.7	6
103	A molecular dynamics study of domain switching in BiFeO ₃ nanofilm under DC electric field. <i>Computational Materials Science</i> , 2021 , 199, 110718	3.2	0
102	Hydrogen-induced tunable electronic and optical properties of a two-dimensional penta-PtN monolayer. <i>Physical Chemistry Chemical Physics</i> , 2021 , 23, 10409-10417	3.6	4
101	Strain-induced work function in h-BN and BCN monolayers. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020 , 123, 114180	3	19
100	On the elastocaloric effect in CuAlBe shape memory alloys: A quantitative phase-field modeling approach. <i>Computational Materials Science</i> , 2020 , 183, 109808	3.2	8
99	Oxidation Induced Stresses in High-Temperature Oxidation of Steel: A Multiphase Field Study. <i>Metals</i> , 2020 , 10, 801	2.3	0
98	StoneWales Defect Induced Performance Improvement of BC ₃ Monolayer for High Capacity Lithium-Ion Rechargeable Battery Anode Applications. <i>Journal of Physical Chemistry C</i> , 2020 , 124, 5910-5919	3.8	29
97	Nanoscale flaw tolerance behaviour of polycrystalline tetragonal zirconia nanopillars. <i>International Journal of Mechanical Sciences</i> , 2020 , 173, 105405	5.5	3
96	Insights on Solidification of Mg and MgAl Alloys by Large Scale Atomistic Simulations. <i>Minerals, Metals and Materials Series</i> , 2020 , 51-53	0.3	
95	Modified embedded-atom method potential for high-temperature crystal-melt properties of TiNi alloys and its application to phase field simulation of solidification. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2020 , 28, 015006	2	11
94	Effects of grain orientations and pre-existing defects on mechanical properties and deformation mechanisms of polycrystalline yttria-stabilized tetragonal zirconia. <i>Materialia</i> , 2020 , 9, 100553	3.2	2
93	An Asymmetric Elasto-Plastic Phase-Field Model for Shape Memory Effect, Pseudoelasticity and Thermomechanical Training in Polycrystalline Shape Memory Alloys. <i>Acta Materialia</i> , 2020 , 201, 580-595	8.4	9
92	Review of Peritectic Solidification Mechanisms and Effects in Steel Casting. <i>Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science</i> , 2020 , 51, 1875-1903	2.5	12
91	Two-Dimensional BoronPhosphorus Monolayer for Reversible NO ₂ Gas Sensing. <i>ACS Applied Nano Materials</i> , 2020 , 3, 10073-10081	5.6	17
90	A new planar BCN lateral heterostructure with outstanding strength and defect-mediated superior semiconducting to metallic properties. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 22066-22077	3.6	15

89	Effects of twin boundaries and pre-existing defects on mechanical properties and deformation mechanisms of yttria-stabilized tetragonal zirconia. <i>Journal of the European Ceramic Society</i> , 2020 , 40, 108-114	6	11
88	A phase-field model for non-isothermal phase transformation and plasticity in polycrystalline yttria-stabilized tetragonal zirconia. <i>Acta Materialia</i> , 2020 , 191, 111-123	8.4	11
87	Predicting effective fracture toughness of ZrB ₂ -based ultra-high temperature ceramics by phase-field modeling. <i>Materials and Design</i> , 2020 , 192, 108713	8.1	10
86	Competition between formation of Al ₂ O ₃ and Cr ₂ O ₃ in oxidation of Al _{0.3} CoCrCuFeNi high entropy alloy: A first-principles study. <i>Scripta Materialia</i> , 2019 , 168, 139-143	5.6	12
85	Nanoscale self-healing mechanisms in shape memory ceramics. <i>Npj Computational Materials</i> , 2019 , 5,	10.9	14
84	Evolution of solidification defects in deformation of nano-polycrystalline aluminum. <i>Computational Materials Science</i> , 2019 , 163, 176-185	3.2	17
83	Understanding specimen- and grain-size effects on nanoscale plastic deformation mechanisms and mechanical properties of polycrystalline yttria-stabilized tetragonal zirconia nanopillars. <i>European Journal of Mechanics, A/Solids</i> , 2019 , 76, 80-90	3.7	10
82	Combined molecular dynamics and phase field simulation investigations of crystal-melt interfacial properties and dendritic solidification of highly undercooled titanium. <i>Computational Materials Science</i> , 2019 , 163, 218-229	3.2	21
81	A Review of Multi-Scale Computational Modeling Tools for Predicting Structures and Properties of Multi-Principal Element Alloys. <i>Metals</i> , 2019 , 9, 254	2.3	4
80	Effects of Crystal Orientation and Pre-existing Defects on Nanoscale Mechanical Properties of Yttria-Stabilized Tetragonal Zirconia Thin Films. <i>Jom</i> , 2019 , 71, 3869-3875	2.1	2
79	Effects of solidification defects on nanoscale mechanical properties of rapid directionally solidified Al-Cu Alloy: A large scale molecular dynamics study. <i>Journal of Crystal Growth</i> , 2019 , 527, 125255	1.6	11
78	Thermodynamic and kinetic behavior of low-alloy steels: An atomic level study using an Fe-Mn-Si-C modified embedded atom method (MEAM) potential. <i>Materialia</i> , 2019 , 8, 100473	3.2	7
77	Size effect in molecular dynamics simulation of nucleation process during solidification of pure metals: investigating modified embedded atom method interatomic potentials. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2019 , 27, 085015	2	6
76	Fatigue-resistant high-performance elastocaloric materials made by additive manufacturing. <i>Science</i> , 2019 , 366, 1116-1121	33.3	103
75	In Situ Bottom-up Synthesis of Porphyrin-Based Covalent Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2019 , 141, 19560-19564	16.4	29
74	A review of computational modeling techniques in study and design of shape memory ceramics. <i>Computational Materials Science</i> , 2019 , 160, 120-136	3.2	16
73	Probing the shear modulus of two-dimensional multiplanar nanostructures and heterostructures. <i>Nanoscale</i> , 2018 , 10, 5280-5294	7.7	40
72	Nickel telluride as a bifunctional electrocatalyst for efficient water splitting in alkaline medium. <i>Journal of Materials Chemistry A</i> , 2018 , 6, 7608-7622	13	140

71	Formation of chromium-iron carbide by carbon diffusion in AlXCoCrFeNiCu high-entropy alloys. <i>Materials Research Letters</i> , 2018 , 6, 321-326	7.4	9
70	Role of grain boundaries in determining strength and plastic deformation of yttria-stabilized tetragonal zirconia bicrystals. <i>Journal of Materials Science</i> , 2018 , 53, 5706-5718	4.3	11
69	A modified phase-field model for quantitative simulation of crack propagation in single-phase and multi-phase materials. <i>Engineering Fracture Mechanics</i> , 2018 , 200, 339-354	4.2	15
68	Phase Exploration and Identification of Multinary Transition-Metal Selenides as High-Efficiency Oxygen Evolution Electrocatalysts through Combinatorial Electrodeposition. <i>ACS Catalysis</i> , 2018 , 8, 8273-8289 ^{13,157}	13.1	57
67	Metastable phase transformation and deformation twinning induced hardening-stiffening mechanism in compression of silicon nanoparticles. <i>Acta Materialia</i> , 2018 , 145, 8-18	8.4	17
66	Understanding homogeneous nucleation in solidification of aluminum by molecular dynamics simulations. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2018 , 26, 025007	2	55
65	Superior structural, elastic and electronic properties of 2D titanium nitride MXenes over carbide MXenes: a comprehensive first principles study. <i>2D Materials</i> , 2018 , 5, 045004	5.9	77
64	Design, Fabrication and Testing of Bioactive Glass Scaffolds for Structural Bone Repair. <i>Ceramic Engineering and Science Proceedings</i> , 2017 , 127-136	0.1	
63	Tough and strong porous bioactive glass-PLA composites for structural bone repair. <i>Journal of Materials Science</i> , 2017 , 52, 9039-9054	4.3	14
62	Investigating phase formations in cast AlFeCoNiCu high entropy alloys by combination of computational modeling and experiments. <i>Materials and Design</i> , 2017 , 127, 224-232	8.1	27
61	Effective elastic properties of two dimensional multiplanar hexagonal nanostructures. <i>2D Materials</i> , 2017 , 4, 025006	5.9	23
60	Effects of specimen size and yttria concentration on mechanical properties of single crystalline yttria-stabilized tetragonal zirconia nanopillars. <i>Journal of Applied Physics</i> , 2017 , 122, 014302	2.5	12
59	Effective mechanical properties of multilayer nano-heterostructures. <i>Scientific Reports</i> , 2017 , 7, 15818	4.9	44
58	Generalized stacking fault energies, ductilities, and twinnabilities of CoCrFeNi-based face-centered cubic high entropy alloys. <i>Scripta Materialia</i> , 2017 , 139, 83-86	5.6	86
57	Solidification Behavior in Reduced Gravity. <i>Jom</i> , 2017 , 69, 1258-1260	2.1	
56	Formation path of Lhydrides in zirconium by multiphase field modeling. <i>Acta Materialia</i> , 2017 , 123, 235-244	2.4	30
55	Effects of SiC, SiO ₂ and CNTs nanoadditives on the properties of porous alumina-zirconia ceramics produced by a hybrid freeze casting-space holder method. <i>Journal of the European Ceramic Society</i> , 2017 , 37, 1635-1642	6	15
54	Quantitative phase-field crystal modeling of solid-liquid interfaces for FCC metals. <i>Computational Materials Science</i> , 2017 , 127, 236-243	3.2	6

53	Competing mechanisms between dislocation and phase transformation in plastic deformation of single crystalline yttria-stabilized tetragonal zirconia nanopillars. <i>Acta Materialia</i> , 2016 , 120, 337-347	8.4	28
52	Comparison of CFD Simulations with Experimental Measurements of Nozzle Clogging in Continuous Casting of Steels. <i>Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science</i> , 2016 , 47, 3384-3393	2.5	12
51	Computational Fluid Dynamics Study of Molten Steel Flow Patterns and Particle-Wall Interactions Inside a Slide-Gate Nozzle by a Hybrid Turbulent Model. <i>Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science</i> , 2016 , 47, 3056-3065	2.5	8
50	The anisotropy of hexagonal close-packed and liquid interface free energy using molecular dynamics simulations based on modified embedded-atom method. <i>Acta Materialia</i> , 2016 , 107, 337-344	8.4	28
49	Predicting Solidification Properties of Magnesium by Molecular Dynamics Simulations 2016 , 53-56		
48	Fatigue Analysis of Ultrafine Grained Al 1050 Alloy Produced by Cyclic Forward Backward Extrusion. <i>Minerals, Metals and Materials Series</i> , 2016 , 357-359	0.3	
47	Creation of bioactive glass (13-93) scaffolds for structural bone repair using a combined finite element modeling and rapid prototyping approach. <i>Materials Science and Engineering C</i> , 2016 , 68, 651-662	8.3	23
46	Rapid Solidification and Phase Transformations in Additive Manufactured Materials. <i>Jom</i> , 2016 , 68, 928-929		5
45	Revisiting phase diagrams of two-mode phase-field crystal models. <i>Computational Materials Science</i> , 2016 , 123, 139-147	3.2	14
44	A phase-field model to study the effects of temperature change on shape evolution of hydrides in zirconium. <i>Journal Physics D: Applied Physics</i> , 2016 , 49, 405302	3	9
43	Quantifying a two-mode phase-field crystal model for BCC metals at melting point. <i>Computational Materials Science</i> , 2015 , 105, 101-109	3.2	15
42	A review on hydride precipitation in zirconium alloys. <i>Journal of Nuclear Materials</i> , 2015 , 466, 12-20	3.3	72
41	A modified two-mode phase-field crystal model applied to face-centered cubic and body-centered cubic orderings. <i>Computational Materials Science</i> , 2015 , 105, 110-113	3.2	25
40	Producing high strength aluminum alloy by combination of equal channel angular pressing and bake hardening. <i>Materials Letters</i> , 2015 , 140, 196-199	3.3	10
39	Advances in Modeling of Solidification Microstructures. <i>Jom</i> , 2015 , 67, 1774-1775	2.1	3
38	Two-phase solid-liquid coexistence of Ni, Cu, and Al by molecular dynamics simulations using the modified embedded-atom method. <i>Acta Materialia</i> , 2015 , 86, 169-181	8.4	73
37	Effect of variant strain accommodation on the three-dimensional microstructure formation during martensitic transformation: Application to zirconia. <i>Acta Materialia</i> , 2015 , 87, 45-55	8.4	30
36	Quantitative modeling of the equilibration of two-phase solid-liquid Fe by atomistic simulations on diffusive time scales. <i>Physical Review B</i> , 2015 , 91,	3.3	50

35	A Review of Quantitative Phase-Field Crystal Modeling of Solid-Liquid Structures. <i>Jom</i> , 2015 , 67, 186-2012.1		36
34	Phase-Field Crystal Model for Fe Connected to MEAM Molecular Dynamics Simulations. <i>Jom</i> , 2014 , 66, 429-436	2.1	29
33	Effect of resistance spot welding parameters on weld pool properties in a DP600 dual-phase steel: A parametric study using thermomechanically-coupled finite element analysis. <i>Materials & Design</i> , 2014 , 56, 387-397		45
32	Phase field modeling of stress-induced tetragonal-to-monoclinic transformation in zirconia and its effect on transformation toughening. <i>Acta Materialia</i> , 2014 , 64, 208-219	8.4	77
31	Algorithm Development in Computational Materials Science. <i>Jom</i> , 2014 , 66, 397-398	2.1	1
30	An elastic phase field model for thermal oxidation of metals: Application to zirconia. <i>Computational Materials Science</i> , 2014 , 89, 122-129	3.2	23
29	Shape memory effect and pseudoelasticity behavior in tetragonal zirconia polycrystals: A phase field study. <i>International Journal of Plasticity</i> , 2014 , 60, 71-86	7.6	59
28	Effect of vacancy defects on generalized stacking fault energy of fcc metals. <i>Journal of Physics Condensed Matter</i> , 2014 , 26, 115404	1.8	17
27	Modeling dendritic solidification of Al ₃ Cu using cellular automaton and phase-field methods. <i>Applied Mathematical Modelling</i> , 2013 , 37, 3495-3503	4.5	51
26	Phase field modeling of the tetragonal-to-monoclinic phase transformation in zirconia. <i>Acta Materialia</i> , 2013 , 61, 5223-5235	8.4	106
25	Transformations and cracks in zirconia films leading to breakaway oxidation of Zircaloy. <i>Acta Materialia</i> , 2013 , 61, 3923-3935	8.4	35
24	A review on phase field modeling of martensitic phase transformation. <i>Computational Materials Science</i> , 2013 , 77, 304-311	3.2	126
23	A Parametric Study of Resistance Spot Welding of a Dual-Phase Steel Using Finite Element Analysis 2013 , 3073-3080		
22	A cyclic forward-backward extrusion process as a novel severe plastic deformation for production of ultrafine grains materials. <i>Materials Letters</i> , 2012 , 68, 204-208	3.3	32
21	Producing ultrafine-grained aluminum rods by cyclic forward-backward extrusion: Study the microstructures and mechanical properties. <i>Materials Letters</i> , 2012 , 74, 147-150	3.3	17
20	Comparison of Cellular Automaton and Phase Field Models to Simulate Dendrite Growth in Hexagonal Crystals. <i>Journal of Materials Science and Technology</i> , 2012 , 28, 137-146	9.1	54
19	Effects of internal stresses and intermediate phases on the coarsening of coherent precipitates: A phase-field study. <i>Current Applied Physics</i> , 2012 , 12, 570-580	2.6	22
18	On laser welding of thin steel sheets. <i>Science and Technology of Welding and Joining</i> , 2012 , 17, 571-580	3.7	1

17	Investigating thermal effects on morphological evolution during crystallisation of hcp metals: three-dimensional phase field study. <i>Materials Technology</i> , 2012 , 27, 355-363	2.1	13
16	Morphological instabilities in thin films: Evolution maps. <i>Computational Materials Science</i> , 2011 , 50, 1030-1036	3.1	30
15	Investigating the effects of grain boundary energy anisotropy and second-phase particles on grain growth using a phase-field model. <i>Computational Materials Science</i> , 2011 , 50, 2488-2492	3.2	46
14	Implantation of HA into Superplastic Ti-6Al-4V: Kinetics and Mechanical Behaviors of Implanted Layer. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2011 , 42, 219-226	2.3	3
13	Effect of the Compositional Strain on the Diffusive Interface Thickness and on the Phase Transformation in a Phase-Field Model for Binary Alloys. <i>Journal of Phase Equilibria and Diffusion</i> , 2011 , 32, 302-308	1	23
12	A Phase-Field Finite Element Model for Instabilities in Multilayer Thin Films. <i>Materials Research Society Symposia Proceedings</i> , 2011 , 1297, 35		
11	THE ROLE OF COMPOSITIONAL STRAIN IN THE INSTABILITY OF SOLID-FLUID THIN FILM INTERFACES. <i>Modern Physics Letters B</i> , 2011 , 25, 1591-1601	1.6	5
10	Embedment of HA into Superplastic Ti-6Al-4V: Effects of Implantation Temperature. <i>Advanced Materials Research</i> , 2010 , 97-101, 3905-3909	0.5	2
9	Finite element method for conserved phase fields: Stress-mediated diffusional phase transformation. <i>Journal of Computational Physics</i> , 2010 , 229, 9135-9149	4.1	33
8	Investigation of Phase Transformation in Thin Film Using Finite Element Method. <i>Solid State Phenomena</i> , 2009 , 150, 29-41	0.4	18
7	Prediction of welding buckling distortion in a thin wall aluminum T joint. <i>Computational Materials Science</i> , 2007 , 38, 588-594	3.2	36
6	Investigation of Global Buckling Distortion in Welding of a Thin Wall Aluminium T Joint. <i>Materials Science Forum</i> , 2006 , 519-521, 1187-1192	0.4	
5	Predicting Solidification Properties of Magnesium by Molecular Dynamics Simulations	53-56	
4	A Finite Element-Phase Field Study of Solid State Phase Transformation: Coarsening of Coherent Precipitates and Instability of Multilayer Thin Films	341-348	
3	Fatigue Analysis of Ultrafine Grained Al 1050 Alloy Produced by Cyclic Forward Backward Extrusion	357-359	
2	Phase Field Modeling of Tetragonal to Monoclinic Phase Transformation at Zirconium Oxide	885-891	
1	Phase-Field Crystal Modeling: Integrating Density Functional Theory, Molecular Dynamics, and Phase-Field Modeling	49-70	1