

Mohsen Asle Zaeem

List of Publications by Year in descending order

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125
papers

3,955
citations

134610

34
h-index

169272

56
g-index

134
all docs

134
docs citations

134
times ranked

3986
citing authors

#	ARTICLE	IF	CITATIONS
1	Fatigue-resistant high-performance elastocaloric materials made by additive manufacturing. <i>Science</i> , 2019, 366, 1116-1121.	6.0	229
2	Nickel telluride as a bifunctional electrocatalyst for efficient water splitting in alkaline medium. <i>Journal of Materials Chemistry A</i> , 2018, 6, 7608-7622.	5.2	223
3	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.	2.0	171
4	A review on phase field modeling of martensitic phase transformation. <i>Computational Materials Science</i> , 2013, 77, 304-311.	1.4	150
5	Phase field modeling of the tetragonal-to-monoclinic phase transformation in zirconia. <i>Acta Materialia</i> , 2013, 61, 5223-5235.	3.8	136
6	Generalized stacking fault energies, ductilities, and twinnabilities of CoCrFeNi-based face-centered cubic high entropy alloys. <i>Scripta Materialia</i> , 2017, 139, 83-86.	2.6	129
7	A review on hydride precipitation in zirconium alloys. <i>Journal of Nuclear Materials</i> , 2015, 466, 12-20.	1.3	109
8	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.	3.8	105
9	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.	3.8	102
10	Understanding homogeneous nucleation in solidification of aluminum by molecular dynamics simulations. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2018, 26, 025007.	0.8	79
11	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.	5.5	76
12	Shape memory effect and pseudoelasticity behavior in tetragonal zirconia polycrystals: A phase field study. <i>International Journal of Plasticity</i> , 2014, 60, 71-86.	4.1	71
13	Modeling dendritic solidification of Al-3%Cu using cellular automaton and phase-field methods. <i>Applied Mathematical Modelling</i> , 2013, 37, 3495-3503.	2.2	68
14	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.	5.6	67
15	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, .	1.1	67
16	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.	5.1	64
17	In Situ Bottom-up Synthesis of Porphyrin-Based Covalent Organic Frameworks. <i>Journal of the American Chemical Society</i> , 2019, 141, 19560-19564.	6.6	55
18	Effective mechanical properties of multilayer nano-heterostructures. <i>Scientific Reports</i> , 2017, 7, 15818.	1.6	53

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19	Stoneâ€“Wales 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.	1.5	52
20	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.	3.8	50
21	Probing the shear modulus of two-dimensional multiplanar nanostructures and heterostructures. <i>Nanoscale</i> , 2018, 10, 5280-5294.	2.8	50
22	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.	1.4	48
23	A Review of Quantitative Phase-Field Crystal Modeling of Solidâ€“Liquid Structures. <i>Jom</i> , 2015, 67, 186-201.	0.9	48
24	Formation path of H ₂ hydrides in zirconium by multiphase field modeling. <i>Acta Materialia</i> , 2017, 123, 235-244.	3.8	45
25	Ca ₂ C MXene monolayer as a superior anode for metal-ion batteries. <i>2D Materials</i> , 2021, 8, 035015.	2.0	44
26	Transformations and cracks in zirconia films leading to breakaway oxidation of Zircaloy. <i>Acta Materialia</i> , 2013, 61, 3923-3935.	3.8	42
27	Strain-induced work function in h-BN and BCN monolayers. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2020, 123, 114180.	1.3	42
28	Prediction of welding buckling distortion in a thin wall aluminum T joint. <i>Computational Materials Science</i> , 2007, 38, 588-594.	1.4	41
29	Two-Dimensional Boronâ€“Phosphorus Monolayer for Reversible NO ₂ Gas Sensing. <i>ACS Applied Nano Materials</i> , 2020, 3, 10073-10081.	2.4	40
30	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.	3.8	37
31	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.	3.8	36
32	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.	1.0	36
33	A cyclic forwardâ€“backward extrusion process as a novel severe plastic deformation for production of ultrafine grains materials. <i>Materials Letters</i> , 2012, 68, 204-208.	1.3	35
34	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.	3.3	35
35	Finite element method for conserved phase fields: Stress-mediated diffusional phase transformation. <i>Journal of Computational Physics</i> , 2010, 229, 9135-9149.	1.9	34
36	Quantitative phase-field modeling of solute trapping in rapid solidification. <i>Acta Materialia</i> , 2021, 205, 116562.	3.8	33

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37	Modified embedded-atom method interatomic potentials for Al-Cu, Al-Fe and Al-Ni binary alloys: From room temperature to melting point. Computational Materials Science, 2022, 201, 110902.	1.4	33
38	Morphological instabilities in thin films: Evolution maps. Computational Materials Science, 2011, 50, 1030-1036.	1.4	32
39	Combined molecular dynamics and phase field simulation investigations of crystal-melt interfacial properties and dendritic solidification of highly undercooled titanium. Computational Materials Science, 2019, 163, 218-229.	1.4	32
40	Phase-Field Crystal Model for Fe Connected to MEAM Molecular Dynamics Simulations. Jom, 2014, 66, 429-436.	0.9	31
41	Effective elastic properties of two dimensional multiplanar hexagonal nanostructures. 2D Materials, 2017, 4, 025006.	2.0	31
42	A new planar BCN lateral heterostructure with outstanding strength and defect-mediated superior semiconducting to metallic properties. Physical Chemistry Chemical Physics, 2020, 22, 22066-22077.	1.3	30
43	Phosgene Gas Sensing of $Ti_{2-x}O_{2-x}$ ($T = F^{+}, O^{+}$) $T_j ETQq1 1 0.784314 rgBT / Overlo$	1.3	30
44	Creation of bioactive glass (13 β 93) scaffolds for structural bone repair using a combined finite element modeling and rapid prototyping approach. Materials Science and Engineering C, 2016, 68, 651-662.	3.8	29
45	A modified two-mode phase-field crystal model applied to face-centered cubic and body-centered cubic orderings. Computational Materials Science, 2015, 105, 110-113.	1.4	28
46	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. Scripta Materialia, 2019, 168, 139-143.	2.6	28
47	Phase-field modeling of crack propagation in polycrystalline materials. Computational Materials Science, 2021, 186, 110057.	1.4	27
48	Evolution of solidification defects in deformation of nano-polycrystalline aluminum. Computational Materials Science, 2019, 163, 176-185.	1.4	26
49	An elastic phase field model for thermal oxidation of metals: Application to zirconia. Computational Materials Science, 2014, 89, 122-129.	1.4	25
50	A review of computational modeling techniques in study and design of shape memory ceramics. Computational Materials Science, 2019, 160, 120-136.	1.4	25
51	Effect of the Compositional Strain on the Diffusive Interface Thickness and on the Phase Transformation in a Phase-Field Model for Binary Alloys. Journal of Phase Equilibria and Diffusion, 2011, 32, 302-308.	0.5	24
52	Effects of solidification defects on nanoscale mechanical properties of rapid directionally solidified Al-Cu Alloy: A large scale molecular dynamics study. Journal of Crystal Growth, 2019, 527, 125255.	0.7	24
53	Modified embedded-atom method potential for high-temperature crystal-melt properties of Ti-Ni alloys and its application to phase field simulation of solidification. Modelling and Simulation in Materials Science and Engineering, 2020, 28, 015006.	0.8	24
54	An Asymmetric Elasto-Plastic Phase-Field Model for Shape Memory Effect, Pseudoelasticity and Thermomechanical Training in Polycrystalline Shape Memory Alloys. Acta Materialia, 2020, 201, 580-595.	3.8	24

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55	Hydrogen-induced tunable electronic and optical properties of a two-dimensional penta-Pt ₂ N ₄ monolayer. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 10409-10417.	1.3	24
56	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.	1.1	23
57	Tough and strong porous bioactive glass-PLA composites for structural bone repair. <i>Journal of Materials Science</i> , 2017, 52, 9039-9054.	1.7	23
58	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.	2.0	23
59	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.	3.1	22
60	Metastable phase transformation and deformation twinning induced hardening-stiffening mechanism in compression of silicon nanoparticles. <i>Acta Materialia</i> , 2018, 145, 8-18.	3.8	22
61	Effect of vacancy defects on generalized stacking fault energy of fcc metals. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 115404.	0.7	21
62	Revisiting phase diagrams of two-mode phase-field crystal models. <i>Computational Materials Science</i> , 2016, 123, 139-147.	1.4	21
63	Nanoscale self-healing mechanisms in shape memory ceramics. <i>Npj Computational Materials</i> , 2019, 5, .	3.5	21
64	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.	2.8	21
65	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.	3.8	21
66	Interactive effects of interfacial energy anisotropy and solute transport on solidification patterns of Al-Cu alloys. <i>Acta Materialia</i> , 2022, 231, 117859.	3.8	21
67	Investigation of Phase Transformation in Thin Film Using Finite Element Method. <i>Solid State Phenomena</i> , 0, 150, 29-41.	0.3	19
68	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.	2.1	19
69	Predicting effective fracture toughness of ZrB ₂ -based ultra-high temperature ceramics by phase-field modeling. <i>Materials and Design</i> , 2020, 192, 108713.	3.3	19
70	Quantifying a two-mode phase-field crystal model for BCC metals at melting point. <i>Computational Materials Science</i> , 2015, 105, 101-109.	1.4	18
71	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.	2.8	18
72	Investigating thermal effects on morphological evolution during crystallisation of hcp metals: three-dimensional phase field study. <i>Materials Technology</i> , 2012, 27, 355-363.	1.5	17

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73	Producing ultrafine-grained aluminum rods by cyclic forward-backward extrusion: Study the microstructures and mechanical properties. <i>Materials Letters</i> , 2012, 74, 147-150.	1.3	17
74	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.	1.0	17
75	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.	0.8	17
76	Transformation-induced fracture toughening in CuAlBe shape memory alloys: A phase-field study. <i>International Journal of Mechanical Sciences</i> , 2021, 192, 106144.	3.6	17
77	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.	3.3	17
78	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.	1.1	15
79	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.	1.3	15
80	A phase-field model to study the effects of temperature change on shape evolution of β -hydrides in zirconium. <i>Journal Physics D: Applied Physics</i> , 2016, 49, 405302.	1.3	14
81	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.	1.7	14
82	On the elastocaloric effect in CuAlBe shape memory alloys: A quantitative phase-field modeling approach. <i>Computational Materials Science</i> , 2020, 183, 109808.	1.4	14
83	Solution processed Ni ₂ Co layered double hydroxides for high performance electrochemical sensors. <i>Applied Surface Science</i> , 2021, 541, 148270.	3.1	14
84	Liquid ordering induced heterogeneities in homogeneous nucleation during solidification of pure metals. <i>Journal of Materials Science and Technology</i> , 2022, 106, 77-89.	5.6	14
85	Producing high strength aluminum alloy by combination of equal channel angular pressing and bake hardening. <i>Materials Letters</i> , 2015, 140, 196-199.	1.3	13
86	Formation of chromium-iron carbide by carbon diffusion in Al _X CoCrFeNiCu high-entropy alloys. <i>Materials Research Letters</i> , 2018, 6, 321-326.	4.1	12
87	Unveiling the role of atomic defects on the electronic, mechanical and elemental diffusion properties in CuS. <i>Scripta Materialia</i> , 2021, 192, 94-99.	2.6	12
88	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.	1.0	11
89	A Review of Multi-Scale Computational Modeling Tools for Predicting Structures and Properties of Multi-Principal Element Alloys. <i>Metals</i> , 2019, 9, 254.	1.0	11
90	Nanotwin-induced strengthening in silicon: A molecular dynamics study. <i>International Journal of Mechanical Sciences</i> , 2021, 189, 105990.	3.6	10

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91	Effects of applied load on formation and reorientation of zirconium hydrides: A multiphase field modeling study. <i>Computational Materials Science</i> , 2021, 192, 110367.	1.4	10
92	Quantitative prediction of rapid solidification by integrated atomistic and phase-field modeling. <i>Acta Materialia</i> , 2021, 211, 116885.	3.8	10
93	From fundamental to CO ₂ and COCl ₂ gas sensing properties of pristine and defective Si ₂ BN monolayers. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 4394-4406.	1.3	10
94	Quantitative phase-field crystal modeling of solid-liquid interfaces for FCC metals. <i>Computational Materials Science</i> , 2017, 127, 236-243.	1.4	9
95	A modified embedded-atom method interatomic potential for bismuth. <i>Modelling and Simulation in Materials Science and Engineering</i> , 0, , .	0.8	7
96	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.	1.4	7
97	A temperature-dependent atomistic-informed phase-field model to study dendritic growth. <i>Journal of Crystal Growth</i> , 2022, 579, 126461.	0.7	7
98	Rapid Solidification and Phase Transformations in Additive Manufactured Materials. <i>Jom</i> , 2016, 68, 928-929.	0.9	6
99	THE ROLE OF COMPOSITIONAL STRAIN IN THE INSTABILITY OF SOLID-FLUID THIN FILM INTERFACES. <i>Modern Physics Letters B</i> , 2011, 25, 1591-1601.	1.0	5
100	Advances in Modeling of Solidification Microstructures. <i>Jom</i> , 2015, 67, 1774-1775.	0.9	5
101	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.	1.3	5
102	Formation energies, electronic properties and elemental diffusion of Cuâ€“Crâ€“Nb (GRCop) alloys. <i>Physica B: Condensed Matter</i> , 2022, 637, 413909.	1.3	5
103	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.	1.1	4
104	Nanoscale flaw tolerance behaviour of polycrystalline tetragonal zirconia nanopillars. <i>International Journal of Mechanical Sciences</i> , 2020, 173, 105405.	3.6	4
105	Unveiling the effect of vacancy defects on structural, mechanical, electronic and diffusion properties of copper (I) iodide. <i>Scripta Materialia</i> , 2022, 213, 114634.	2.6	4
106	Defect-induced asymmetrical mechanical behavior in shape memory zirconia: A phase-field investigation. <i>Journal of the European Ceramic Society</i> , 2022, , .	2.8	4
107	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.	0.9	3
108	Superelasticity and shape memory effect in zirconia nanoparticles. <i>Extreme Mechanics Letters</i> , 2021, 46, 101301.	2.0	3

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109	Embedment of HA into Superplastic Ti-6Al-4V: Effects of Implantation Temperature. <i>Advanced Materials Research</i> , 2010, 97-101, 3905-3909.	0.3	2
110	Oxidation Induced Stresses in High-Temperature Oxidation of Steel: A Multiphase Field Study. <i>Metals</i> , 2020, 10, 801.	1.0	2
111	Finite Element Modeling of a Diffusion-Controlled Phase Transformation in Thin Film. , 2008, , .		1
112	On laser welding of thin steel sheets. <i>Science and Technology of Welding and Joining</i> , 2012, 17, 571-580.	1.5	1
113	Algorithm Development in Computational Materials Science. <i>Jom</i> , 2014, 66, 397-398.	0.9	1
114	Recent Advances in Study of Solid-Liquid Interfaces and Solidification of Metals. <i>Metals</i> , 2018, 8, 120.	1.0	1
115	A molecular dynamics study of domain switching in BiFeO ₃ nanofilm under DC electric field. <i>Computational Materials Science</i> , 2021, 199, 110718.	1.4	1
116	Investigation of Global Buckling Distortion in Welding of a Thin Wall Aluminium T Joint. <i>Materials Science Forum</i> , 2006, 519-521, 1187-1192.	0.3	0
117	A Phase-Field “ Finite Element Model for Instabilities in Multilayer Thin Films. <i>Materials Research Society Symposia Proceedings</i> , 2011, 1297, 35.	0.1	0
118	Solidification Behavior in Reduced Gravity. <i>Jom</i> , 2017, 69, 1258-1260.	0.9	0
119	Finite Element Modeling of the Flexural Mechanical Response of Polymer-Coated Bioactive Glass Scaffolds Composed of Thermally-Bonded Unidirectional Fibers. <i>Biomedical Glasses</i> , 2017, 3, .	2.4	0
120	Dendritic Solidification of Crystals. , 2017, , .		0
121	Prediction of Residual Stresses and Buckling Distortion in Welding of a Thin Wall Aluminum Butt Joint. , 2006, , .		0
122	Predicting Solidification Properties of Magnesium by Molecular Dynamics Simulations. , 2016, , 53-56.		0
123	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	0
124	Insights on Solidification of Mg and Mg“Al Alloys by Large Scale Atomistic Simulations. <i>Minerals, Metals and Materials Series</i> , 2020, , 51-53.	0.3	0
125	Additively Manufactured High-Performance Elastocaloric Materials with Long Fatigue Life. , 2022, , .		0