Nele Moelans

List of Publications by Year
in descending order

96 papers	3,383 citations	236833 25 h-index	149623 56 g-index
101 all docs	101 docs citations	101 times ranked	2210 citing authors

#	Article	IF	Citations
1	An introduction to phase-field modeling of microstructure evolution. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2008, 32, 268-294.	0.7	717
2	Quantitative analysis of grain boundary properties in a generalized phase field model for grain growth in anisotropic systems. Physical Review B, 2008, 78, .	1.1	291
3	A quantitative and thermodynamically consistent phase-field interpolation function for multi-phase systems. Acta Materialia, 2011, 59, 1077-1086.	3.8	195
4	Plasma-enhanced chemical vapour deposition growth of Si nanowires with low melting point metal catalysts: an effective alternative to Au-mediated growth. Nanotechnology, 2007, 18, 505307.	1.3	120
5	Phase field simulations of grain growth in two-dimensional systems containing finely dispersed second-phase particles. Acta Materialia, 2006, 54, 1175-1184.	3.8	114
6	Pinning effect of second-phase particles on grain growth in polycrystalline films studied by 3-D phase field simulations. Acta Materialia, 2007, 55, 2173-2182.	3.8	114
7	Quantitative Phase-Field Approach for Simulating Grain Growth in Anisotropic Systems with Arbitrary Inclination and Misorientation Dependence. Physical Review Letters, 2008, 101, 025502.	2.9	113
8	A phase field model for the simulation of grain growth in materials containing finely dispersed incoherent second-phase particles. Acta Materialia, 2005, 53, 1771-1781.	3.8	107
9	Comparative study of two phase-field models for grain growth. Computational Materials Science, 2009, 46, 479-490.	1.4	91
10	Thermodynamic optimization of the lead-free solder system Biâ€“Inâ€“Snâ€“Zn. Journal of Alloys and Compounds, 2003, 360, 98-106.	2.8	80
11	Pinning effect of spheroid second-phase particles on grain growth studied by three-dimensional phase-field simulations. Computational Materials Science, 2010, 49, 340-350.	1.4	80
12	Metal losses in pyrometallurgical operations - A review. Advances in Colloid and Interface Science, 2018, 255, 47-63.	7.0	67
13	Phase-field simulation study of the migration of recrystallization boundaries. Physical Review B, 2013, 88, .	1.1	60
14	Study of Mn absorption by complex oxide inclusions in Al Ti Mg killed steels. Acta Materialia, 2016, 118, 8-16.	3.8	54
15	Investigation of diffusion behavior in Cuâ€“Sn solid state diffusion couples. Journal of Alloys and Compounds, 2016, 661, 282-293.	2.8	51
16	Bounding box algorithm for three-dimensional phase-field simulations of microstructural evolution in polycrystalline materials. Physical Review E, 2007, 76, 056702.	0.8	46
17	Evaluation of interfacial excess contributions in different phase-field models for elastically inhomogeneous systems. Modelling and Simulation in Materials Science and Engineering, 2013, 21, 055018.	0.8	45
18	Effect of grain boundary energy anisotropy on highly textured grain structures studied by phase-field simulations. Acta Materialia, 2014, 64, 443-454.	3.8	44

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19	Effect of strong nonuniformity in grain boundary energy on 3-D grain growth behavior: A phase-field simulation study. Computational Materials Science, 2017, 127, 67-77.	1.4	44
20	A phase field model for isothermal crystallization of oxide melts. Acta Materialia, 2011, 59, 2156-2165.	3.8	41
21	Effects of LaAlO3 and La2O2S inclusions on the initialization of localized corrosion of pipeline steels in NaCl solution. Scripta Materialia, 2020, 177, 151-156.	2.6	38
22	Microstructure and degradation performance of biodegradable Mg-Si-Sr implant alloys. Materials Science and Engineering C, 2017, 71, 25-34.	3.8	37
23	Formation of compounds and Kirkendall vacancy in the Cuâ€“Sn system. Microelectronic Engineering, 2014, 120, 133-137.	1.1	35
24	Origin and sedimentation of Cu-droplets sticking to spinel solids in pyrometallurgical slags. Materials Science and Technology, 2016, 32, 1911-1924.	0.8	30
25	Combining multi-phase field simulation with neural network analysis to unravel thermomigration accelerated growth behavior of Cu6Sn5 IMC at cold side Cuâ€“Sn interface. International Journal of Mechanical Sciences, 2020, 184, 105843.	3.6	27
26	Phase-field study of IMC growth in Snâ€“Cu/Cu solder joints including elastoplastic effects. Acta Materialia, 2020, 188, 241-258.	3.8	27
27	A quantitative phase-field model for two-phase elastically inhomogeneous systems. Computational Materials Science, 2015, 99, 81-95.	1.4	25
28	Formation and autocatalytic nucleation of co-zone <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.gif" overflow="scroll"><mml:mrow><mml:mrow><mml:mo>{</mml:mo><mml:mrow><mml:mn>10</mml:mn><mml:mrow><mml:mover accent="true"><mml:mn>1</mml:mn><mml:mo>Â¯</mml:mo></mml:mover></mml:mrow><mml:mn>2</mml:mn></mml:mrow><mml: deformation twins in polycrystalline Mg: A phase field simulation study. Acta Materialia, 2018, 153, 86-107.	3.8	25
29	DFT study on the mechanism of inclusion-induced initial pitting corrosion of Al-Ti-Ca complex deoxidized steel with Ce treatment. Physica B: Condensed Matter, 2019, 558, 10-19.	1.3	25
30	Integration of machine learning with phase field method to model the electromigration induced Cu6Sn5 IMC growth at anode side Cu/Sn interface. Journal of Materials Science and Technology, 2020, 59, 203-219.	5.6	25
31	Three-dimensional phase-field study of grain coarsening and grain shape accommodation in the final stage of liquid-phase sintering. Journal of the European Ceramic Society, 2017, 37, 2265-2275.	2.8	23
32	Grain growth in thin films with a fibre texture studied by phase-field simulations and mean field modelling. Philosophical Magazine, 2010, 90, 501-523.	0.7	21
33	Bounding box framework for efficient phase field simulation of grain growth in anisotropic systems. Computational Materials Science, 2011, 50, 2221-2231.	1.4	20
34	Analysis of the isothermal crystallization of CaSiO3 in a CaOâ€“Al2O3â€“SiO2 melt through in situ observations. Journal of the European Ceramic Society, 2011, 31, 1873-1879.	2.8	20
35	Investigation of High-Temperature Slag/Copper/Spinel Interactions. Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science, 2016, 47, 3421-3434.	1.0	20
36	Investigation on the existence of a â€˜Hillert regimeâ€™ in normal grain growth. Scripta Materialia, 2018, 142, 148-152.	2.6	19

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37	Wetting behaviour of Cu based alloys on spinel substrates in pyrometallurgical context. Materials Science and Technology, 2015, 31, 1925-1933.	0.8	18
38	Three-dimensional phase-field simulation of microstructural evolution in three-phase materials with different interfacial energies and different diffusivities. Journal of Materials Science, 2017, 52, 13852-13867.	1.7	17
39	In-situ observation of isothermal CaSiO3 crystallization in CaOâ€“Al2O3â€“SiO2 melts: A study of the effects of temperature and composition. Journal of Crystal Growth, 2014, 402, 1-8.	0.7	16
40	Phase-field simulations of the interaction between a grain boundary and an evolving second-phase particle. Philosophical Magazine Letters, 2015, 95, 202-210.	0.5	15
41	Phase field modelling of the attachment of metallic droplets to solid particles in liquid slags: Influence of interfacial energies and slag supersaturation. Computational Materials Science, 2015, 108, 348-357.	1.4	15
42	Study of the Effect of Spinel Composition on Metallic Copper Losses in Slags. Journal of Sustainable Metallurgy, 2017, 3, 416-427.	1.1	15
43	Analysis of grain topology and volumetric growth rate relation in three-dimensional normal grain growth. Acta Materialia, 2018, 156, 275-286.	3.8	15
44	Combining thermodynamics with tensor completion techniques to enable multicomponent microstructure prediction. Npj Computational Materials, 2020, 6, .	3.5	15
45	Effect of volume fractions on microstructure evolution in isotropic volume-conserved two-phase alloys: A phase-field study. Computational Materials Science, 2016, 125, 297-308.	1.4	14
46	A grand-potential based phase-field approach for simulating growth of intermetallic phases in multicomponent alloy systems. Acta Materialia, 2021, 206, 116630.	3.8	14
47	Microstructure simulation of grain growth in Cu through silicon vias using phase-field modeling. Microelectronics Reliability, 2015, 55, 765-770.	0.9	13
48	Sessile drop evaluation of high temperature copper/spinel and slag/spinel interactions. Transactions of Nonferrous Metals Society of China, 2016, 26, 2770-2783.	1.7	13
49	Phase field simulation study of the dissolution behavior of Al2O3 into CaOâ€“Al2O3â€“SiO2 slags. Computational Materials Science, 2016, 119, 9-18.	1.4	13
50	Calculation of phase equilibria for an alloy nanoparticle in contact with a solid nanowire. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2011, 35, 173-182.	0.7	12
51	Influence of the solubility range of intermetallic compounds on their growth behavior in hetero-junctions. Journal of Alloys and Compounds, 2015, 635, 289-299.	2.8	12
52	Influence of geometrical alignment of the deformation microstructure on local migration of grain boundaries during recrystallization: A phase-field study. Scripta Materialia, 2021, 191, 116-119	2.6	12
53	Multi-phase field simulation of Al<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e1157" altimg="si16.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub></mml:math>Ni<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e1165" altimg="si17.svg"><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:math> intermetallic growth at	3.6	12
54	Phase field modeling of the crystallization of FeOxâ€“SiO2 melts in contact with an oxygen-containing atmosphere. Chemical Geology, 2011, 290, 156-162.	1.4	11

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55	Three-dimensional phase-field simulation of microstructural evolution in three-phase materials with different diffusivities. Journal of Materials Science, 2014, 49, 7066-7072.	1.7	11
56	Microstructure and mechanical characterization of cast Mg-Ca-Si alloys. Journal of Alloys and Compounds, 2017, 694, 767-776.	2.8	11
57	Study of the effect of Sn grain boundaries on IMC morphology in solid state inter-diffusion soldering. Scientific Reports, 2019, 9, 14862.	1.6	11
58	Phase-field analysis of a ternary two-phase diffusion couple with multiple analytical solutions. Acta Materialia, 2011, 59, 3946-3954.	3.8	10
59	A phase-field simulation study of irregular grain boundary migration during recrystallization. IOP Conference Series: Materials Science and Engineering, 2015, 89, 012037.	0.3	10
60	Investigation of Origin of Attached Cu-Ag Droplets to Solid Particles During High-Temperature Slag/Copper/Spinel Interactions. Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science, 2017, 48, 3058-3073.	1.0	10
61	New phase-field model for polycrystalline systems with anisotropic grain boundary properties. Materials and Design, 2022, 217, 110592.	3.3	10
62	Phase field modelling of the attachment of metallic droplets to solid particles in liquid slags: Influence of particle characteristics. Acta Materialia, 2015, 101, 172-180.	3.8	9
63	Investigation of the diffusion behavior in Sn-xAg-yCu/Cu solid state diffusion couples. Journal of Alloys and Compounds, 2016, 686, 794-802.	2.8	9
64	Phase-Field Modelling in Extractive Metallurgy. Critical Reviews in Solid State and Materials Sciences, 2018, 43, 417-454.	6.8	9
65	Metal Droplet Entrainment by Solid Particles in Slags: An Experimental Approach. Journal of Sustainable Metallurgy, 2018, 4, 15-32.	1.1	9
66	Variant selection of primaryâ€“secondary extension twin pairs in magnesium: An analytical calculation study. Acta Materialia, 2021, 219, 117221.	3.8	9
67	Effects of dislocation boundary spacings and stored energy on boundary migration during recrystallization: A phase-field analysis. Acta Materialia, 2021, 221, 117377.	3.8	9
68	Identification and description of intermetallic compounds in Mgâ€“Siâ€“Sr cast and heat-treated alloys. Journal of Alloys and Compounds, 2016, 669, 123-133.	2.8	8
69	Diffusion multiple study of the Co-Fe-Ni system at 800â€¯Â°C. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2019, 64, 149-159.	0.7	8
70	Phase-field simulation and analytical modelling of CaSiO3 growth in CaO-Al2O3-SiO2 melts. Computational Materials Science, 2018, 144, 126-132.	1.4	7
71	Phase-field approach to simulate BCC-B2 phase separation in the AlnCrFe2Ni2 medium-entropy alloy. Journal of Materials Science, 0, , 1.	1.7	7
72	Phase field simulations of FCC to BCC phase transformation in (Al)CrFeNi medium entropy alloys. Materials Theory, 2022, 6, .	2.2	7

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73	A Phase Field Model for grain Growth and Thermal Grooving in Thin Films with Orientation Dependent Surface Energy. Solid State Phenomena, 2007, 129, 89-94.	0.3	6
74	On the rotation invariance of multi-order parameter models for grain growth. Scripta Materialia, 2010, 62, 827-830.	2.6	6
75	Comments on â€œA numerical method to determine interdiffusion coefficients of Cu6Sn5 and Cu3Sn intermetallic compoundsâ€. Intermetallics, 2016, 69, 95-97.	1.8	6
76	Investigation of Reactive Origin for Attachment of Cu Droplets to Solid Particles. Metallurgical and Materials Transactions B: Process Metallurgy and Materials Processing Science, 2017, 48, 2459-2468.	1.0	6
77	Study of the interfacial reactions controlling the spreading of Al on Ni. Applied Surface Science, 2022, 571, 151272.	3.1	6
78	Phase field simulation study of the attachment of metallic droplets to solid particles in liquid slags based on real slagâ€“spinel micrographs. Computational Materials Science, 2016, 118, 269-278.	1.4	5
79	Comparison of coarsening behaviour in non-conserved and volume-conserved isotropic two-phase grain structures. Scripta Materialia, 2018, 146, 142-145.	2.6	5
80	Phase field analysis of the growth of fast and slow crystallites. European Physical Journal: Special Topics, 2020, 229, 433-437.	1.2	5
81	Phase field model derivation for rapid crystal growth in polycrystalline alloys. European Physical Journal: Special Topics, 2020, 229, 453-458.	1.2	5
82	Influence of 5 at.%Al-Additions on the FCC to BCC Phase Transformation in CrFeNi Concentrated Alloys. Journal of Phase Equilibria and Diffusion, 0, , 1.	0.5	5
83	Diffusion multiple study of Co-Ni-Ti system at 1073â€¯K. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2018, 63, 156-163.	0.7	4
84	3D Phase-Field Simulation and Characterization of Microstructure Evolution during Liquid Phase Sintering. Advances in Science and Technology, 0, , .	0.2	3
85	A phase-field investigation of recrystallization boundary migration into heterogeneous deformation energy fields: Effects of dislocation boundary sharpness. IOP Conference Series: Materials Science and Engineering, 2021, 1121, 012013.	0.3	3
86	An efficient and quantitative phase-field model for elastically heterogeneous two-phase solids based on a partial rank-one homogenization scheme. International Journal of Solids and Structures, 2022, 250, 111709.	1.3	3
87	Alternative Catalysts For Si-Technology Compatible Growth Of Si Nanowires. Materials Research Society Symposia Proceedings, 2007, 1017, 14.	0.1	2
88	Isothermal Crystal Growth Behavior of CaSiO$lt;inf$gt;3$lt;/inf$gt; in Ternary Oxide Melts. Wuji Cailiao Xuebao/Journal of Inorganic Materials, 2016, 31, 547.	0.6	2
89	The effect of voids on boundary migration during recrystallization in additive manufactured samplesâ€”a phase field study. Scripta Materialia, 2022, 214, 114675.	2.6	2
90	Threeâ€dimensional phase field simulations of grain growth in materials containing finely dispersed secondâ€phase particles. Proceedings in Applied Mathematics and Mechanics, 2007, 7, 2020001-2020002.	0.2	1

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91	Towards more realistic simulations of microstructural evolution in oxidic systems. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2022, 77, 102402.	0.7	1
92	Indium-assisted Growth of Si Nanowires: Perspectives on Controlled Growth for CMOS Applications. Materials Research Society Symposia Proceedings, 2008, 1080, 1.	0.1	0
93	Microstructure simulation of grain growth in Cu Through Silicon Via using phase-field modeling. , 2014, , .		0
94	Study on Mgâ€“Siâ€“Sr Ternary Alloys for Biomedical Applications. Minerals, Metals and Materials Series, 2018, , 413-424.	0.3	0
95	Influence of rigid body motion on the attachment of metallic droplets to solid particles in liquid slags ï¿½ A phase field study. Minerals and Metallurgical Processing, 2018, 35, 87-97.	0.7	0
96	Correlation between Mechanical Behaviour and Microstructure in the Mg-Ca-Si-Sr System for Degradable Biomaterials Based on Thermodynamic Calculations. , 2015, , 431-436.		0