Yasushi Shibuta

List of Publications by Year
in descending order

161 papers	4,858 citations	81900 39 h-index	118850 62 g-index
162 all docs	162 docs citations	162 times ranked	3498 citing authors

#	Article	IF	Citations
1	Molecular dynamics simulation of formation process of single-walled carbon nanotubes by CCVD method. Chemical Physics Letters, 2003, 382, 381-386.	2.6	224
2	Heterogeneity in homogeneous nucleation from billion-atom molecular dynamics simulation of solidification of pure metal. Nature Communications, 2017, 8, 10.	12.8	219
3	Catalyzed Growth of Carbon Nanotube with Definable Chirality by Hybrid Molecular Dynamicsâ^'Force Biased Monte Carlo Simulations. ACS Nano, 2010, 4, 6665-6672.	14.6	162
4	Melting and nucleation of iron nanoparticles: A molecular dynamics study. Chemical Physics Letters, 2007, 445, 265-270.	2.6	144
5	A molecular dynamics study of the phase transition in bcc metal nanoparticles. Journal of Chemical Physics, 2008, 129, 144102.	3.0	124
6	A Molecular Dynamics Study of the Energy and Structure of the Symmetric Tilt Boundary of Iron. ISIJ International, 2008, 48, 1582-1591.	1.4	112
7	Interaction between two graphene sheets with a turbostratic orientational relationship. Chemical Physics Letters, 2011, 512, 146-150.	2.6	109
8	Bond-order potential for transition metal carbide cluster for the growth simulation of a single-walled carbon nanotube. Computational Materials Science, 2007, 39, 842-848.	3.0	96
9	Solidification in a Supercomputer: From Crystal Nuclei to Dendrite Assemblages. Jom, 2015, 67, 1793-1804.	1.9	92
10	Atomistic modelling of CVD synthesis of carbon nanotubes and graphene. Nanoscale, 2013, 5, 6662.	5.6	88
11	Primary arm array during directional solidification of a single-crystal binary alloy: Large-scale phase-field study. Acta Materialia, 2016, 118, 230-243.	7.9	87
12	Submicrometer-scale molecular dynamics simulation of nucleation and solidification from undercooled melt: Linkage between empirical interpretation and atomistic nature. Acta Materialia, 2016, 105, 328-337.	7.9	86
13	Homogeneous nucleation and microstructure evolution in million-atom molecular dynamics simulation. Scientific Reports, 2015, 5, 13534.	3.3	84
14	Multi-GPUs parallel computation of dendrite growth in forced convection using the phase-field-lattice Boltzmann model. Journal of Crystal Growth, 2017, 474, 154-159.	1.5	81
15	Melting and solidification point of fcc-metal nanoparticles with respect to particle size: A molecular dynamics study. Chemical Physics Letters, 2010, 498, 323-327.	2.6	77
16	Ultra-large-scale phase-field simulation study of ideal grain growth. Npj Computational Materials, 2017, 3, .	8.7	77
17	Two-dimensional phase-field study of competitive grain growth during directional solidification of polycrystalline binary alloy. Journal of Crystal Growth, 2016, 442, 14-24.	1.5	76
18	A molecular dynamics study of the fccâ€“bcc phase transformation kinetics of iron. Scripta Materialia, 2008, 59, 971-974.	5.2	67

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19	Molecular dynamics simulation of generation process of SWNTs. Physica B: Condensed Matter, 2002, 323, 187-189.	2.7	66
20	Phase-field lattice Boltzmann simulations of multiple dendrite growth with motion, collision, and coalescence and subsequent grain growth. Computational Materials Science, 2018, 147, 124-131.	3.0	66
21	Phase-field modeling for electrodeposition process. Science and Technology of Advanced Materials, 2007, 8, 511-518.	6.1	63
22	A phase-field model for electrode reactions with Butlerâ€“Volmer kinetics. Computational Materials Science, 2010, 50, 118-124.	3.0	63
23	Phase-field-lattice Boltzmann studies for dendritic growth with natural convection. Journal of Crystal Growth, 2017, 474, 146-153.	1.5	61
24	A molecular dynamics study of the effect of a substrate on catalytic metal clusters in nucleation process of single-walled carbon nanotubes. Chemical Physics Letters, 2007, 437, 218-223.	2.6	60
25	A Molecular Dynamics Study of Thermodynamic and Kinetic Properties of Solidâ€“Liquid Interface for Bcc Iron. ISIJ International, 2010, 50, 1158-1164.	1.4	60
26	Inverse Hall-Petch relationship of high-entropy alloy by atomistic simulation. Materials Letters, 2020, 274, 128024.	2.6	60
27	Proton Migration on Hydrated Surface of Cubic ZrO₂: Ab initio Molecular Dynamics Simulation. Journal of Physical Chemistry C, 2015, 119, 28925-28933.	3.1	57
28	Competitive grain growth during directional solidification of a polycrystalline binary alloy: Three-dimensional large-scale phase-field study. Materialia, 2018, 1, 104-113.	2.7	57
29	A molecular dynamics study of cooling rate during solidification of metal nanoparticles. Chemical Physics Letters, 2011, 502, 82-86.	2.6	55
30	Ab initio molecular dynamics simulation of dissociation of methane on nickel(1 1 1) surface: Unravelling initial stage of graphene growth via a CVD technique. Chemical Physics Letters, 2013, 565, 92-97.	2.6	54
31	Interaction between nano-voids and migrating grain boundary by molecular dynamics simulation. Acta Materialia, 2019, 173, 206-224.	7.9	52
32	Direction Control of Chemical Wave Propagation in Self-Oscillating Gel Array. Journal of Physical Chemistry B, 2008, 112, 1777-1782.	2.6	47
33	Growth and melting of nanoparticles in liquid iron: A molecular dynamics study. Chemical Physics Letters, 2009, 475, 264-268.	2.6	47
34	Wafer-scale fabrication and growth dynamics of suspended graphene nanoribbon arrays. Nature Communications, 2016, 7, 11797.	12.8	43
35	Grain boundary induced deformation mechanisms in nanocrystalline Al by molecular dynamics simulation: From interatomic potential perspective. Computational Materials Science, 2019, 156, 421-433.	3.0	42
36	Largeâ€“scale phaseâ€“field lattice Boltzmann study on the effects of natural convection on dendrite morphology formed during directional solidification of a binary alloy. Computational Materials Science, 2020, 171, 109209.	3.0	42

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37	Dynamic interaction between grain boundary and stacking fault tetrahedron. Scripta Materialia, 2018, 144, 78-83.	5.2	41
38	A molecular dynamics study of the carbonâ€“catalyst interaction energy for multi-scale modelling of single wall carbon nanotube growth. Chemical Physics Letters, 2006, 427, 365-370.	2.6	40
39	Advent of Crossâ€Scale Modeling: Highâ€Performance Computing of Solidification and Grain Growth. Advanced Theory and Simulations, 2018, 1, 1800065.	2.8	40
40	Ultrastrong underwater adhesion on diverse substrates using non-canonical phenolic groups. Nature Communications, 2022, 13, 1892.	12.8	40
41	Large-scale Phase-field Studies of Three-dimensional Dendrite Competitive Growth at the Converging Grain Boundary during Directional Solidification of a Bicrystal Binary Alloy. ISIJ International, 2016, 56, 1427-1435.	1.4	39
42	Three-dimensional morphologies of inclined equiaxed dendrites growing under forced convection by phase-field-lattice Boltzmann method. Journal of Crystal Growth, 2018, 483, 147-155.	1.5	39
43	Two-dimensional large-scale phase-field lattice Boltzmann simulation of polycrystalline equiaxed solidification with motion of a massive number of dendrites. Computational Materials Science, 2020, 178, 109639.	3.0	39
44	Phase transition in substrate-supported molybdenumnanoparticles: a molecular dynamics study. Physical Chemistry Chemical Physics, 2010, 12, 731-739.	2.8	38
45	Permeability prediction for flow normal to columnar solidification structures by largeâ€“scale simulations of phaseâ€“field and lattice Boltzmann methods. Acta Materialia, 2019, 164, 237-249.	7.9	37
46	Grain growth kinetics in submicrometer-scale molecular dynamics simulation. Acta Materialia, 2018, 153, 108-116.	7.9	36
47	Dependence of the grain boundary energy on the alloy composition in the bcc ironâ€“chromium alloy: A molecular dynamics study. Computational Materials Science, 2009, 44, 1025-1029.	3.0	34
48	Estimation of Solid-liquid Interfacial Energy from Gibbs-Thomson Effect: A Molecular Dynamics Study. ISIJ International, 2011, 51, 1664-1667.	1.4	33
49	A phase-field simulation of bridge formation process in a nanometer-scale switch. Scripta Materialia, 2006, 55, 1095-1098.	5.2	32
50	A molecular dynamics study of the graphitization ability of transition metals for catalysis of carbon nanotube growth via chemical vapor deposition. Chemical Physics Letters, 2009, 472, 200-206.	2.6	32
51	Molecular dynamics simulation and machine learning of mechanical response in non-equiatomic FeCrNiCoMn high-entropy alloy. Journal of Materials Research and Technology, 2021, 13, 2043-2054.	5.8	32
52	Ab Initio Molecular Dynamics Simulation of the Dissociation of Ethanol on a Nickel Cluster: Understanding the Initial Stage of Metal-Catalyzed Growth of Carbon Nanotubes. Journal of Physical Chemistry C, 2013, 117, 9983-9990.	3.1	31
53	Variational formulation and numerical accuracy of a quantitative phase-field model for binary alloy solidification with two-sided diffusion. Physical Review E, 2016, 93, 012802.	2.1	31
54	Variational formulation of a quantitative phase-field model for nonisothermal solidification in a multicomponent alloy. Physical Review E, 2017, 96, 033311.	2.1	31

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55	Million-atom molecular dynamics simulation on spontaneous evolution of anisotropy in solid nucleus during solidification of iron. Scripta Materialia, 2014, 86, 20-23.	5.2	29
56	Large-scale phase-field study of anisotropic grain growth: Effects of misorientation-dependent grain boundary energy and mobility. Computational Materials Science, 2021, 186, 109992.	3.0	29
57	Generation of Single-Walled Carbon Nanotubes from Alcohol and Generation Mechanism by Molecular Dynamics Simulations. Journal of Nanoscience and Nanotechnology, 2004, 4, 360-367.	0.9	28
58	Orientation Relationship in Fccâ€“Bcc Phase Transformation Kinetics of Iron: a Molecular Dynamics Study. ISIJ International, 2010, 50, 1211-1216.	1.4	28
59	Molecular dynamics simulation of athermal heterogeneous nucleation of solidification. Computational Materials Science, 2019, 164, 74-81.	3.0	28
60	Bond dissociation mechanism of ethanol during carbon nanotube synthesis via alcohol catalytic CVD technique: Ab initio molecular dynamics simulation. Chemical Physics Letters, 2014, 595-596, 185-191.	2.6	27
61	Permeability tensor for columnar dendritic structures: Phase-field and lattice Boltzmann study. Acta Materialia, 2020, 188, 282-287.	7.9	27
62	A numerical approach to the metal-catalyzed growth process of carbon nanotubes. Diamond and Related Materials, 2011, 20, 334-338.	3.9	25
63	Simulation method based on phase-field lattice Boltzmann model for long-distance sedimentation of single equiaxed dendrite. Computational Materials Science, 2019, 164, 39-45.	3.0	25
64	Estimation of Thermodynamic and Interfacial Parameters of Metallic Materials by Molecular Dynamics Simulations. Materials Transactions, 2019, 60, 180-188.	1.2	24
65	Free energy barriers from biased molecular dynamics simulations. Journal of Chemical Physics, 2020, 153, 114118.	3.0	24
66	Prediction on Mechanical Properties of Non-Equiatomic High-Entropy Alloy by Atomistic Simulation and Machine Learning. Metals, 2021, 11, 922.	2.3	24
67	Molecular dynamics simulations investigating consecutive nucleation, solidification and grain growth in a twelve-million-atom Fe-system. Journal of Crystal Growth, 2017, 474, 140-145.	1.5	23
68	Ab Initio Molecular Dynamics Simulation of Ethylene Reaction on Nickel (111) Surface. Journal of Physical Chemistry C, 2015, 119, 3210-3216.	3.1	22
69	Composition dependence of solid-liquid interfacial energy of Fe-Cr binary alloy from molecular dynamics simulations. Computational Materials Science, 2019, 167, 1-7.	3.0	22
70	Bayesian inference of solid-liquid interfacial properties out of equilibrium. Physical Review E, 2020, 101, 052121.	2.1	22
71	Machine learning approach to automated analysis of atomic configuration of molecular dynamics simulation. Computational Materials Science, 2020, 184, 109880.	3.0	22
72	Bridging molecular dynamics and phase-field methods for grain growth prediction. Computational Materials Science, 2018, 152, 118-124.	3.0	21

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73	Effect of wettability on phase transition in substrate-supported bcc-metal nanoparticles: A molecular dynamics study. Chemical Physics Letters, 2010, 486, 137-143.	2.6	20
74	Interaction between graphene and nickel(111) surfaces with commensurate and incommensurate orientational relationships. Chemical Physics Letters, 2012, 538, 112-117.	2.6	20
75	Numerical testing of quantitative phase-field models with different polynomials for isothermal solidification in binary alloys. Journal of Computational Physics, 2017, 335, 621-636.	3.8	20
76	A multiscale approach for modeling the early stage growth of single and multiwall carbon nanotubes produced by a metal-catalyzed synthesis process. Journal of Chemical Physics, 2009, 130, 034704.	3.0	19
77	Large-scale Molecular Dynamics Study on Evolution of Grain Boundary Groove of Iron. ISIJ International, 2012, 52, 2205-2209.	1.4	19
78	Low reactivity of methane on copper surface during graphene synthesis via CVD process: Ab initio molecular dynamics simulation. Chemical Physics Letters, 2014, 610-611, 33-38.	2.6	19
79	Role of oxygen vacancy in dissociation of oxygen molecule on SOFC cathode: Ab initio molecular dynamics simulation. Solid State Ionics, 2016, 285, 209-214.	2.7	19
80	Shear response of grain boundaries with metastable structures by molecular dynamics simulations. Modelling and Simulation in Materials Science and Engineering, 2018, 26, 035008.	2.0	19
81	Acceleration of phase-field lattice Boltzmann simulation of dendrite growth with thermosolutal convection by the multi-GPUs parallel computation with multiple mesh and time step method. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 054004.	2.0	19
82	Accuracy Evaluation of Phase-field Models for Grain Growth Simulation with Anisotropic Grain Boundary Properties. ISIJ International, 2020, 60, 160-167.	1.4	19
83	A Molecular Dynamics Study of Bidirectional Phase Transformation between bcc and fcc Iron. ISIJ International, 2011, 51, 1710-1716.	1.4	18
84	A phase-field simulation of uranium dendrite growth on the cathode in the electrorefining process. Journal of Nuclear Materials, 2011, 414, 114-119.	2.7	17
85	Preferential synthesis of (6,4) single-walled carbon nanotubes by controlling oxidation degree of Co catalyst. Scientific Reports, 2017, 7, 11149.	3.3	16
86	A parametric study of morphology selection in equiaxed dendritic solidification. Computational Materials Science, 2019, 162, 76-81.	3.0	16
87	Distinctive Potential Behavior at the Oxidized Surface of a Semiconductor Device in a Concentrated Aqueous Salt Solution. ChemElectroChem, 2014, 1, 1516-1524.	3.4	15
88	Calculation of surface potentials at the silicaâ€“water interface using molecular dynamics: Challenges and opportunities. Japanese Journal of Applied Physics, 2018, 57, 04FM02.	1.5	15
89	Molecular dynamics in formation process of swnt s. Molecular Crystals and Liquid Crystals, 2002, 387, 87-92.	0.9	14
90	Morphology of uranium electrodeposits on cathode in electrorefining process: A phase-field simulation. Journal of Nuclear Materials, 2013, 436, 61-67.	2.7	14

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91	First principles calculation of CH4 decomposition on nickel (111) surface. European Physical Journal B, 2015, 88, 1.	1.5	14
92	Effect of double-stranded DNA on electrical double layer structure at oxide/electrolyte interface in classical molecular dynamics simulation. Chemical Physics Letters, 2015, 619, 152-157.	2.6	14
93	A Molecular Dynamics Study of Partitionless Solidification and Melting of Alâ€“Cu Alloys. ISIJ International, 2017, 57, 1774-1779.	1.4	14
94	Large-scale phase-field simulation of three-dimensional isotropic grain growth in polycrystalline thin films. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 054003.	2.0	14
95	Micrometer-scale molecular dynamics simulation of microstructure formation linked with multi-phase-field simulation in same space scale. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 054002.	2.0	14
96	Charge Behaviors around Oxide Device/Pseudo-Physiological Solution Interface with Molecular Dynamic Simulations. Japanese Journal of Applied Physics, 2013, 52, 127001.	1.5	13
97	Competitive growth during directional solidification of a binary alloy with natural convection: two-dimensional phase-field study. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 054001.	2.0	13
98	Molecular Dynamics Simulation of Nucleation from Undercooled Melt of Nickelâ€“Aluminum Alloy and Discussion on Polymorphism in Nucleation. Materials Transactions, 2020, 61, 750-757.	1.2	13
99	Accelerated molecular dynamics simulation of large systems with parallel collective variable-driven hyperdynamics. Computational Materials Science, 2020, 177, 109581.	3.0	13
100	Novel estimation method for anisotropic grain boundary properties based on Bayesian data assimilation and phase-field simulation. Materials and Design, 2021, 210, 110089.	7.0	13
101	Accelerating Molecular Dynamics Simulation Performed on GPU. Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals, 2012, 76, 462-467.	0.4	12
102	Correlation between three-dimensional and cross-sectional characteristics of ideal grain growth: large-scale phase-field simulation study. Journal of Materials Science, 2018, 53, 15165-15180.	3.7	12
103	Non-classical nucleation in vaporâ€“liquidâ€“solid growth of monolayer WS2 revealed by in-situ monitoring chemical vapor deposition. Scientific Reports, 2021, 11, 22285.	3.3	12
104	Modeling electrochemistry in metallurgical processes. Jom, 2007, 59, 35-43.	1.9	11
105	Particle size dependence of polarization of Ni/YSZ cermet anodes for solid oxide fuel cells. Journal of Power Sources, 2013, 234, 147-153.	7.8	11
106	Grain Growth in Large-Scale Molecular Dynamics Simulation: Linkage between Atomic Configuration and von Neumann-Mullins Relation. ISIJ International, 2016, 56, 2199-2207.	1.4	11
107	Conformation and catalytic activity of nickel â€“ carbon cluster for ethanol dissociation in carbon nanotube synthesis: Ab initio molecular dynamics simulation. Chemical Physics Letters, 2017, 679, 164-171.	2.6	11
108	Solute partition at solid-liquid interface of binary alloy from molecular dynamics simulation. Materialia, 2018, 4, 553-557.	2.7	11

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109	Bayesian Data Assimilation of Temperature Dependence of Solidâ€“Liquid Interfacial Properties of Nickel. Nanomaterials, 2021, 11, 2308.	4.1	11
110	Phase-field study on an array of tilted columnar dendrites during the directional solidification of a binary alloy. Computational Materials Science, 2022, 203, 111143.	3.0	11
111	A semi-empirical molecular orbital study of freestanding and fullerene-encapsulated Mo nanoclusters. Molecular Simulation, 2008, 34, 891-903.	2.0	10
112	Ab initio molecular dynamics simulation of ethanol decomposition on platinum cluster at initial stage of carbon nanotube growth. Chemical Physics Letters, 2015, 636, 110-116.	2.6	10
113	Effects of CO₂ adsorption on proton migration on a hydrated ZrO₂ surface: an ab initio molecular dynamics study. Physical Chemistry Chemical Physics, 2017, 19, 20198-20205.	2.8	10
114	Mechanical response and plastic deformation of coherent twin boundary with perfect and defective structures. Mechanics of Materials, 2020, 141, 103266.	3.2	10
115	Phase transition of metal nanowires confined in a low-dimensional nanospace. Chemical Physics Letters, 2012, 532, 84-89.	2.6	9
116	Multi-Phase-Field Modeling of Transformation Kinetics at Multiple Scales and Its Application to Welding of Steel. Materials Transactions, 2019, 60, 170-179.	1.2	9
117	Overgrowth behavior at converging grain boundaries during competitive grain growth: A two-dimensional phase-field study. International Journal of Heat and Mass Transfer, 2020, 160, 120196.	4.8	9
118	Molecular dynamics of the generation process of double-walled carbon nanotubes from peapods. Heat Transfer - Asian Research, 2006, 35, 254-264.	2.8	8
119	Dewetting dynamics of nickel thin film on alpha-quartz substrate: A molecular dynamics study. Chemical Physics Letters, 2016, 658, 30-36.	2.6	8
120	Nucleation dynamics in Al solidification with Al-Ti refiners by molecular dynamics simulation. Computational Materials Science, 2020, 182, 109763.	3.0	8
121	Uniquely selected primary dendrite arm spacing during competitive growth of columnar grains in Alâ€“Cu alloy. Journal of Crystal Growth, 2021, 558, 126014.	1.5	8
122	Molecular dynamics simulation of interfacial growth of SiC from Siâ€“C solution on different growth planes. Journal of Crystal Growth, 2018, 494, 36-43.	1.5	7
123	Ab initio molecular dynamics simulation of ethanol dissociation reactions on alloy catalysts in carbon nanotube growth. Chemical Physics Letters, 2019, 731, 136619.	2.6	7
124	Accelerated molecular dynamics simulation of vacancy diffusion in substitutional alloy with collective variable-driven hyperdynamics. Computational Materials Science, 2021, 196, 110577.	3.0	7
125	Solid-liquid Interfacial Energy for Feâ€“Cr Alloy under Temperature Gradient from Molecular Dynamics Simulation. ISIJ International, 2020, 60, 2301-2305.	1.4	7
126	Molecular dynamics in the formation process of single-walled carbon nanotubes. Heat Transfer - Asian Research, 2003, 32, 690-699.	2.8	6

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127	Numerical Simulation of Switching Behavior in Cu/Cu₂S Nanometer-Scale Switch. Applied Physics Express, 2010, 3, 065202.	2.4	6
128	A Molecular Dynamics Study of Effects of Size and Cooling Rate on the Structure of Molybdenum Nanoparticles. Journal of Thermal Science and Technology, 2012, 7, 45-57.	1.1	5
129	Semi-grand canonical Monte Carlo simulation for derivation of thermodynamic properties of binary alloy. IOP Conference Series: Materials Science and Engineering, 2019, 529, 012037.	0.6	5
130	Entropic and enthalpic factors determining the thermodynamics and kinetics of carbon segregation from transition metal nanoparticles. Carbon, 2021, 171, 806-813.	10.3	5
131	Hierarchical Clustering of Structural and Electronic Characteristics Obtained from Molecular Dynamics Simulation of Catalytic Reaction on Metal Nanoparticle. Materials Transactions, 2021, 62, 829-835.	1.2	5
132	Fast-Decoding Algorithm for Electrode Processes at Electrified Interfaces by Mean-Field Kinetic Model and Bayesian Data Assimilation: An Active-Data-Mining Approach for the Efficient Search and Discovery of Electrocatalysts. ACS Applied Materials & Interfaces, 2022, 14, 22889-22902.	8.0	5
133	Silicon Crystal Pulling from the Melt of Si-45mass%Ni Alloy. Tetsu-To-Hagane/Journal of the Iron and Steel Institute of Japan, 2008, 94, 496-501.	0.4	4
134	Phase-Field Simulation of Dendrite Growth during Electrodeposition. Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals, 2009, 73, 601-607.	0.4	4
135	Effect of Ionic Atmosphere around DNA/Electrolyte Interface on Potentiometric Signal. Journal of the Electrochemical Society, 2017, 164, B548-B552.	2.9	4
136	Atomistic Simulation of the Interaction Between Point Defects and Twin Boundary. Physica Status Solidi (B): Basic Research, 2018, 255, 1800228.	1.5	3
137	Time invariance of three-dimensional morphology of equiaxed dendrite: A phase-field study. Computational Materials Science, 2022, 204, 111173.	3.0	3
138	Numerical Approach to the Phase Transformation of Iron and Related Properties at the Interface by Molecular Simulation. Materia Japan, 2009, 48, 61-66.	0.1	2
139	Numerical Simulation of Silver Pillar Growth and Switching Behavior in Ag/Ag2S Nanometer Scale Switch. Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals, 2009, 73, 589-594.	0.4	2
140	Elucidation of Semiconductor/Bio-Interface Structure with Massive Classical Molecular Dynamics Simulation. Hyomen Gijutsu/Journal of the Surface Finishing Society of Japan, 2014, 65, 251-256.	0.2	2
141	Molecular Dynamics in Formation Process of Single-Walled Carbon Nanotubes.. 880-02 Nihon Kikai Gakkai RonbunshÅ« Transactions of the Japan Society of Mechanical Engineers Series B B-hen, 2002, 68, 3087-3092.	0.2	1
142	The Effect of Catalytic Metals of Various Elements in Nucleation Process of Single-Walled Carbon Nanotubes. 880-02 Nihon Kikai Gakkai RonbunshÅ« Transactions of the Japan Society of Mechanical Engineers Series B B-hen, 2006, 72, 2513-2518.	0.2	1
143	Synthesis of Single Walled Carbon Nanotubes by Laser Vaporized Catalytic Chemical Vapor Deposition Technique. , 2007, , .		1
144	Numerical Simulation of Two-dimensional Meniscus Surface and Its Application to Estimation of Wetting Behavior between Solid Substrate and Melt. Tetsu-To-Hagane/Journal of the Iron and Steel Institute of Japan, 2010, 96, 138-140.	0.4	1

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145	Distinctive Potential Behavior at Oxidized Surface of Semiconductor Device in Concentrated Aqueous Salt Solution. ChemElectroChem, 2014, 1, 1427-1427.	3.4	1
146	Reaction of ethylene molecules with a nickel cluster: <i>ab initio</i> molecular dynamics study. Transactions of the Materials Research Society of Japan, 2015, 40, 215-218.	0.2	1
147	Molecular dynamics simulation of heterogeneous nucleation via grain refiner inoculated in aluminium melt. IOP Conference Series: Materials Science and Engineering, 2019, 529, 012047.	0.6	1
148	Free energy surface of initial cap formation in carbon nanotube growth. Nanoscale Advances, 0, , .	4.6	1
149	Dendrite Growth of Silicon along the Undercooled Melt Surface of Si-45mass%Ni Alloy. Tetsu-To-Hagane/Journal of the Iron and Steel Institute of Japan, 2009, 95, 22-25.	0.4	1
150	Molecular Dynamics of Generation Process of Double-Walled Carbon Nanotubes from Peapods. 880-02 Nihon Kikai Gakkai RonbunshÅ« Transactions of the Japan Society of Mechanical Engineers Series B B-hen, 2005, 71, 2117-2122.	0.2	0
151	Molecular Dynamics of Nucleation Process of Single-Walled Carbon Nanotubes in Catalytic CVD Method. 880-02 Nihon Kikai Gakkai RonbunshÅ« Transactions of the Japan Society of Mechanical Engineers Series B B-hen, 2006, 72, 2505-2512.	0.2	0
152	Molecular Dynamics Simulation of Nucleation Process of Single-Walled Carbon Nanotubes from a Metal Cluster on a Substrate. 880-02 Nihon Kikai Gakkai RonbunshÅ« Transactions of the Japan Society of Mechanical Engineers Series B B-hen, 2006, 72, 2519-2523.	0.2	0
153	Atomistic Simulation of the Interaction Between Point Defects and Twin Boundary (Phys. Status Solidi) Tj ETQq1 1 0.784314 rgBT /Over	1.5	0
154	Molecular Dynamics Study of the Effect of Carbon Atoms on the Surface Tension of Siliconâ€“carbon Alloy. ISIJ International, 2020, 60, 199-204.	1.4	0
155	116 A phase-field model for electrochemical processes. The Proceedings of the Computational Mechanics Conference, 2008, 2008.21, 127-128.	0.0	0
156	348 Effects of catalyst difference in production of SWNT by laser ablation. The Proceedings of the JSME Annual Meeting, 2008, 2008.8, 95-96.	0.0	0
157	Variational formulation of quantitative phase-field model. The Proceedings of the Computational Mechanics Conference, 2016, 2016.29, 4_133.	0.0	0
158	Interaction Between Nano-Voids and Migrating Grain Boundary by Molecular Dynamics Simulation. SSRN Electronic Journal, 0, , .	0.4	0
159	High Performance Computing of Solidification Microstructures and Emergence of Cross-scale Approach. Materia Japan, 2020, 59, 139-144.	0.1	0
160	Temperature Dependence of Solid-Liquid Interfacial Energy for Pure Metals by Metadynamics-Based Simulations. Materials Transactions, 2021, 63, .	1.2	0
161	Inverse analysis of anisotropy of solid-liquid interfacial free energy based on machine learning. Computational Materials Science, 2022, 207, 111294.	3.0	0