Yasushi Shibuta

List of Publications by Year in Descending Order

157 papers	3,694 citations	34 h-index	54 g-index
162 ext. papers	4,218 ext. citations	3.4 avg, IF	6.06 L-index

#	Paper	IF	Citations
157	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**,	9.5	1
156	Phase-field study on an array of tilted columnar dendrites during the directional solidification of a binary alloy. *Computational Materials Science*, **2022**, 203, 111143	3.2	1
155	Time invariance of three-dimensional morphology of equiaxed dendrite: A phase-field study. *Computational Materials Science*, **2022**, 204, 111173	3.2	1
154	Inverse analysis of anisotropy of solid-liquid interfacial free energy based on machine learning. *Computational Materials Science*, **2022**, 207, 111294	3.2	
153	Ultrastrong underwater adhesion on diverse substrates using non-canonical phenolic groups.. *Nature Communications*, **2022**, 13, 1892	17.4	6
152	Non-classical nucleation in vapor-liquid-solid growth of monolayer WS revealed by in-situ monitoring chemical vapor deposition. *Scientific Reports*, **2021**, 11, 22285	4.9	0
151	Uniquely selected primary dendrite arm spacing during competitive growth of columnar grains in Al□u alloy. *Journal of Crystal Growth*, **2021**, 558, 126014	1.6	2
150	Prediction on Mechanical Properties of Non-Equiatomic High-Entropy Alloy by Atomistic Simulation and Machine Learning. *Metals*, **2021**, 11, 922	2.3	7
149	Hierarchical Clustering of Structural and Electronic Characteristics Obtained from Molecular Dynamics Simulation of Catalytic Reaction on Metal Nanoparticle. *Materials Transactions*, **2021**, 62, 829-835	1.3	
148	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	5.5	5
147	Entropic and enthalpic factors determining the thermodynamics and kinetics of carbon segregation from transition metal nanoparticles. *Carbon*, **2021**, 171, 806-813	10.4	3
146	Large-scale phase-field study of anisotropic grain growth: Effects of misorientation-dependent grain boundary energy and mobility. *Computational Materials Science*, **2021**, 186, 109992	3.2	9
145	Accelerated molecular dynamics simulation of vacancy diffusion in substitutional alloy with collective variable-driven hyperdynamics. *Computational Materials Science*, **2021**, 196, 110577	3.2	0
144	Bayesian Data Assimilation of Temperature Dependence of Solid-Liquid Interfacial Properties of Nickel. *Nanomaterials*, **2021**, 11,	5.4	2
143	Novel estimation method for anisotropic grain boundary properties based on Bayesian data assimilation and phase-field simulation. *Materials and Design*, **2021**, 210, 110089	8.1	1
142	Molecular Dynamics Simulation of Nucleation from Undercooled Melt of Nickel□luminum Alloy and Discussion on Polymorphism in Nucleation. *Materials Transactions*, **2020**, 61, 750-757	1.3	8
141	Bayesian inference of solid-liquid interfacial properties out of equilibrium. *Physical Review E*, **2020**, 101, 052121	2.4	12

140	Nucleation dynamics in Al solidification with Al-Ti refiners by molecular dynamics simulation. *Computational Materials Science*, **2020**, 182, 109763	3.2	5
139	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	3.2	23
138	Machine learning approach to automated analysis of atomic configuration of molecular dynamics simulation. *Computational Materials Science*, **2020**, 184, 109880	3.2	5
137	Permeability tensor for columnar dendritic structures: Phase-field and lattice Boltzmann study. *Acta Materialia*, **2020**, 188, 282-287	8.4	13
136	Accelerated molecular dynamics simulation of large systems with parallel collective variable-driven hyperdynamics. *Computational Materials Science*, **2020**, 177, 109581	3.2	4
135	Accuracy Evaluation of Phase-field Models for Grain Growth Simulation with Anisotropic Grain Boundary Properties. *ISIJ International*, **2020**, 60, 160-167	1.7	8
134	Molecular Dynamics Study of the Effect of Carbon Atoms on the Surface Tension of Silicon–carbon Alloy. *ISIJ International*, **2020**, 60, 199-204	1.7	
133	High Performance Computing of Solidification Microstructures and Emergence of Cross-scale Approach. *Materia Japan*, **2020**, 59, 139-144	0.1	
132	Solid-liquid Interfacial Energy for Fe–Cr Alloy under Temperature Gradient from Molecular Dynamics Simulation. *ISIJ International*, **2020**, 60, 2301-2305	1.7	1
131	Inverse Hall-Petch relationship of high-entropy alloy by atomistic simulation. *Materials Letters*, **2020**, 274, 128024	3.3	21
130	Mechanical response and plastic deformation of coherent twin boundary with perfect and defective structures. *Mechanics of Materials*, **2020**, 141, 103266	3.3	4
129	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	4.9	5
128	Free energy barriers from biased molecular dynamics simulations. *Journal of Chemical Physics*, **2020**, 153, 114118	3.9	15
127	Large-scale phase-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	3.2	21
126	Composition dependence of solid-liquid interfacial energy of Fe-Cr binary alloy from molecular dynamics simulations. *Computational Materials Science*, **2019**, 167, 1-7	3.2	12
125	Interaction between nano-voids and migrating grain boundary by molecular dynamics simulation. *Acta Materialia*, **2019**, 173, 206-224	8.4	24
124	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	12
123	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	7

122	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	7
121	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	8
120	Estimation of Thermodynamic and Interfacial Parameters of Metallic Materials by Molecular Dynamics Simulations. *Materials Transactions*, **2019**, 60, 180-188	1.3	17
119	A parametric study of morphology selection in equiaxed dendritic solidification. *Computational Materials Science*, **2019**, 162, 76-81	3.2	11
118	Molecular dynamics simulation of athermal heterogeneous nucleation of solidification. *Computational Materials Science*, **2019**, 164, 74-81	3.2	14
117	Simulation method based on phase-field lattice Boltzmann model for long-distance sedimentation of single equiaxed dendrite. *Computational Materials Science*, **2019**, 164, 39-45	3.2	16
116	Ab initio molecular dynamics simulation of ethanol dissociation reactions on alloy catalysts in carbon nanotube growth. *Chemical Physics Letters*, **2019**, 731, 136619	2.5	6
115	Multi-Phase-Field Modeling of Transformation Kinetics at Multiple Scales and Its Application to Welding of Steel. *Materials Transactions*, **2019**, 60, 170-179	1.3	6
114	Semi-grand canonical Monte Carlo simulation for derivation of thermodynamic properties of binary alloy. *IOP Conference Series: Materials Science and Engineering*, **2019**, 529, 012037	0.4	4
113	Molecular dynamics simulation of heterogeneous nucleation via grain refiner inoculated in aluminium melt. *IOP Conference Series: Materials Science and Engineering*, **2019**, 529, 012047	0.4	1
112	Permeability prediction for flow normal to columnar solidification structures by large-scale simulations of phase-field and lattice Boltzmann methods. *Acta Materialia*, **2019**, 164, 237-249	8.4	26
111	Grain boundary induced deformation mechanisms in nanocrystalline Al by molecular dynamics simulation: From interatomic potential perspective. *Computational Materials Science*, **2019**, 156, 421-433	3.2	25
110	Shear response of grain boundaries with metastable structures by molecular dynamics simulations. *Modelling and Simulation in Materials Science and Engineering*, **2018**, 26, 035008	2	14
109	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	3.2	54
108	Grain growth kinetics in submicrometer-scale molecular dynamics simulation. *Acta Materialia*, **2018**, 153, 108-116	8.4	26
107	Calculation of surface potentials at the silica-water interface using molecular dynamics: Challenges and opportunities. *Japanese Journal of Applied Physics*, **2018**, 57, 04FM02	1.4	11
106	Dynamic interaction between grain boundary and stacking fault tetrahedron. *Scripta Materialia*, **2018**, 144, 78-83	5.6	31
105	Advent of Cross-Scale Modeling: High-Performance Computing of Solidification and Grain Growth. *Advanced Theory and Simulations*, **2018**, 1, 1800065	3.5	30

104	Atomistic Simulation of the Interaction Between Point Defects and Twin Boundary. *Physica Status Solidi (B): Basic Research*, **2018**, 255, 1800228	1.3	2
103	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	4.3	7
102	Molecular dynamics simulation of interfacial growth of SiC from Si□ solution on different growth planes. *Journal of Crystal Growth*, **2018**, 494, 36-43	1.6	4
101	Bridging molecular dynamics and phase-field methods for grain growth prediction. *Computational Materials Science*, **2018**, 152, 118-124	3.2	15
100	Competitive grain growth during directional solidification of a polycrystalline binary alloy: Three-dimensional large-scale phase-field study. *Materialia*, **2018**, 1, 104-113	3.2	34
99	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	1.6	33
98	Solute partition at solid-liquid interface of binary alloy from molecular dynamics simulation. *Materialia*, **2018**, 4, 553-557	3.2	9
97	Atomistic Simulation of the Interaction Between Point Defects and Twin Boundary (Phys. Status Solidi B 9/2018). *Physica Status Solidi (B): Basic Research*, **2018**, 255, 1870133	1.3	
96	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	1.6	59
95	Heterogeneity in homogeneous nucleation from billion-atom molecular dynamics simulation of solidification of pure metal. *Nature Communications*, **2017**, 8, 10	17.4	152
94	Conformation and catalytic activity of nickel□carbon cluster for ethanol dissociation in carbon nanotube synthesis: Ab initio molecular dynamics simulation. *Chemical Physics Letters*, **2017**, 679, 164-171	2.5	8
93	Numerical testing of quantitative phase-field models with different polynomials for isothermal solidification in binary alloys. *Journal of Computational Physics*, **2017**, 335, 621-636	4.1	16
92	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	1.6	16
91	Phase-field-lattice Boltzmann studies for dendritic growth with natural convection. *Journal of Crystal Growth*, **2017**, 474, 146-153	1.6	45
90	Effect of Ionic Atmosphere around DNA/Electrolyte Interface on Potentiometric Signal. *Journal of the Electrochemical Society*, **2017**, 164, B548-B552	3.9	2
89	Preferential synthesis of (6,4) single-walled carbon nanotubes by controlling oxidation degree of Co catalyst. *Scientific Reports*, **2017**, 7, 11149	4.9	11
88	Effects of CO adsorption on proton migration on a hydrated ZrO surface: an ab initio molecular dynamics study. *Physical Chemistry Chemical Physics*, **2017**, 19, 20198-20205	3.6	6
87	Variational formulation of a quantitative phase-field model for nonisothermal solidification in a multicomponent alloy. *Physical Review E*, **2017**, 96, 033311	2.4	19

86	Ultra-large-scale phase-field simulation study of ideal grain growth. *Npj Computational Materials*, **2017**, 3,	10.9	48
85	A Molecular Dynamics Study of Partitionless Solidification and Melting of Al□u Alloys. *ISIJ International*, **2017**, 57, 1774-1779	1.7	11
84	Role of oxygen vacancy in dissociation of oxygen molecule on SOFC cathode: Ab initio molecular dynamics simulation. *Solid State Ionics*, **2016**, 285, 209-214	3.3	14
83	Primary arm array during directional solidification of a single-crystal binary alloy: Large-scale phase-field study. *Acta Materialia*, **2016**, 118, 230-243	8.4	72
82	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	2.4	24
81	Wafer-scale fabrication and growth dynamics of suspended graphene nanoribbon arrays. *Nature Communications*, **2016**, 7, 11797	17.4	35
80	Dewetting dynamics of nickel thin film on alpha-quartz substrate: A molecular dynamics study. *Chemical Physics Letters*, **2016**, 658, 30-36	2.5	8
79	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	8.4	72
78	Two-dimensional phase-field study of competitive grain growth during directional solidification of polycrystalline binary alloy. *Journal of Crystal Growth*, **2016**, 442, 14-24	1.6	63
77	Variational formulation of quantitative phase-field model. *The Proceedings of the Computational Mechanics Conference*, **2016**, 2016.29, 4_133	0	
76	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	1.7	33
75	Grain Growth in Large-Scale Molecular Dynamics Simulation: Linkage between Atomic Configuration and von Neumann-Mullins Relation. *ISIJ International*, **2016**, 56, 2199-2207	1.7	11
74	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	2.5	6
73	First principles calculation of CH4 decomposition on nickel (111) surface. *European Physical Journal B*, **2015**, 88, 1	1.2	8
72	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	2.5	12
71	Homogeneous nucleation and microstructure evolution in million-atom molecular dynamics simulation. *Scientific Reports*, **2015**, 5, 13534	4.9	69
70	Reaction of ethylene molecules with a nickel cluster: ab initio molecular dynamics study. *Transactions of the Materials Research Society of Japan*, **2015**, 40, 215-218	0.2	1
69	Solidification in a Supercomputer: From Crystal Nuclei to Dendrite Assemblages. *Jom*, **2015**, 67, 1793-1804	2.1	80

68	Proton Migration on Hydrated Surface of Cubic ZrO2: Ab initio Molecular Dynamics Simulation. *Journal of Physical Chemistry C*, **2015**, 119, 28925-28933	3.8	39
67	Ab Initio Molecular Dynamics Simulation of Ethylene Reaction on Nickel (111) Surface. *Journal of Physical Chemistry C*, **2015**, 119, 3210-3216	3.8	15
66	Million-atom molecular dynamics simulation on spontaneous evolution of anisotropy in solid nucleus during solidification of iron. *Scripta Materialia*, **2014**, 86, 20-23	5.6	26
65	Distinctive Potential Behavior at Oxidized Surface of Semiconductor Device in Concentrated Aqueous Salt Solution. *ChemElectroChem*, **2014**, 1, 1427-1427	4.3	1
64	Distinctive Potential Behavior at the Oxidized Surface of a Semiconductor Device in a Concentrated Aqueous Salt Solution. *ChemElectroChem*, **2014**, 1, 1516-1524	4.3	13
63	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	2.5	16
62	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	2.5	25
61	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	0.1	2
60	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	2.5	47
59	Particle size dependence of polarization of Ni/YSZ cermet anodes for solid oxide fuel cells. *Journal of Power Sources*, **2013**, 234, 147-153	8.9	9
58	Morphology of uranium electrodeposits on cathode in electrorefining process: A phase-field simulation. *Journal of Nuclear Materials*, **2013**, 436, 61-67	3.3	10
57	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	3.8	27
56	Atomistic modelling of CVD synthesis of carbon nanotubes and graphene. *Nanoscale*, **2013**, 5, 6662-76	7.7	75
55	Charge Behaviors around Oxide Device/Pseudo-Physiological Solution Interface with Molecular Dynamic Simulations. *Japanese Journal of Applied Physics*, **2013**, 52, 127001	1.4	13
54	Phase transition of metal nanowires confined in a low-dimensional nanospace. *Chemical Physics Letters*, **2012**, 532, 84-89	2.5	9
53	Interaction between graphene and nickel(111) surfaces with commensurate and incommensurate orientational relationships. *Chemical Physics Letters*, **2012**, 538, 112-117	2.5	19
52	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	0.6	5
51	Large-scale Molecular Dynamics Study on Evolution of Grain Boundary Groove of Iron. *ISIJ International*, **2012**, 52, 2205-2209	1.7	17

50	Accelerating Molecular Dynamics Simulation Performed on GPU. *Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals*, **2012**, 76, 462-467	0.4	11
49	A numerical approach to the metal-catalyzed growth process of carbon nanotubes. *Diamond and Related Materials*, **2011**, 20, 334-338	3.5	25
48	A Molecular Dynamics Study of Bidirectional Phase Transformation between bcc and fcc Iron. *ISIJ International*, **2011**, 51, 1710-1716	1.7	16
47	Estimation of Solid-liquid Interfacial Energy from Gibbs-Thomson Effect: A Molecular Dynamics Study. *ISIJ International*, **2011**, 51, 1664-1667	1.7	28
46	Interaction between two graphene sheets with a turbostratic orientational relationship. *Chemical Physics Letters*, **2011**, 512, 146-150	2.5	95
45	A phase-field simulation of uranium dendrite growth on the cathode in the electrorefining process. *Journal of Nuclear Materials*, **2011**, 414, 114-119	3.3	12
44	A molecular dynamics study of cooling rate during solidification of metal nanoparticles. *Chemical Physics Letters*, **2011**, 502, 82-86	2.5	47
43	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	0.5	
42	Numerical Simulation of Switching Behavior in Cu/Cu2S Nanometer-Scale Switch. *Applied Physics Express*, **2010**, 3, 065202	2.4	4
41	A phase-field model for electrode reactions with Butler□Volmer kinetics. *Computational Materials Science*, **2010**, 50, 118-124	3.2	47
40	Phase transition in substrate-supported molybdenum nanoparticles: a molecular dynamics study. *Physical Chemistry Chemical Physics*, **2010**, 12, 731-9	3.6	35
39	Catalyzed growth of carbon nanotube with definable chirality by hybrid molecular dynamics-force biased Monte Carlo simulations. *ACS Nano*, **2010**, 4, 6665-72	16.7	149
38	A Molecular Dynamics Study of Thermodynamic and Kinetic Properties of Solid□Liquid Interface for Bcc Iron. *ISIJ International*, **2010**, 50, 1158-1164	1.7	51
37	Orientation Relationship in Fcc□Bcc Phase Transformation Kinetics of Iron: a Molecular Dynamics Study. *ISIJ International*, **2010**, 50, 1211-1216	1.7	21
36	Effect of wettability on phase transition in substrate-supported bcc-metal nanoparticles: A molecular dynamics study. *Chemical Physics Letters*, **2010**, 486, 137-143	2.5	18
35	Melting and solidification point of fcc-metal nanoparticles with respect to particle size: A molecular dynamics study. *Chemical Physics Letters*, **2010**, 498, 323-327	2.5	69
34	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	17
33	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	2.5	28

32	Growth and melting of nanoparticles in liquid iron: A molecular dynamics study. *Chemical Physics Letters*, **2009**, 475, 264-268	2.5	44
31	Dependence of the grain boundary energy on the alloy composition in the bcc iron□hromium alloy: A molecular dynamics study. *Computational Materials Science*, **2009**, 44, 1025-1029	3.2	31
30	Phase-Field Simulation of Dendrite Growth during Electrodeposition. *Nippon Kinzoku Gakkaishi/Journal of the Japan Institute of Metals*, **2009**, 73, 601-607	0.4	3
29	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	1
28	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
27	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	0.5	1
26	A molecular dynamics study of the fcc□bcc phase transformation kinetics of iron. *Scripta Materialia*, **2008**, 59, 971-974	5.6	57
25	Direction control of chemical wave propagation in self-oscillating gel array. *Journal of Physical Chemistry B*, **2008**, 112, 1777-82	3.4	44
24	A semi-empirical molecular orbital study of freestanding and fullerene-encapsulated Mo nanoclusters. *Molecular Simulation*, **2008**, 34, 891-903	2	7
23	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	0.5	4
22	A Molecular Dynamics Study of the Energy and Structure of the Symmetric Tilt Boundary of Iron. *ISIJ International*, **2008**, 48, 1582-1591	1.7	97
21	A molecular dynamics study of the phase transition in bcc metal nanoparticles. *Journal of Chemical Physics*, **2008**, 129, 144102	3.9	112
20	116 A phase-field model for electrochemical processes. *The Proceedings of the Computational Mechanics Conference*, **2008**, 2008.21, 127-128	0	
19	348 Effects of catalyst difference in production of SWNT by laser ablation. *The Proceedings of the JSME Annual Meeting*, **2008**, 2008.8, 95-96		
18	Synthesis of Single Walled Carbon Nanotubes by Laser Vaporized Catalytic Chemical Vapor Deposition Technique **2007**,		1
17	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	2.5	53
16	Melting and nucleation of iron nanoparticles: A molecular dynamics study. *Chemical Physics Letters*, **2007**, 445, 265-270	2.5	130
15	Modeling electrochemistry in metallurgical processes. *Jom*, **2007**, 59, 35-43	2.1	10

14	Phase-field modeling for electrodeposition process. *Science and Technology of Advanced Materials*, **2007**, 8, 511-518	7.1	41
13	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	3.2	83
12	A phase-field simulation of bridge formation process in a nanometer-scale switch. *Scripta Materialia* , **2006**, 55, 1095-1098	5.6	29
11	Molecular dynamics of the generation process of double-walled carbon nanotubes from peapods. *Heat Transfer - Asian Research*, **2006**, 35, 254-264	2.8	8
10	Molecular Dynamics of Nucleation Process of Single-Walled Carbon Nanotubes in Catalytic CVD Method. *880-02 Nihon Kikai Gakkai Ronbunsh Transactions of the Japan Society of Mechanical Engineers Series B B-hen*, **2006**, 72, 2505-2512		
9	The Effect of Catalytic Metals of Various Elements in Nucleation Process of Single-Walled Carbon Nanotubes. *880-02 Nihon Kikai Gakkai Ronbunsh Transactions of the Japan Society of Mechanical Engineers Series B B-hen*, **2006**, 72, 2513-2518		
8	Molecular Dynamics Simulation of Nucleation Process of Single-Walled Carbon Nanotubes from a Metal Cluster on a Substrate. *880-02 Nihon Kikai Gakkai Ronbunsh Transactions of the Japan Society of Mechanical Engineers Series B B-hen*, **2006**, 72, 2519-2523		
7	A molecular dynamics study of the carbon catalyst interaction energy for multi-scale modelling of single wall carbon nanotube growth. *Chemical Physics Letters*, **2006**, 427, 365-370	2.5	38
6	Molecular Dynamics of Generation Process of Double-Walled Carbon Nanotubes from Peapods. *880-02 Nihon Kikai Gakkai Ronbunsh Transactions of the Japan Society of Mechanical Engineers Series B B-hen*, **2005**, 71, 2117-2122		
5	Generation of single-walled carbon nanotubes from alcohol and generation mechanism by molecular dynamics simulations. *Journal of Nanoscience and Nanotechnology*, **2004**, 4, 360-7	1.3	24
4	Molecular dynamics in the formation process of single-walled carbon nanotubes. *Heat Transfer - Asian Research*, **2003**, 32, 690-699	2.8	5
3	Molecular dynamics simulation of formation process of single-walled carbon nanotubes by CCVD method. *Chemical Physics Letters*, **2003**, 382, 381-386	2.5	205
2	Molecular dynamics simulation of generation process of SWNTs. *Physica B: Condensed Matter*, **2002**, 323, 187-189	2.8	60
1	Molecular dynamics in formation process of swnt s. *Molecular Crystals and Liquid Crystals*, **2002**, 387, 87-92	0.5	12