

Chong-Yu Wang

List of Publications by Year in Descending Order

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

77
papers

1,259
citations

21
h-index

32
g-index

81
ext. papers

1,464
ext. citations

3.1
avg, IF

4.85
L-index

#	Paper	IF	Citations
77	Synergistic strengthening mechanisms of rhenium in nickel-based single crystal superalloys. <i>Intermetallics</i> , 2021 , 132, 107133	3.5	2
76	Transition metal solutes in Ni-based ternary model superalloys: Partitioning and effects on elastic properties from first-principles calculations. <i>Computational Materials Science</i> , 2021 , 195, 110447	3.2	0
75	Novel structures and mechanical properties of Zr ₂ N: Ab initio description under high pressures. <i>Chinese Physics B</i> , 2021 , 30, 016403	1.2	1
74	Construction of Ni ₃ Al ₂ W EAM potential and application in misfit dislocation system. <i>Progress in Natural Science: Materials International</i> , 2020 , 30, 539-544	3.6	1
73	Compressive behavior and elastic properties of Ni-based ternary model superalloys: First-principles calculations and rule of mixtures predications. <i>Journal of Alloys and Compounds</i> , 2020 , 839, 155661	5.7	3
72	Alloying-element dependence of structural, elastic and electronic properties of nickel-based superalloys: Influence of γ' volume fraction. <i>Journal of Alloys and Compounds</i> , 2020 , 838, 155141	5.7	6
71	First-principles study of Ni/Ni ₃ Al interface doped with Re, Ta and W. <i>Computational Materials Science</i> , 2020 , 175, 109586	3.2	8
70	Re effects in model Ni-based superalloys investigated with first-principles calculations and atom probe tomography. <i>Chinese Physics B</i> , 2020 , 29, 043103	1.2	4
69	Predicting creep rupture life of Ni-based single crystal superalloys using divide-and-conquer approach based machine learning. <i>Acta Materialia</i> , 2020 , 195, 454-467	8.4	35
68	Doping effects on the stacking fault energies of the γ' phase in Ni-based superalloys. <i>Chinese Physics B</i> , 2020 , 29, 026401	1.2	1
67	Dependence of mechanical properties on the site occupancy of ternary alloying elements in γ' -Ni ₃ Al: Ab initio description for shear and tensile deformation. <i>Chinese Physics B</i> , 2020 , 29, 078103	1.2	4
66	Transition-metal-element dependence of ideal shear strength and elastic behaviors of γ' -Ni ₃ Al: ab initio study to guide rational alloy design. <i>Journal of Alloys and Compounds</i> , 2019 , 806, 1260-1266	5.7	13
65	Effects of Re, W and Co on dislocation nucleation at the crack tip in the γ' -phase of Ni-based single-crystal superalloys by atomistic simulation. <i>Royal Society Open Science</i> , 2019 , 6, 190441	3.3	2
64	Transition-metal alloying of γ' -Ni ₃ Al: Effects on the ideal uniaxial compressive strength from first-principles calculations. <i>Physical Review B</i> , 2018 , 97,	3.3	15
63	The effects of combining alloying elements on the elastic properties of γ' -Ni in Ni-based superalloy: High-throughput first-principles calculations. <i>Chinese Physics B</i> , 2018 , 27, 077104	1.2	3
62	Anisotropic elastic properties and ideal uniaxial compressive strength of TiB ₂ from first principles calculations. <i>Chinese Physics B</i> , 2018 , 27, 077103	1.2	2
61	Multiscale energy density algorithm and application to surface structure of Ni matrix of superalloy. <i>Chinese Physics B</i> , 2018 , 27, 097105	1.2	

60	Site preferences of alloying transition metal elements in Ni-based superalloy: A first-principles study. <i>Chinese Physics B</i> , 2018 , 27, 097102	1.2	2
59	Effect of interactions between elements on the diffusion of solutes in Ni X Y systems and γ -coarsening in model Ni-based superalloys. <i>Scripta Materialia</i> , 2017 , 138, 100-104	5.6	20
58	Partitioning and diffusion of transition metal solutes in ternary model Ni-based single crystal superalloys. <i>Materials and Design</i> , 2017 , 130, 157-165	8.1	28
57	Electronic structure and multi-scale behaviour for the dislocation-looping complex in the gamma phase of nickel-base superalloys. <i>RSC Advances</i> , 2017 , 7, 19124-19135	3.7	6
56	Lattice stability and the effect of Co and Re on the ideal strength of Ni: First-principles study of uniaxial tensile deformation. <i>Chinese Physics B</i> , 2017 , 26, 093106	1.2	4
55	Influence of alloying elements upon the theoretical tensile strength of Ni-based model superalloy: γ -Ni/ γ -Ni ₃ Al multilayer. <i>Computational Materials Science</i> , 2016 , 119, 120-129	3.2	7
54	First principles study of the diffusional phenomena across the clean and Re-doped γ -Ni/ γ -Ni ₃ Al interface of Ni-based single crystal superalloy. <i>Chinese Physics B</i> , 2016 , 25, 067104	1.2	2
53	Effect of the alloying element on the temperature-dependent ideal shear strength of γ -Ni ₃ Al. <i>RSC Advances</i> , 2016 , 6, 20551-20558	3.7	10
52	Diffusion in Ni-Based Single Crystal Superalloys with Density Functional Theory and Kinetic Monte Carlo Method. <i>Communications in Computational Physics</i> , 2016 , 20, 603-618	2.4	6
51	Construction of ternary Ni-Ta potential and its application in the effect of Ta on [1 1 0] edge dislocation slipping in γ -Ni ₃ Al. <i>Computational Materials Science</i> , 2016 , 118, 288-296	3.2	2
50	Effect of alloying elements on the ideal strength and charge redistribution of γ -Ni ₃ Al: a first-principles study of tensile deformation. <i>RSC Advances</i> , 2016 , 6, 77489-77498	3.7	14
49	Density functional theory study of the thermodynamic and elastic properties of Ni-based superalloys. <i>Journal of Physics Condensed Matter</i> , 2015 , 27, 295401	1.8	13
48	Effect of Re and W upon brittle fracture in Ni ₃ Al cracks by atomic simulation. <i>Computational Materials Science</i> , 2015 , 110, 261-269	3.2	6
47	Effect of Re on dislocation nucleation from crack tip in Ni by atomistic simulation. <i>Computational Materials Science</i> , 2015 , 97, 127-135	3.2	6
46	Effect of Re on lattice trapping in γ -Ni ₃ Al cracks by atomistic simulation. <i>Computational Materials Science</i> , 2015 , 97, 102-108	3.2	11
45	A ternary Ni-Ta-W EAM potential for Ni-based single crystal superalloys. <i>Physica B: Condensed Matter</i> , 2015 , 456, 283-292	2.8	11
44	Influence of the alloying elements Re, Co and W on the propagation of the Ni/Ni ₃ Al interface crack. <i>RSC Advances</i> , 2015 , 5, 52473-52480	3.7	16
43	Molecular dynamics simulations of influence of Re on lattice trapping and fracture stress of cracks in Ni. <i>Computational Materials Science</i> , 2014 , 83, 196-206	3.2	19

42	The ternary NiAlCo embedded-atom-method potential for γ -Ni-based single-crystal superalloys: Construction and application. <i>Chinese Physics B</i> , 2014 , 23, 033401	1.2	7
41	Cross-slip process in model Ni(Al) solid solution: An embedded-atom method study. <i>Computational Materials Science</i> , 2014 , 91, 192-199	3.2	5
40	Effect of Re on stacking fault nucleation under shear strain in Ni by atomistic simulation. <i>Chinese Physics B</i> , 2014 , 23, 110208	1.2	1
39	First-principles study of point defects in solar cell semiconductor CuI. <i>Physica B: Condensed Matter</i> , 2013 , 413, 116-119	2.8	21
38	Influence of Re on the propagation of a Ni/Ni3Al interface crack by molecular dynamics simulation. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2013 , 21, 045009	2	25
37	The effects of alloying elements on generalized stacking fault energies, strength and ductility of γ -Ni3Al. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2012 , 539, 38-41	5.3	47
36	Effect of alloying element on dislocation cross-slip in γ -Ni3Al: a first-principles study. <i>Philosophical Magazine</i> , 2012 , 92, 4028-4039	1.6	12
35	First-principle investigation of 3d transition metal elements in γ -Co3(Al,W). <i>Journal of Applied Physics</i> , 2010 , 107, 093705	2.5	28
34	Multiscale analysis and numerical algorithm for the Schrödinger equations in heterogeneous media. <i>Applied Mathematics and Computation</i> , 2010 , 217, 3955-3973	2.7	4
33	Effect of Re in γ phase, γ' phase and γ/γ' interface of Ni-based single-crystal superalloys. <i>Acta Materialia</i> , 2010 , 58, 2045-2055	8.4	44
32	A comparison of the ideal strength between L12Co3(Al,W) and Ni3Al under tension and shear from first-principles calculations. <i>Applied Physics Letters</i> , 2009 , 94, 261909	3.4	62
31	Mechanical properties and electronic structure of superhard diamondlike BC5: A first-principles study. <i>Journal of Applied Physics</i> , 2009 , 106, 043513	2.5	14
30	Influence of alloying elements on the elastic properties of ternary and quaternary nickel-base superalloys. <i>Philosophical Magazine</i> , 2009 , 89, 2935-2947	1.6	19
29	Influence of the alloying element Re on the ideal tensile and shear strength of γ -Ni3Al. <i>Scripta Materialia</i> , 2009 , 61, 197-200	5.6	44
28	Ni/Ni3Al interface: A density functional theory study. <i>Applied Surface Science</i> , 2009 , 255, 3669-3675	6.7	33
27	The effect of alloying elements on the dislocation climbing velocity in Ni: A first-principles study. <i>Acta Materialia</i> , 2009 , 57, 5914-5920	8.4	65
26	Motion of misfit dislocation in an Ni/Ni3Al interface: a molecular dynamics simulations study. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2009 , 17, 055007	2	33
25	Vacancy-assisted diffusion mechanism of group-III elements in ZnO: An ab initio study. <i>Journal of Applied Physics</i> , 2009 , 105, 073504	2.5	18

24	Effect of alloying elements on the elastic properties of γ -Ni and γ -Ni ₃ Al from first-principles calculations. <i>Materials Research Society Symposia Proceedings</i> , 2009 , 1224, 1		9
23	A first-principles survey of the partitioning behaviors of alloying elements on γ/γ' interface. <i>Journal of Applied Physics</i> , 2008 , 104, 013109	2.5	15
22	First-principles study of a hybrid carbon material: Imperfect fullerenes covalently bonded to defective single-walled carbon nanotubes. <i>Physical Review B</i> , 2008 , 77,	3.3	19
21	Atomistic simulation of fracture in Ni ₃ Al. <i>Journal of Materials Research</i> , 2008 , 23, 1597-1603	2.5	14
20	First-principles study for transport properties of armchair carbon nanotubes with a double vacancy under strain. <i>Journal of Applied Physics</i> , 2008 , 103, 113714	2.5	5
19	Electronic structure analysis of self-consistent embedding theory for quantum/molecular mechanics simulations. <i>Physical Review B</i> , 2008 , 78,	3.3	13
18	Density functional theory study of Ni/Ni ₃ Al interface alloying with Re and Ru. <i>Surface Science</i> , 2008 , 602, 2604-2609	1.8	25
17	The alloying mechanisms of Re, Ru in the quaternary Ni-based superalloys interface: A first principles calculation. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2008 , 490, 242-249	5.3	35
16	First-principles investigation of 3d transition elements in L10 TiAl. <i>Journal of Applied Physics</i> , 2007 , 101, 083702	2.5	9
15	Dimer-breaking-assisted exchange mechanism in surfactant-mediated epitaxial growth of Ge on Si(001): Ab initio total energy calculations. <i>Physical Review B</i> , 2007 , 76,	3.3	3
14	First-principles study of contact between Ti surface and semiconducting carbon nanotube. <i>Journal of Applied Physics</i> , 2007 , 102, 013709	2.5	23
13	Atomistic study of lattice trapping behavior for brittle fracture in bcc-iron. <i>Computational Materials Science</i> , 2007 , 40, 376-381	3.2	18
12	Adsorption, diffusion, and site exchange for Ge ad-dimers on Sb-covered Si(001) from first-principles total-energy calculations. <i>Physical Review B</i> , 2006 , 74,	3.3	7
11	Atomistic simulation for configuration evolution and energetic calculation of crack in body-centered-cubic iron. <i>Journal of Materials Research</i> , 2006 , 21, 2542-2549	2.5	9
10	Misfit dislocation networks in the γ/γ' phase interface of a Ni-based single-crystal superalloy: Molecular dynamics simulations. <i>Physical Review B</i> , 2005 , 72,	3.3	57
9	First-principles study on the effect of impurities at the front of cracks in Fe. <i>Physical Review B</i> , 2005 , 72,	3.3	7
8	First-Principles Study of the Electronic Properties of γ/γ' Interface in Ni Based Superalloys. <i>Materials Transactions</i> , 2005 , 46, 1122-1126	1.3	1
7	CLUSTER-SIMULATED DISLOCATION CORE: MOTION AND TRAP FOR IMPURITY ATOMS. <i>International Journal of Modern Physics B</i> , 2005 , 19, 2353-2358	1.1	

6	Energetics and local spin magnetic moment of single 3,4d impurities encapsulated in an icosahedral Au ₁₂ cage. <i>Physical Review B</i> , 2004 , 70,	3-3	68
5	Electronic states and doping effect of carbon in the edge-dislocation core of bcc iron. <i>Physical Review B</i> , 2004 , 69,	3-3	23
4	Electronic structure of edge dislocation of core-doped Ti in Fe. <i>Progress in Natural Science: Materials International</i> , 2004 , 14, 477-482	3-6	6
3	Phase Diagram of Ising Nano-Particles with Cubic Structures. <i>Physica Status Solidi (B): Basic Research</i> , 2002 , 232, 254-263	1-3	47
2	First-principles study of the stability of the icosahedral Ti ₁₃ , Ti ₁₃ □, and Ti ₁₃ +1 clusters. <i>Physical Review B</i> , 2002 , 65,	3-3	39
1	Energetics and electronic structure of Re and Ta in the γ phase of Ni-based superalloys. <i>Physical Review B</i> , 2001 , 65,	3-3	42