

David Holec

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.

167
papers

3,669
citations

34
h-index

52
g-index

174
ext. papers

4,307
ext. citations

4.4
avg, IF

5.72
L-index

#	Paper	IF	Citations
167	Stabilization of Al ₃ Zr allotropes in dilute aluminum alloys via the addition of ternary elements. <i>Materialia</i> , 2022 , 21, 101321	3.2	2
166	Stability and ordering of bcc and hcp TiAl+Mo phases: An ab initio study. <i>Computational Materials Science</i> , 2022 , 205, 111163	3.2	1
165	Probing the onset of wurtzite phase formation in (V,Al)N thin films by transmission electron microscopy and atom probe tomography. <i>Surface and Coatings Technology</i> , 2022 , 128235	4.4	1
164	W 4f electron binding energies in amorphous W-B-C systems. <i>Applied Surface Science</i> , 2022 , 152824	6.7	1
163	Influence of B content on microstructure, phase composition and mechanical properties of CVD Ti(B,N) coatings. <i>Materialia</i> , 2022 , 21, 101323	3.2	1
162	Strain-stabilized Al-containing high-entropy sublattice nitrides. <i>Acta Materialia</i> , 2022 , 224, 117483	8.4	2
161	Ab initio-guided X-ray photoelectron spectroscopy quantification of Ti vacancies in Ti _{1-x} N. <i>Acta Materialia</i> , 2022 , 230, 117778	8.4	0
160	Atomistic mechanisms underlying plasticity and crack growth in ceramics: a case study of AlN/TiN superlattices. <i>Acta Materialia</i> , 2022 , 229, 117809	8.4	3
159	Heavy-element-alloying for toughness enhancement of hard nitrides on the example Ti-W-N. <i>Acta Materialia</i> , 2022 , 231, 117897	8.4	0
158	Structural stability and mechanical properties of TiAl+Mo alloys: A comprehensive ab initio study. <i>Acta Materialia</i> , 2021 , 221, 117427	8.4	0
157	High-throughput first-principles search for ceramic superlattices with improved ductility and fracture resistance. <i>Acta Materialia</i> , 2021 , 206, 116615	8.4	7
156	Real-time atomic-resolution observation of coherent twin boundary migration in CrN. <i>Acta Materialia</i> , 2021 , 208, 116732	8.4	4
155	The MoN-TaN system: Role of vacancies in phase stability and mechanical properties. <i>Materials and Design</i> , 2021 , 202, 109568	8.1	2
154	Enhanced fracture toughness in ceramic superlattice thin films: On the role of coherency stresses and misfit dislocations. <i>Materials and Design</i> , 2021 , 202, 109517	8.1	4
153	Fracture toughness trends of modulus-matched TiN/(Cr,Al)N thin film superlattices. <i>Acta Materialia</i> , 2021 , 202, 376-386	8.4	11
152	Surface stress of gold nanoparticles revisited. <i>International Journal of Solids and Structures</i> , 2021 , 224, 111044	3.1	2
151	Atomic insights on intermixing of nanoscale nitride multilayer triggered by nanoindentation. <i>Acta Materialia</i> , 2021 , 214, 117004	8.4	7

150	Pressure- and temperature-dependent diffusion from first-principles: A case study of V and Ti in a TiN matrix. <i>Surface and Coatings Technology</i> , 2021 , 422, 127491	4.4	0
149	Correlating point defects with mechanical properties in nanocrystalline TiN thin films. <i>Materials and Design</i> , 2021 , 207, 109844	8.1	4
148	Enhanced thermal stability of (Ti,Al)N coatings by oxygen incorporation. <i>Acta Materialia</i> , 2021 , 218, 117204	8.4	6
147	Mechanical properties of CrN-based superlattices: Impact of magnetism. <i>Acta Materialia</i> , 2021 , 218, 117095	8.5	1
146	Adsorption of H ₂ on Penta-Octa-Penta Graphene: Grand Canonical Monte Carlo Study. <i>Journal of Carbon Research</i> , 2020 , 6, 20	3.3	
145	Modelling of short-range ordering kinetics in dilute multicomponent substitutional solid solutions. <i>Philosophical Magazine</i> , 2020 , 100, 1942-1961	1.6	
144	Fracture properties of thin film TiN at elevated temperatures. <i>Materials and Design</i> , 2020 , 194, 108885	8.1	18
143	Surface Energy of Au Nanoparticles Depending on Their Size and Shape. <i>Nanomaterials</i> , 2020 , 10,	5.4	20
142	Unexpected softness of bilayer graphene and softening of A-A stacked graphene layers. <i>Physical Review B</i> , 2020 , 101,	3.3	6
141	Structure, stress, and mechanical properties of Mo-Al-N thin films deposited by dc reactive magnetron cosputtering: Role of point defects. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2020 , 38, 053401	2.9	6
140	Chemical bonding effects on the brittle-to-ductile transition in metallic glasses. <i>Acta Materialia</i> , 2020 , 188, 273-281	8.4	17
139	Ab initio study of chemical disorder as an effective stabilizing mechanism of bcc-based TiAl(+Mo). <i>Physical Review Materials</i> , 2020 , 4,	3.2	3
138	Mapping the mechanical properties in nitride coatings at the nanometer scale. <i>Acta Materialia</i> , 2020 , 194, 343-353	8.4	2
137	Impact of V, Hf and Si on oxidation processes in TiAlN: Insights from ab initio molecular dynamics. <i>Surface and Coatings Technology</i> , 2020 , 381, 125125	4.4	10
136	Point-defect engineering of MoN/TaN superlattice films: A first-principles and experimental study. <i>Materials and Design</i> , 2020 , 186, 108211	8.1	7
135	Unravelling local environments in mixed TiO ₂ BiO ₂ thin films by XPS and ab initio calculations. <i>Applied Surface Science</i> , 2020 , 510, 145056	6.7	11
134	The effect of chemical composition on the structure, chemistry and mechanical properties of magnetron sputtered W-B-C coatings: Modeling and experiments. <i>Surface and Coatings Technology</i> , 2020 , 383, 125274	4.4	9
133	The Effect of Local Arrangement of Excess Mn on Phase Stability in NiMnGa Martensite: An Ab Initio Study. <i>Shape Memory and Superelasticity</i> , 2020 , 6, 35-44	2.8	3

132	Erosion and cathodic arc plasma of Nb ₃ Al cathodes: composite versus intermetallic. <i>Plasma Sources Science and Technology</i> , 2020 , 29, 025022	3.5	6
131	Mechanistic study of superlattice-enabled high toughness and hardness in MoN/TaN coatings. <i>Communications Materials</i> , 2020 , 1,	6	12
130	Multi-phase ELAStic Aggregates (MELASA) software tool for modeling anisotropic elastic properties of lamellar composites. <i>Computer Physics Communications</i> , 2020 , 247, 106863	4.2	4
129	Interactions between a H ₂ Molecule and Carbon Nanostructures: A DFT Study. <i>Journal of Carbon Research</i> , 2020 , 6, 16	3.3	3
128	Elasticity of Phases in Fe-Al-Ti Superalloys: Impact of Atomic Order and Anti-Phase Boundaries. <i>Crystals</i> , 2019 , 9, 299	2.3	8
127	An Ab Initio Study of Vacancies in Disordered Magnetic Systems: A Case Study of Fe-Rich Fe-Al Phases. <i>Materials</i> , 2019 , 12,	3.5	9
126	Toughness enhancement in TiN/WN superlattice thin films. <i>Acta Materialia</i> , 2019 , 172, 18-29	8.4	44
125	Thermal Expansion and Other Thermodynamic Properties of -TiAl and -TiAl Intermetallic Phases from First Principles Methods. <i>Materials</i> , 2019 , 12,	3.5	9
124	Correlating structural and mechanical properties of AlN/TiN superlattice films. <i>Scripta Materialia</i> , 2019 , 165, 159-163	5.6	21
123	Experimental Chemistry and Structural Stability of AlNb Enabled by Antisite Defects Formation. <i>Materials</i> , 2019 , 12,	3.5	6
122	Crystallographic orientation dependent maximum layer thickness of cubic AlN in CrN/AlN multilayers. <i>Acta Materialia</i> , 2019 , 168, 190-202	8.4	18
121	An Ab Initio Study of Magnetism in Disordered Fe-Al Alloys with Thermal Antiphase Boundaries. <i>Nanomaterials</i> , 2019 , 10,	5.4	3
120	Assessment of ductile character in superhard Ta-C-N thin films. <i>Acta Materialia</i> , 2019 , 179, 17-25	8.4	20
119	Structural evolution of oxygen on the surface of TiAlN: Ab initio molecular dynamics simulations. <i>Applied Surface Science</i> , 2019 , 470, 520-525	6.7	8
118	Stability and elasticity of metastable solid solutions and superlattices in the MoN/TaN system: First-principles calculations. <i>Materials and Design</i> , 2018 , 144, 310-322	8.1	23
117	An ab initio study of mechanical and dynamical stability of MoSi ₂ . <i>Journal of Alloys and Compounds</i> , 2018 , 746, 720-728	5.7	11
116	Predicting Optical Properties from Ab Initio Calculations. <i>Springer Series in Surface Sciences</i> , 2018 , 83-104.	4	
115	Pathways of phase transformation in ϵ -phase-stabilized γ -TiAl alloys subjected to two-step heat treatments. <i>Scripta Materialia</i> , 2018 , 149, 70-74	5.6	11

114	Influence of carbon deficiency on phase formation and thermal stability of super-hard TaC _y thin films. <i>Scripta Materialia</i> , 2018 , 149, 150-154	5.6	21
113	Theory-guided metal-decoration of nanoporous carbon for hydrogen storage applications. <i>Surface and Coatings Technology</i> , 2018 , 351, 42-49	4.4	10
112	Graphite under compression: shift of layer breathing and shear modes frequencies with interlayer spacing. <i>Journal of Physics Communications</i> , 2018 , 2, 045004	1.2	5
111	Ab initio inspired design of ternary boride thin films. <i>Scientific Reports</i> , 2018 , 8, 9288	4.9	40
110	Multi-Scale Microstructural Characterization. <i>Praktische Metallographie/Practical Metallography</i> , 2018 , 55, 584-602	0.3	2
109	Non-equilibrium solid solution of molybdenum and sodium: Atomic scale experimental and first principles studies. <i>Acta Materialia</i> , 2018 , 144, 700-706	8.4	6
108	Study of Local Mechanical Properties of Fe78Al22 Alloy. <i>Key Engineering Materials</i> , 2018 , 784, 27-32	0.4	1
107	An Ab Initio Study of Connections between Tensorial Elastic Properties and Chemical Bonds in $\Sigma(210)$ Grain Boundaries in Ni ₃ Si. <i>Materials</i> , 2018 , 11,	3.5	3
106	Origin of the Low Magnetic Moment in Fe ₃ AlTi: An Ab Initio Study. <i>Materials</i> , 2018 , 11,	3.5	14
105	Strength and Brittleness of Interfaces in Fe-Al Superalloy Nanocomposites under Multiaxial Loading: An ab initio and Atomistic Study. <i>Nanomaterials</i> , 2018 , 8,	5.4	18
104	Self-structuring in ZrAlN films as a function of composition and growth temperature. <i>Scientific Reports</i> , 2018 , 8, 16327	4.9	5
103	Impact of Nano-Scale Distribution of Atoms on Electronic and Magnetic Properties of Phases in Fe-Al Nanocomposites: An Ab Initio Study. <i>Nanomaterials</i> , 2018 , 8,	5.4	10
102	An Ab Initio Study of Pressure-Induced Reversal of Elastically Stiff and Soft Directions in YN and ScN and Its Effect in Nanocomposites Containing These Nitrides. <i>Nanomaterials</i> , 2018 , 8,	5.4	1
101	Quantum-Mechanical Study of Nanocomposites with Low and Ultra-Low Interface Energies. <i>Nanomaterials</i> , 2018 , 8,	5.4	10
100	An Study of Thermodynamic and Mechanical Stability of Heusler-Based Fe ₃ AlCo Polymorphs. <i>Materials</i> , 2018 , 11,	3.5	10
99	Tuning structure and mechanical properties of Ta-C coatings by N-alloying and vacancy population. <i>Scientific Reports</i> , 2018 , 8, 17669	4.9	21
98	Surface energy of nanoparticles - influence of particle size and structure. <i>Beilstein Journal of Nanotechnology</i> , 2018 , 9, 2265-2276	3	73
97	Atomistic Modeling-Based Design of Novel Materials . <i>Advanced Engineering Materials</i> , 2017 , 19, 1600683.5	3.5	10

96	Systematic ab initio investigation of the elastic modulus in quaternary transition metal nitride alloys and their coherent multilayers. <i>Acta Materialia</i> , 2017 , 127, 124-132	8.4	36
95	Intermetallic β -Solidifying β -TiAl Based Alloys From Fundamental Research to Application . <i>Advanced Engineering Materials</i> , 2017 , 19, 1600735	3.5	99
94	Impact of Mo on the β phase in β -solidifying TiAl alloys: An experimental and computational approach. <i>Intermetallics</i> , 2017 , 85, 26-33	3.5	12
93	Structure and surface energy of Au 55 nanoparticles: An ab initio study. <i>Computational Materials Science</i> , 2017 , 134, 137-144	3.2	13
92	Thermal stability and oxidation resistance of sputtered Ti Al Cr N hard coatings. <i>Surface and Coatings Technology</i> , 2017 , 324, 48-56	4.4	52
91	Peculiarity of self-assembled cubic nanolamellae in the TiN/AlN system: Epitaxial self-stabilization by element deficiency/excess. <i>Acta Materialia</i> , 2017 , 131, 391-399	8.4	22
90	Au, a stable glassy cluster: results of ab initio calculations. <i>Beilstein Journal of Nanotechnology</i> , 2017 , 8, 2221-2229	3	5
89	On grain boundary segregation in molybdenum materials. <i>Materials and Design</i> , 2017 , 135, 204-212	8.1	32
88	Interface-induced electronic structure toughening of nitride superlattices. <i>Surface and Coatings Technology</i> , 2017 , 325, 410-416	4.4	25
87	Vacancy-driven extended stability of cubic metastable Ta-Al-N and Nb-Al-N phases. <i>Surface and Coatings Technology</i> , 2017 , 326, 37-44	4.4	14
86	Magnetic properties of the CrMnFeCoNi high-entropy alloy. <i>Physical Review B</i> , 2017 , 96,	3.3	74
85	Optical properties of $\text{Ti}_x\text{Si}_{1-x}\text{O}_2$ solid solutions. <i>Physical Review B</i> , 2017 , 95,	3.3	8
84	Quantum-mechanical study of tensorial elastic and high-temperature thermodynamic properties of grain boundary states in superalloy-phase Ni β Al. <i>IOP Conference Series: Materials Science and Engineering</i> , 2017 , 219, 012019	0.4	6
83	Superlattice-induced oscillations of interplanar distances and strain effects in the CrN/AlN system. <i>Physical Review B</i> , 2017 , 95,	3.3	12
82	Thermal expansion of Ti-Al-N and Cr-Al-N coatings. <i>Scripta Materialia</i> , 2017 , 127, 182-185	5.6	37
81	Non-reactively sputtered ultra-high temperature Hf-C and Ta-C coatings. <i>Surface and Coatings Technology</i> , 2017 , 309, 436-444	4.4	27
80	Impact of Alloying on Stacking Fault Energies in β -TiAl. <i>Applied Sciences (Switzerland)</i> , 2017 , 7, 1193	2.6	14
79	Tensorial elastic properties and stability of interface states associated with β (210) grain boundaries in Ni(Al,Si). <i>Science and Technology of Advanced Materials</i> , 2017 , 18, 273-282	7.1	13

78	Influence of varying nitrogen partial pressures on microstructure, mechanical and optical properties of sputtered TiAlON coatings. <i>Acta Materialia</i> , 2016 , 119, 26-34	8.4	14
77	Structural and mechanical properties of nitrogen-deficient cubic CrMoN and CrWN systems. <i>Scripta Materialia</i> , 2016 , 123, 34-37	5.6	19
76	Microstructure, mechanical and optical properties of TiAlON coatings sputter-deposited with varying oxygen partial pressures. <i>Journal Physics D: Applied Physics</i> , 2016 , 49, 025307	3	9
75	Silicon distribution and silicide precipitation during annealing in an advanced multi-phase TiAl based alloy. <i>Acta Materialia</i> , 2016 , 110, 236-245	8.4	60
74	On the chemistry of the carbides in a molybdenum base Mo-Hf-C alloy produced by powder metallurgy. <i>Journal of Alloys and Compounds</i> , 2016 , 654, 445-454	5.7	15
73	Controlling microstructure, preferred orientation, and mechanical properties of Cr-Al-N by bombardment and alloying with Ta. <i>Journal of Applied Physics</i> , 2016 , 119, 065304	2.5	14
72	First Principles Study of Water-Based Self-Assembled Nanobearing Effect in CrN/TiN Multilayer Coatings. <i>Solid State Phenomena</i> , 2016 , 258, 373-378	0.4	3
71	The impact of nitrogen content and vacancies on structure and mechanical properties of MoN thin films. <i>Journal of Applied Physics</i> , 2016 , 120, 185301	2.5	42
70	Preferential site occupancy of alloying elements in TiAl-based phases. <i>Journal of Applied Physics</i> , 2016 , 119, 205104	2.5	39
69	Point defects stabilise cubic Mo-N and Ta-N. <i>Journal Physics D: Applied Physics</i> , 2016 , 49, 375303	3	49
68	First principles studies on the impact of point defects on the phase stability of (Al _x Cr _{1-x}) ₂ O ₃ solid solutions. <i>AIP Advances</i> , 2016 , 6, 025002	1.5	15
67	Predicting an alloying strategy for improving fracture toughness of C15 NbCr ₂ Laves phase: A first-principles study. <i>Computational Materials Science</i> , 2016 , 123, 59-64	3.2	9
66	Accurate prediction of band gaps and optical properties of HfO ₂ . <i>Journal Physics D: Applied Physics</i> , 2016 , 49, 395301	3	15
65	Nitrogen atom shift and the structural change in chromium nitride. <i>Acta Materialia</i> , 2015 , 98, 119-127	8.4	4
64	Complementary ab initio and X-ray nanodiffraction studies of TaO. <i>Acta Materialia</i> , 2015 , 83, 276-284	8.4	20
63	Interplay between effect of Mo and chemical disorder on the stability of β-TiAl phase. <i>Intermetallics</i> , 2015 , 61, 85-90	3.5	31
62	Ab initio studies on the adsorption and implantation of Al and Fe to nitride materials. <i>Journal of Applied Physics</i> , 2015 , 118, 125306	2.5	2
61	Thermal expansion of rock-salt cubic AlN. <i>Applied Physics Letters</i> , 2015 , 107, 071602	3.4	22

60	Origin of temperature-induced low friction of sputtered Si-containing amorphous carbon coatings. <i>Acta Materialia</i> , 2015 , 82, 437-446	8.4	30
59	Graphite under uniaxial compression along the c axis: A parameter to relate out-of-plane strain to in-plane phonon frequency. <i>Physical Review B</i> , 2015 , 92,	3.3	8
58	Synergy of atom-probe structural data and quantum-mechanical calculations in a theory-guided design of extreme-stiffness superlattices containing metastable phases. <i>New Journal of Physics</i> , 2015 , 17, 093004	2.9	13
57	Facet-controlled phase separation in supersaturated Au-Ni nanoparticles upon shape equilibration. <i>Applied Physics Letters</i> , 2015 , 107, 073109	3.4	18
56	Evaluation of dislocation energy in thin films. <i>Philosophical Magazine</i> , 2015 , 95, 186-209	1.6	2
55	Ab initio study of point defects in NiTi-based alloys. <i>Physical Review B</i> , 2014 , 89,	3.3	23
54	On the Behavior of Yttria/Yttrium during Mechanical Alloying of a Fe - Y2O3 Model Alloy System. <i>Advanced Materials Research</i> , 2014 , 922, 598-603	0.5	
53	The effect of interlayer composition and thickness on the stabilization of cubic AlN in AlN/TiAlN superlattices. <i>Thin Solid Films</i> , 2014 , 565, 94-100	2.2	20
52	Buckling of ZnS-filled single-walled carbon nanotubes The influence of aspect ratio. <i>Carbon</i> , 2014 , 79, 529-537	10.4	9
51	Atomistic insights into milling mechanisms in an Fe γ 2O3 model alloy. <i>Applied Physics A: Materials Science and Processing</i> , 2014 , 115, 851-858	2.6	12
50	Structural and mechanical evolution of reactively and non-reactively sputtered Zr-Al-N thin films during annealing. <i>Surface and Coatings Technology</i> , 2014 , 244, 52-56	4.4	38
49	Protective Transition Metal Nitride Coatings 2014 , 355-388		19
48	Structural stability and thermodynamics of CrN magnetic phases from ab initio calculations and experiment. <i>Physical Review B</i> , 2014 , 90,	3.3	78
47	Macroscopic elastic properties of textured ZrN-AlN polycrystalline aggregates: From ab initio calculations to grain-scale interactions. <i>Physical Review B</i> , 2014 , 90,	3.3	28
46	A combinatorial X-ray sub-micron diffraction study of microstructure, residual stress and phase stability in TiAlN coatings. <i>Surface and Coatings Technology</i> , 2014 , 257, 108-113	4.4	8
45	Nanomechanics of Carbon Nanotubes. <i>Proceedings in Applied Mathematics and Mechanics</i> , 2013 , 13, 7-10	0.2	7
44	Phase stability, mechanical properties and thermal stability of Y alloyed TiAlN coatings. <i>Surface and Coatings Technology</i> , 2013 , 235, 174-180	4.4	43
43	Magnetic field strength influence on the reactive magnetron sputter deposition of Ta2O5. <i>Journal Physics D: Applied Physics</i> , 2013 , 46, 335203	3	11

42	Elastic constants and critical thicknesses of ScGaN and ScAlN. <i>Journal of Applied Physics</i> , 2013 , 114, 243516	6	64
41	Stabilization criteria for cubic AlN in TiN/AlN and CrN/AlN bi-layer systems. <i>Journal Physics D: Applied Physics</i> , 2013 , 46, 045305	3	31
40	Critical thickness for GaN thin film on AlN substrate 2013 ,		2
39	Alloying-related trends from first principles: An application to the TiAl _x N system. <i>Journal of Applied Physics</i> , 2013 , 113, 113510	2.5	49
38	Ab initio study of the alloying effect of transition metals on structure, stability and ductility of CrN. <i>Journal Physics D: Applied Physics</i> , 2013 , 46, 365301	3	33
37	Tunable optoelectronic and ferroelectric properties in Sc-based III-nitrides. <i>Journal of Applied Physics</i> , 2013 , 114, 133510	2.5	84
36	First-principles study of elastic properties of cubic Cr _{1-x} Al _x N alloys. <i>Journal of Applied Physics</i> , 2013 , 113, 043511	2.5	50
35	Effect of Hf on structure and age hardening of TiAl-N thin films. <i>Surface and Coatings Technology</i> , 2012 , 206, 2667-2672	4.4	37
34	Interfacial coherency stress distribution in TiN/AlN bilayer and multilayer films studied by FEM analysis. <i>Computational Materials Science</i> , 2012 , 55, 211-216	3.2	8
33	Increased thermal stability of TiAl _x N thin films by Ta alloying. <i>Surface and Coatings Technology</i> , 2012 , 211, 98-103	4.4	87
32	Surface energies of AlN allotropes from first principles. <i>Scripta Materialia</i> , 2012 , 67, 760-762	5.6	57
31	Trends in the elastic response of binary early transition metal nitrides. <i>Physical Review B</i> , 2012 , 85,	3.3	121
30	First-principles study of the thermodynamic and elastic properties of eutectic Fe ₃ Ti alloys. <i>Acta Materialia</i> , 2012 , 60, 1594-1602	8.4	33
29	Theory-Guided Materials Design of Multi-Phase Ti-Nb Alloys with Bone-Matching Elastic Properties. <i>Materials</i> , 2012 , 5, 1853-1872	3.5	62
28	Strain-induced effects on the electronic structure and N K-edge ELNES of wurtzite AlN and Al _x Ga _{1-x} N. <i>Journal of Physics: Conference Series</i> , 2011 , 326, 012016	0.3	1
27	Electronic origin of structure and mechanical properties in Y and Nb alloyed TiAl _x N thin films. <i>International Journal of Materials Research</i> , 2011 , 102, 735-742	0.5	32
26	Phase stability and alloy-related trends in TiAl _x N, ZrAl _x N and HfAl _x N systems from first principles. <i>Surface and Coatings Technology</i> , 2011 , 206, 1698-1704	4.4	89
25	Methodological challenges in combining quantum-mechanical and continuum approaches for materials science applications. <i>European Physical Journal Plus</i> , 2011 , 126, 1	3.1	20

24	Size effect of thermal expansion and thermal/intrinsic stresses in nanostructured thin films: Experiment and model. <i>Acta Materialia</i> , 2011 , 59, 6631-6645	8.4	61
23	Decomposition pathways in age hardening of Ti-Al-N films. <i>Journal of Applied Physics</i> , 2011 , 110, 023515	2.5	131
22	Continuum modeling of van der Waals interactions between carbon onion layers. <i>Carbon</i> , 2011 , 49, 1620-1627	2.3	23
21	Influence of Zr on structure, mechanical and thermal properties of Ti-Al-N. <i>Thin Solid Films</i> , 2011 , 519, 5503-5510	2.2	90
20	Towards predictive modeling of near-edge structures in electron energy-loss spectra of AlN-based ternary alloys. <i>Physical Review B</i> , 2011 , 83,	3.3	33
19	Ab initio study of pressure stabilized NiTi allotropes: Pressure-induced transformations and hysteresis loops. <i>Physical Review B</i> , 2011 , 84,	3.3	29
18	Phase stability and decomposition products of TiAl _{0.5} N thin films. <i>Applied Physics Letters</i> , 2010 , 97, 151901	3.4	53
17	Structure and stability of phases within the NbN/AlN system. <i>Journal Physics D: Applied Physics</i> , 2010 , 43, 145403	3	43
16	Curvature-induced excess surface energy of fullerenes: Density functional theory and Monte Carlo simulations. <i>Physical Review B</i> , 2010 , 81,	3.3	24
15	Imaging dislocations in gallium nitride across broad areas using atomic force microscopy. <i>Review of Scientific Instruments</i> , 2010 , 81, 063701	1.7	5
14	Pressure-dependent stability of cubic and wurtzite phases within the TiN/AlN and CrN/AlN systems. <i>Scripta Materialia</i> , 2010 , 62, 349-352	5.6	62
13	Influence of Nb on the phase stability of TiAlN. <i>Scripta Materialia</i> , 2010 , 63, 807-810	5.6	37
12	Combined structure-factor phase measurement and theoretical calculations for mapping of chemical bonds in GaN. <i>Acta Crystallographica Section A: Foundations and Advances</i> , 2010 , 66, 446-50		7
11	Structural properties of wurtzitelike ScGaN films grown by NH ₃ -molecular beam epitaxy. <i>Journal of Applied Physics</i> , 2009 , 106, 113533	2.5	23
10	HANSIS software tool for the automated analysis of HOLZ lines. <i>Ultramicroscopy</i> , 2009 , 109, 837-44	3.1	1
9	A theoretical study of ELNES spectra of . <i>Computational Materials Science</i> , 2008 , 44, 91-96	3.2	5
8	Equilibrium critical thickness for misfit dislocations in III-nitrides. <i>Journal of Applied Physics</i> , 2008 , 104, 123514	2.5	79
7	Electron energy loss near edge structure (ELNES) spectra of AlN and AlGa _{0.5} N: a theoretical study using the Wien2k and Telnes programs. <i>Micron</i> , 2008 , 39, 690-7	2.3	12

6	Ni ₄ Ti ₃ precipitate structures in Ni-rich NiTi shape memory alloys. <i>Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2008 , 481-482, 462-465	5.3	12
5	Critical thickness calculations for InGaN/GaN. <i>Journal of Crystal Growth</i> , 2007 , 303, 314-317	1.6	166
4	Calculations of Equilibrium Critical Thickness for Non-Polar Wurtzite InGaN/GaN Systems. <i>Materials Science Forum</i> , 2007 , 567-568, 209-212	0.4	1
3	Interactions between particles and low-angle dislocation boundaries during high-temperature deformation. <i>International Journal of Materials Research</i> , 2005 , 96, 558-565		10
2	Stability and Motion of Low Angle Dislocation Boundaries in Precipitation Hardened Crystals. <i>Materials Science Forum</i> , 2005 , 482, 159-162	0.4	2
1	Electrons Meet Alloy Development: A TiAl-Based Alloy Showcase. <i>Advanced Engineering Materials</i> , 2009 , 11, 37	3.7	1