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List of Publications by Year
in descending order

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55 papers	2,125 citations	159585 30 h-index	233421 45 g-index
56 all docs	56 docs citations	56 times ranked	1407 citing authors

#	Article	IF	Citations
1	Predicting elastic properties of hard-coating alloys using ab-initio and machine learning methods. Npj Computational Materials, 2022, 8, .	8.7	16
2	Atomistic mechanisms underlying plasticity and crack growth in ceramics: a case study of AlN/TiN superlattices. Acta Materialia, 2022, 229, 117809.	7.9	29
3	Color and pseudogap tunability in multicomponent carbonitrides. Materials and Design, 2022, 217, 110600.	7.0	2
4	MOCVD of AlN on epitaxial graphene at extreme temperatures. CrystEngComm, 2021, 23, 385-390.	2.6	46
5	Temperature-dependent elastic properties of binary and multicomponent high-entropy refractory carbides. Materials and Design, 2021, 204, 109634.	7.0	26
6	Enhancing plasticity in high-entropy refractory ceramics via tailoring valence electron concentration. Materials and Design, 2021, 209, 109932.	7.0	32
7	Thermally induced structural evolution and age-hardening of polycrystalline V1â€“xMoxN (xÂâ‰ˆÂ0.4) thin films. Surface and Coatings Technology, 2021, 405, 126723.	4.8	11
8	Room-temperature diffusion of metal clusters on graphene. Physical Chemistry Chemical Physics, 2021, 23, 13087-13094.	2.8	6
9	Nanoscale phenomena ruling deposition and intercalation of AlN at the graphene/SiC interface. Nanoscale, 2020, 12, 19470-19476.	5.6	54
10	Anomalous versus Normal Room-Temperature Diffusion of Metal Adatoms on Graphene. Journal of Physical Chemistry Letters, 2020, 11, 8930-8936.	4.6	14
11	Adaptive hard and tough mechanical response in single-crystal B1 VNx ceramics via control of anion vacancies. Acta Materialia, 2020, 192, 78-88.	7.9	46
12	Atomistic description of self-diffusion in molybdenum: A comparative theoretical study of non-Arrhenius behavior. Physical Review Materials, 2020, 4, .	2.4	14
13	Strength, transformation toughening, and fracture dynamics of rocksalt-structure <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">T</mml:mi><mml:msub><mml:mi mathvariant="normal">i</mml:mi><mml:mrow><mml:mn>1</mml:mn><mml:mo>â^’</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub><mml:mi mathvariant="normal">A</mml:mi><mml:msub><mml:mi mathvariant="normal">l</mml:mi><mml:mi>x</mml:mi></mml:msub><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math>	2.4	12
14	A review of the intrinsic ductility and toughness of hard transition-metal nitride alloy thin films. Thin Solid Films, 2019, 688, 137479.	1.8	71
15	Mechanical properties of VMoNO as a function of oxygen concentration: Toward development of hard and tough refractory oxynitrides. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2019, 37, .	2.1	1
16	Superionic‐like Diffusion in an Elemental Crystal: bcc Titanium. Physical Review Letters, 2019, 123, 105501.	7.8	28
17	Semi-Empirical Force-Field Model for the Ti1â^’xAlxN (0 â‰¤ x â‰¤ 1) System. Materials, 2019, 12, 215.	2.9	22
18	TiN film growth on misoriented TiN grains with simultaneous low-energy bombardment: Restructuring leading to epitaxy. Thin Solid Films, 2019, 688, 137380.	1.8	7

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19	Mass transport properties of quasiharmonic vs. anharmonic transition-metal nitrides. Thin Solid Films, 2019, 688, 137297.	1.8	7
20	Atomic-scale diffusion rates during growth of thin metal films on weakly-interacting substrates. Scientific Reports, 2019, 9, 6640.	3.3	35
21	First-principles characterization of reversible martensitic transformations. Physical Review B, 2019, 99, .	3.2	12
22	Adsorption-controlled growth and properties of epitaxial SnO films. Physical Review Materials, 2019, 3, .	2.4	15
23	Effects of surface vibrations on interlayer mass transport: Ab initio molecular dynamics investigation of Ti adatom descent pathways and rates from TiN/TiN(001) islands. Physical Review B, 2018, 97, .	3.2	21
24	Inherent toughness and fracture mechanisms of refractory transition-metal nitrides via density-functional molecular dynamics. Acta Materialia, 2018, 151, 11-20.	7.9	49
25	Elastic properties and plastic deformation of TiC- and VC-based pseudobinary alloys. Acta Materialia, 2018, 144, 376-385.	7.9	45
26	Effect of dispersion corrections on ab initio predictions of graphite and diamond properties under pressure. Physical Review B, 2018, 98, .	3.2	24
27	Copper adatom, admolecule transport, and island nucleation on TiN(0â€¯0â€¯1) via ab initio molecular dynamics. Applied Surface Science, 2018, 450, 180-189.	6.1	12
28	Ab initio molecular dynamics of atomic-scale surface reactions: insights into metal organic chemical vapor deposition of AlN on graphene. Physical Chemistry Chemical Physics, 2018, 20, 17751-17761.	2.8	68
29	Effects of incident N atom kinetic energy on TiN/TiN(001) film growth dynamics: A molecular dynamics investigation. Journal of Applied Physics, 2017, 121, .	2.5	31
30	Thermally induced age hardening in tough Ta-Al-N coatings via spinodal decomposition. Journal of Applied Physics, 2017, 121, .	2.5	14
31	Experimental and computational studies on toughness enhancement in Ti-Al-Ta-N quaternaries. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2017, 35, .	2.1	34
32	Nonequilibrium ab initio molecular dynamics determination of Ti monovacancy migration rates in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>B</mml:mi><mml:mn>1</mml:mn></mml:mrow></mml:m TiN. Physical Review B, 2017, 96, .	3.2	15
33	Phonon and electron contributions to the thermal conductivity of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi mathvariant="normal">V</mml:mi><mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mi>x</mml:mi></mml:msub></mml:mrow></mml:math> epitaxial layers. Physical Review Materials, 2017, 1, .	2.4	34
34	Large-scale molecular dynamics simulations of TiN/TiN(001) epitaxial film growth. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2016, 34, .	2.1	30
35	Toughness enhancement in highly NbN-alloyed Ti-Al-N hard coatings. Acta Materialia, 2016, 121, 59-67.	7.9	69
36	Growth, nanostructure, and optical properties of epitaxial VN_x/MgO(001) (0.80 â‰¤ x â‰¤ 1.00) layers deposited by reactive magnetron sputtering. Journal of Materials Chemistry C, 2016, 4, 7924-7938.	5.5	30

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37	Efficient and accurate determination of lattice-vacancy diffusion coefficients via non equilibriumab initiomolecular dynamics. Physical Review B, 2016, 93, .	3.2	11
38	Ab Initio Molecular Dynamics Simulations of Nitrogen/VN(001) Surface Reactions: Vacancy-Catalyzed N₂ Dissociative Chemisorption, N Adatom Migration, and N₂ Desorption. Journal of Physical Chemistry C, 2016, 120, 12503-12516.	3.1	39
39	Effects of phase stability, lattice ordering, and electron density on plastic deformation in cubic TiWN pseudobinary transition-metal nitride alloys. Acta Materialia, 2016, 103, 823-835.	7.9	56
40	N and Ti adatom dynamics on stoichiometric polar TiN(111) surfaces. Surface Science, 2016, 649, 72-79.	1.9	32
41	Dynamic and structural stability of cubic vanadium nitride. Physical Review B, 2015, 91, .	3.2	71
42	The dynamics of TiNx (x = 1â€“3) admolecule interlayer and intralayer transport on TiN/TiN(001) islands. Thin Solid Films, 2015, 589, 133-144.	1.8	12
43	Nitrogen vacancy, self-interstitial diffusion, and Frenkel-pair formation/dissociation in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>B</mml:mi><mml:mn>1</mml:mn></mml:mrow></mml studied byab initioand classical molecular dynamics with optimized potentials. Physical Review B, 2015, 91, .	3.2	53
44	Vacancy-induced toughening in hard single-crystal V 0.5 Mo 0.5 N x /MgO(0 0 1) thin films. Acta Materialia, 2014, 77, 394-400.	7.9	75
45	Effect of WN content on toughness enhancement in V1â^'xWxN/MgO(001) thin films. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2014, 32, .	2.1	45
46	Ti adatom diffusion on TiN(001): Ab initio and classical molecular dynamics simulations. Surface Science, 2014, 627, 34-41.	1.9	40
47	Effects of atomic ordering on the elastic properties of TiN- and VN-based ternary alloys. Thin Solid Films, 2014, 571, 145-153.	1.8	34
48	Ab initio and classical molecular dynamics simulations of N2 desorption from TiN(001) surfaces. Surface Science, 2014, 624, 25-31.	1.9	52
49	Ti and N adatom descent pathways to the terrace from atop two-dimensional TiN/TiN(001) islands. Thin Solid Films, 2014, 558, 37-46.	1.8	29
50	Toughness enhancement in hard ceramic thin films by alloy design. APL Materials, 2013, 1, .	5.1	109
51	Dynamics of Ti, N, and TiN<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mi>x</mml:mi></mml:msub></mml:math>(<mml:math) Tj ETQq1 1 0.784314 rgBT admolecule transport on TiN(001) surfaces. Physical Review B, 2012, 86, .	3.2	47
52	Toughness enhancement in TiAlN-based quarternary alloys. Thin Solid Films, 2012, 520, 4080-4088.	1.8	79
53	Supertoughening in B1 transition metal nitride alloys by increased valence electron concentration. Acta Materialia, 2011, 59, 2121-2134.	7.9	166
54	Structure and mechanical properties of TiAlNâ€“WNx thin films. Surface and Coatings Technology, 2011, 205, 4821-4827.	4.8	47

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	Universal mechanism for toughness enhancement in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"		
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