Avinash Dongare

List of Publications by Year
in descending order

77 papers	1,723 citations	218592 26 h-index	302012 39 g-index
78 all docs	78 docs citations	78 times ranked	1881 citing authors

#	Article	IF	Citations
1	Sulfur-Doped Titanium Carbide MXenes for Room-Temperature Gas Sensing. ACS Sensors, 2020, 5, 2915-2924.	4.0	92
2	Effects of Uniaxial and Biaxial Strain on Few-Layered Terrace Structures of MoS₂ Grown by Vapor Transport. ACS Nano, 2016, 10, 3186-3197.	7.3	83
3	Dislocation evolution and peak spall strengths in single crystal and nanocrystalline Cu. Journal of Applied Physics, 2016, 119, .	1.1	77
4	Atomic scale simulations of ductile failure micromechanisms in nanocrystalline Cu at high strain rates. Physical Review B, 2009, 80, .	1.1	71
5	Atomic scale studies of spall behavior in nanocrystalline Cu. Journal of Applied Physics, 2010, 108, .	1.1	71
6	Partial Surface Selenization of Cobalt Sulfide Microspheres for Enhancing the Hydrogen Evolution Reaction. ACS Catalysis, 2019, 9, 456-465.	5.5	71
7	Theoretical study on strain-induced variations in electronic properties of monolayer MoS2. Journal of Materials Science, 2014, 49, 6762-6771.	1.7	65
8	Insight into point defects and impurities in titanium from first principles. Npj Computational Materials, 2018, 4, .	3.5	62
9	Temperature dependent structural, elastic, and polar properties of ferroelectric polyvinylidene fluoride (PVDF) and trifluoroethylene (TrFE) copolymers. Journal of Materials Chemistry C, 2015, 3, 8389-8396.	2.7	51
10	Mesoscale modeling of jet initiation behavior and microstructural evolution during cold spray single particle impact. Acta Materialia, 2020, 182, 197-206.	3.8	48
11	Synthesis and characterization of copper-stabilized zirconia as an anode material for SOFC. Solid State Ionics, 2002, 152-153, 455-462.	1.3	46
12	Shock wave propagation and spall failure in single crystal Mg at atomic scales. Journal of Applied Physics, 2016, 119, .	1.1	42
13	Defect and damage evolution during spallation of single crystal Al: Comparison between molecular dynamics and quasi-coarse-grained dynamics simulations. Computational Materials Science, 2018, 145, 68-79.	1.4	39
14	Atomic scale modeling of shock response of fused silica and Î±-quartz. Journal of Materials Science, 2015, 50, 8128-8141.	1.7	37
15	Theoretical study on strain induced variations in electronic properties of 2<i>H</i>-MoS2 bilayer sheets. Applied Physics Letters, 2014, 104, .	1.5	36
16	Giant Mechano-Optoelectronic Effect in an Atomically Thin Semiconductor. Nano Letters, 2018, 18, 2351-2357.	4.5	36
17	Angular-dependent embedded atom method potential for atomistic simulations of metal-covalent systems. Physical Review B, 2009, 80, .	1.1	35
18	Understanding and predicting damage and failure at grain boundaries in BCC Ta. Journal of Applied Physics, 2019, 126, .	1.1	35

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19	Shock wave compression behavior and dislocation density evolution in Al microstructures at the atomic scales and the mesoscales. International Journal of Plasticity, 2020, 128, 102678.	4.1	35
20	Atomic Scale Studies of Spall Behavior in Single Crystal Cu. Procedia Engineering, 2011, 10, 3636-3641.	1.2	31
21	Unraveling the Mesoscale Evolution of Microstructure during Supersonic Impact of Aluminum Powder Particles. Scientific Reports, 2018, 8, 10075.	1.6	31
22	Role of grain boundary character on oxygen and hydrogen segregation-induced embrittlement in polycrystalline Ni. Journal of Materials Science, 2017, 52, 30-45.	1.7	30
23	Dynamic evolution of microstructure during laser shock loading and spall failure of single crystal Al at the atomic scales. Journal of Applied Physics, 2018, 124, .	1.1	30
24	Shock wave propagation and spall failure of nanocrystalline Cu/Ta alloys: Effect of Ta in solid-solution. Journal of Applied Physics, 2017, 122, .	1.1	29
25	Microstructure and Micromechanical Response in Gas-Atomized Al 6061 Alloy Powder and Cold-Sprayed Splats. Journal of Thermal Spray Technology, 2018, 27, 1563-1578.	1.6	29
26	Quasi-coarse-grained dynamics: modelling of metallic materials at mesoscales. Philosophical Magazine, 2014, 94, 3877-3897.	0.7	28
27	Role of nanoscale Cu/Ta interfaces on the shock compression and spall failure of nanocrystalline Cu/Ta systems at the atomic scales. Journal of Materials Science, 2018, 53, 5745-5765.	1.7	27
28	Tensionâ€“compression asymmetry in nanocrystalline Cu: High strain rate vs. quasi-static deformation. Computational Materials Science, 2010, 49, 260-265.	1.4	26
29	Correlations between dislocation density evolution and spall strengths of Cu/Ta multilayered systems at the atomic scales: The role of spacing of KS interfaces. Materialia, 2019, 5, 100192.	1.3	25
30	The Quasi-Coarse-Grained Dynamics Method to Unravel the Mesoscale Evolution of Defects/Damage during Shock Loading and Spall Failure of Polycrystalline Al Microstructures. Scientific Reports, 2017, 7, 12376.	1.6	22
31	Unraveling the Role of Interfaces on the Spall Failure of Cu/Ta Multilayered Systems. Scientific Reports, 2020, 10, 208.	1.6	22
32	An angular-dependent embedded atom method (A-EAM) interatomic potential to model thermodynamic and mechanical behavior of Al/Si composite materials. Modelling and Simulation in Materials Science and Engineering, 2012, 20, 035007.	0.8	21
33	Deformation Twinning in Polycrystalline Mg Microstructures at High Strain Rates at the Atomic Scales. Scientific Reports, 2019, 9, 3550.	1.6	21
34	Atomic-Scale Study of Plastic-Yield Criterion in Nanocrystalline Cu at High Strain Rates. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2010, 41, 523-531.	1.1	20
35	Edge effects on band gap energy in bilayer 2<i>H</i>-MoS2 under uniaxial strain. Journal of Applied Physics, 2015, 117, .	1.1	20
36	Modeling the thermodynamic behavior and shock response of Ti systems at the atomic scales and the mesoscales. Journal of Materials Science, 2017, 52, 10853-10870.	1.7	19

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37	Modeling the damage evolution and recompression behavior during laser shock loading of aluminum microstructures at the mesoscales. Journal of Materials Science, 2021, 56, 4446-4469.	1.7	19
38	Shock-induced deformation twinning and softening in magnesium single crystals. Materials and Design, 2020, 194, 108884.	3.3	17
39	Understanding the plasticity contributions during laser-shock loading and spall failure of Cu microstructures at the atomic scales. Computational Materials Science, 2021, 198, 110668.	1.4	16
40	Interatomic potentials for atomic scale modeling of metalâ€“matrix ceramic particle reinforced nanocomposites. Composites Part B: Engineering, 2009, 40, 461-467.	5.9	15
41	Vertically Stacked 2Hâ€•1T Dualâ€•Phase MoS₂ Microstructures during Lithium Intercalation: A First Principles Study. Journal of the American Ceramic Society, 2020, 103, 6603-6614.	1.9	15
42	Surface states of gas-atomized Al 6061 powders â€“ Effects of heat treatment. Applied Surface Science, 2020, 534, 147643.	3.1	14
43	Role of pre-existing dislocations on the shock compression and spall behavior in single-crystal copper at atomic scales. Journal of Applied Physics, 2021, 129, .	1.1	14
44	Challenges to model the role of heterogeneities on the shock response and spall failure of metallic materials at the mesoscales. Journal of Materials Science, 2020, 55, 3157-3166.	1.7	13
45	Mechanical properties of supersonic-impacted Al6061 powder particles. Scripta Materialia, 2019, 171, 52-56.	2.6	11
46	Atomistic study of shock Hugoniot of single crystal Mg. AIP Conference Proceedings, 2017, , .	0.3	10
47	Phase evolution and structural modulation during in situ lithiation of MoS2, WS2 and graphite in TEM. Scientific Reports, 2021, 11, 9014.	1.6	10
48	Origins of Ripples in CVD-Grown Few-layered MoS2 Structures under Applied Strain at Atomic Scales. Scientific Reports, 2017, 7, 40862.	1.6	9
49	Virtual texture analysis to investigate the deformation mechanisms in metal microstructures at the atomic scale. Journal of Materials Science, 2022, 57, 10549-10568.	1.7	9
50	Origin of High Interfacial Resistance in Solidâ€•State Batteries: LLTO/LCO Halfâ€•Cells**. ChemElectroChem, 2021, 8, 1847-1857.	1.7	8
51	Understanding the phase transformation mechanisms that affect the dynamic response of Fe-based microstructures at the atomic scales. Journal of Applied Physics, 2021, 130, .	1.1	8
52	<i>In Situ</i> Studies of Single-Nanoparticle-Level Nickel Thermal Oxidation: From Early Oxide Nucleation to Diffusion-Balanced Oxide Thickening. ACS Nano, 2022, 16, 6468-6479.	7.3	8
53	Understanding mechanical behavior of interfaces in materials. Journal of Materials Science, 2018, 53, 5511-5514.	1.7	7
54	Fingerprinting shock-induced deformations via diffraction. Scientific Reports, 2021, 11, 9872.	1.6	7

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55	Strong, ductile, and thermally stable Cu-based metal-intermetallic nanostructured composites. Scientific Reports, 2017, 7, 40409.	1.6	6
56	Density functional theory study of electronic structure of defects and the role on the strain relaxation behavior of MoS2 bilayer structures. Journal of Materials Science, 2018, 53, 9064-9075.	1.7	6
57	Recent advances in computational materials design: methods, applications, algorithms, and informatics. Journal of Materials Science, 2022, 57, 10471-10474.	1.7	6
58	Role of $${varvec{alpha}} o {varvec{varepsilon}} o {varvec{alpha}}$$ phase transformation on the spall behavior of iron at atomic scales. Journal of Materials Science, 2022, 57, 12556-12571.	1.7	5
59	Virtual diffraction simulations using the quasi-coarse-grained dynamics method to understand and interpret plasticity contributions during in situ shock experiments. Journal of Materials Science, 2022, 57, 12782-12796.	1.7	4
60	Shock Hugoniot behavior of single crystal titanium using atomistic simulations. AIP Conference Proceedings, 2017, , .	0.3	3
61	Structures of Layered Materials After Reaction with Li/Na. Microscopy and Microanalysis, 2020, 26, 2356-2357.	0.2	3
62	HRTEM and EELS Studies on the Structural and Chemical Modification of MoS₂ and Graphite During In-situ Reactions with Li and Na. Microscopy and Microanalysis, 2020, 26, 2410-2412.	0.2	3
63	Computational Study of Nanomaterials: From Large-Scale Atomistic Simulations to Mesoscopic Modeling. , 2016, , 633-645.		3
64	Origins of MoirÃ© Patterns in CVD-grown MoS2 Bilayer Structures at the Atomic Scales. Scientific Reports, 2018, 8, 9439.	1.6	2
65	Deformation and Failure Mechanisms in Ceramic-Reinforced Metal-Matrix Composites at Atomic Scales. , 2011, , .		1
66	Atomistic Study of Deformation and Failure Behavior in Nanocrystalline Mg. MRS Advances, 2016, 1, 3859-3864.	0.5	1
67	In-situ TEM Studies of Structural Modification in WS₂ during Intercalation of Li and Na. Microscopy and Microanalysis, 2021, 27, 654-656.	0.2	1
68	Computational Study of Nanomaterials: From Large-Scale Atomistic Simulations to Mesoscopic Modeling. , 2012, , 470-480.		1
69	Characterizing Li in partially lithiated layer materials using atomicâ€resolution imaging, modeling, and simulation. Journal of the American Ceramic Society, 2022, 105, 1581.	1.9	1
70	Atomistic study of silicon alloying in the spallation behavior of nanocrystalline aluminum systems. AIP Conference Proceedings, 2020, , .	0.3	1
71	Atomistic simulation study of misfit strain relaxation mechanisms in heteroepitaxial islands. Materials Research Society Symposia Proceedings, 2002, 749, 1.	0.1	0
72	Dynamic Evolution of Defect Structures during Spall Failure of Nanocrystalline Al. MRS Advances, 2016, 1, 3853-3858.	0.5	0

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73	Observing the Lithiation of M0S2. Microscopy and Microanalysis, 2018, 24, 1858-1859.	0.2	0
74	TEM Studies of Nanoscale Phase Transformation during in-situ reaction of Li with 2D Materials (MoS2,) Tj ETQq0 0 0 rgBT /Overlock 10 T	0.2	0
75	COMPUTATIONAL INVESTIGATION OF THE EFFECT OF CLUSTER IMPACT ENERGY ON THE MICROSTRUCTURE OF FILMS GROWN BY CLUSTER DEPOSITION. , 2005, , .		0
76	Computational Study of Nanomaterials: From Large-Scale Atomistic Simulations to Mesoscopic Modeling. , 2015, , 1-14.		0
77	Damage initiation and evolution in Al-Si layered microstructures under shock loading conditions at atomic scales. AIP Conference Proceedings, 2020, , .	0.3	0