Avinash Dongare

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	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
2	<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
3	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
4	Recent advances in computational materials design: methods, applications, algorithms, and informatics. Journal of Materials Science, 2022, 57, 10471-10474.	1.7	6
5	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
6	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
7	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
8	Phase evolution and structural modulation during in situ lithiation of MoS2, WS2 and graphite in TEM. Scientific Reports, 2021, 11, 9014.	1.6	10
9	Origin of High Interfacial Resistance in Solid‣tate Batteries: LLTO/LCO Half ells**. ChemElectroChem, 2021, 8, 1847-1857.	1.7	8
10	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
11	Fingerprinting shock-induced deformations via diffraction. Scientific Reports, 2021, 11, 9872.	1.6	7
12	TEM Studies of Nanoscale Phase Transformation during in-situ reaction of Li with 2D Materials (MoS2,) Tj ETQc	10 0 8.12BT	/Overlock 10
13	In-situ TEM Studies of Structural Modification in WS ₂ during Intercalation of Li and Na. Microscopy and Microanalysis, 2021, 27, 654-656.	0.2	1
14	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
15	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
16	Mesoscale modeling of jet initiation behavior and microstructural evolution during cold spray single particle impact. Acta Materialia, 2020, 182, 197-206.	3.8	48
17	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

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

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19	Vertically Stacked 2Hâ€1T Dualâ€Phase MoS ₂ Microstructures during Lithium Intercalation: A First Principles Study. Journal of the American Ceramic Society, 2020, 103, 6603-6614.	1.9	15
20	Structures of Layered Materials After Reaction with Li/Na. Microscopy and Microanalysis, 2020, 26, 2356-2357.	0.2	3
21	HRTEM and EELS Studies on the Structural and Chemical Modification of MoS ₂ and Graphite During In-situ Reactions with Li and Na. Microscopy and Microanalysis, 2020, 26, 2410-2412.	0.2	3
22	Sulfur-Doped Titanium Carbide MXenes for Room-Temperature Gas Sensing. ACS Sensors, 2020, 5, 2915-2924.	4.0	92
23	Surface states of gas-atomized Al 6061 powders – Effects of heat treatment. Applied Surface Science, 2020, 534, 147643.	3.1	14
24	Shock-induced deformation twinning and softening in magnesium single crystals. Materials and Design, 2020, 194, 108884.	3.3	17
25	Unraveling the Role of Interfaces on the Spall Failure of Cu/Ta Multilayered Systems. Scientific Reports, 2020, 10, 208.	1.6	22
26	Atomistic study of silicon alloying in the spallation behavior of nanocrystalline aluminum systems. AIP Conference Proceedings, 2020, , .	0.3	1
27	Damage initiation and evolution in Al-Si layered microstructures under shock loading conditions at atomic scales. AIP Conference Proceedings, 2020, , .	0.3	0
28	Mechanical properties of supersonic-impacted Al6061 powder particles. Scripta Materialia, 2019, 171, 52-56.	2.6	11
29	Understanding and predicting damage and failure at grain boundaries in BCC Ta. Journal of Applied Physics, 2019, 126, .	1.1	35
30	Deformation Twinning in Polycrystalline Mg Microstructures at High Strain Rates at the Atomic Scales. Scientific Reports, 2019, 9, 3550.	1.6	21
31	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
32	Partial Surface Selenization of Cobalt Sulfide Microspheres for Enhancing the Hydrogen Evolution Reaction. ACS Catalysis, 2019, 9, 456-465.	5.5	71
33	Understanding mechanical behavior of interfaces in materials. Journal of Materials Science, 2018, 53, 5511-5514.	1.7	7
34	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
35	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
36	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

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37	Insight into point defects and impurities in titanium from first principles. Npj Computational Materials, 2018, 4, .	3.5	62
38	Giant Mechano-Optoelectronic Effect in an Atomically Thin Semiconductor. Nano Letters, 2018, 18, 2351-2357.	4.5	36
39	Observing the Lithiation of M0S2. Microscopy and Microanalysis, 2018, 24, 1858-1859.	0.2	0
40	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
41	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
42	Unraveling the Mesoscale Evolution of Microstructure during Supersonic Impact of Aluminum Powder Particles. Scientific Reports, 2018, 8, 10075.	1.6	31
43	Origins of Moiré Patterns in CVD-grown MoS2 Bilayer Structures at the Atomic Scales. Scientific Reports, 2018, 8, 9439.	1.6	2
44	Origins of Ripples in CVD-Grown Few-layered MoS2 Structures under Applied Strain at Atomic Scales. Scientific Reports, 2017, 7, 40862.	1.6	9
45	Atomistic study of shock Hugoniot of single crystal Mg. AIP Conference Proceedings, 2017, , .	0.3	10
46	Strong, ductile, and thermally stable Cu-based metal-intermetallic nanostructured composites. Scientific Reports, 2017, 7, 40409.	1.6	6
47	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
48	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
49	Shock Hugoniot behavior of single crystal titanium using atomistic simulations. AIP Conference Proceedings, 2017, , .	0.3	3
50	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
51	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
52	Dislocation evolution and peak spall strengths in single crystal and nanocrystalline Cu. Journal of Applied Physics, 2016, 119, .	1.1	77
53	Shock wave propagation and spall failure in single crystal Mg at atomic scales. Journal of Applied Physics, 2016, 119, .	1.1	42
54	Atomistic Study of Deformation and Failure Behavior in Nanocrystalline Mg. MRS Advances, 2016, 1, 3859-3864.	0.5	1

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55	Dynamic Evolution of Defect Structures during Spall Failure of Nanocrystalline Al. MRS Advances, 2016, 1, 3853-3858.	0.5	0
56	Effects of Uniaxial and Biaxial Strain on Few-Layered Terrace Structures of MoS ₂ Grown by Vapor Transport. ACS Nano, 2016, 10, 3186-3197.	7.3	83
57	Computational Study of Nanomaterials: From Large-Scale Atomistic Simulations to Mesoscopic Modeling. , 2016, , 633-645.		3
58	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
59	Atomic scale modeling of shock response of fused silica and α-quartz. Journal of Materials Science, 2015, 50, 8128-8141.	1.7	37
60	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
61	Computational Study of Nanomaterials: From Large-Scale Atomistic Simulations to Mesoscopic Modeling. , 2015, , 1-14.		0
62	Quasi-coarse-grained dynamics: modelling of metallic materials at mesoscales. Philosophical Magazine, 2014, 94, 3877-3897.	0.7	28
63	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
64	Theoretical study on strain-induced variations in electronic properties of monolayer MoS2. Journal of Materials Science, 2014, 49, 6762-6771.	1.7	65
65	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
66	Computational Study of Nanomaterials: From Large-Scale Atomistic Simulations to Mesoscopic Modeling. , 2012, , 470-480.		1
67	Deformation and Failure Mechanisms in Ceramic-Reinforced Metal-Matrix Composites at Atomic Scales. , 2011, , .		1
68	Atomic Scale Studies of Spall Behavior in Single Crystal Cu. Procedia Engineering, 2011, 10, 3636-3641.	1.2	31
69	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
70	Tension–compression asymmetry in nanocrystalline Cu: High strain rate vs. quasi-static deformation. Computational Materials Science, 2010, 49, 260-265.	1.4	26
71	Atomic scale studies of spall behavior in nanocrystalline Cu. Journal of Applied Physics, 2010, 108, .	1.1	71
72	Atomic scale simulations of ductile failure micromechanisms in nanocrystalline Cu at high strain rates. Physical Review B, 2009, 80, .	1.1	71

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73	Interatomic potentials for atomic scale modeling of metal–matrix ceramic particle reinforced nanocomposites. Composites Part B: Engineering, 2009, 40, 461-467.	5.9	15
74	Angular-dependent embedded atom method potential for atomistic simulations of metal-covalent systems. Physical Review B, 2009, 80, .	1.1	35
75	COMPUTATIONAL INVESTIGATION OF THE EFFECT OF CLUSTER IMPACT ENERGY ON THE MICROSTRUCTURE OF FILMS GROWN BY CLUSTER DEPOSITION. , 2005, , .		Ο
76	Atomistic simulation study of misfit strain relaxation mechanisms in heteroepitaxial islands. Materials Research Society Symposia Proceedings, 2002, 749, 1.	0.1	0
77	Synthesis and characterization of copper-stabilized zirconia as an anode material for SOFC. Solid State Ionics, 2002, 152-153, 455-462.	1.3	46