Douglas E Spearot

List of Publications by Year in Descending Order

83 papers	1,938 citations	23 h-index	41 g-index
87 ext. papers	2,208 ext. citations	4 avg, IF	5.46 L-index

#	Paper	IF	Citations
83	Molecular dynamics simulation of the shock response of materials: A tutorial. *Journal of Applied Physics*, **2022**, 131, 051101	2.5	3
82	Data-driven analysis of neutron diffraction line profiles: application to plastically deformed Ta.. *Scientific Reports*, **2022**, 12, 5628	4.9	
81	Disclination-dislocation based model for grain boundary stress field evolution due to slip transmission history and influence on subsequent dislocation transmission. *Journal of the Mechanics and Physics of Solids*, **2022**, 104920	5	0
80	Role of equilibrium and non-equilibrium grain boundary stress fields on dislocation transmission. *Journal of Materials Research*, **2021**, 36, 2687-2704	2.5	2
79	Effect of the initial temperature on the shock response of Cu50Zr50 bulk metallic glass by molecular dynamics simulation. *Journal of Applied Physics*, **2021**, 129, 165103	2.5	5
78	On shockwave propagation and attenuation in poly(ethylene glycol) diacrylate hydrogels. *Journal of the Mechanical Behavior of Biomedical Materials*, **2021**, 118, 104423	4.1	1
77	Spectrum of embrittling potencies and relation to properties of symmetric-tilt grain boundaries. *Acta Materialia*, **2021**, 205, 116527	8.4	8
76	Validated tensile characterization of the strain rate dependence in soft materials. *International Journal of Impact Engineering*, **2021**, 156, 103949	4	3
75	Hyperelastic constitutive modeling of hydrogels based on primary deformation modes and validation under 3D stress states. *International Journal of Engineering Science*, **2020**, 154, 103314	5.7	18
74	Role of grain boundary structure on diffusion and dissolution during Ni/Al nanolaminate combustion. *Journal of Applied Physics*, **2020**, 127, 125111	2.5	6
73	Effect of Loop Defects on the High Strain Rate Behavior of PEGDA Hydrogels: A Molecular Dynamics Study. *Journal of Physical Chemistry B*, **2020**, 124, 2029-2039	3.4	4
72	Zr segregation in Ni□r alloy: implication on deformation mechanism during shear loading and bending creep. *Journal of Materials Science*, **2020**, 55, 6172-6186	4.3	4
71	Visco-hyperelastic constitutive modeling of strain rate sensitive soft materials. *Journal of the Mechanics and Physics of Solids*, **2020**, 135, 103777	5	27
70	Virtual diffraction analysis of dislocations and dislocation networks in discrete dislocation dynamics simulations. *Computational Materials Science*, **2020**, 174, 109473	3.2	5
69	Mechanical behavior of core□hell nanostructures. *Journal of Materials Science*, **2020**, 55, 4303-4310	4.3	5
68	Structure and kinetics of three-dimensional defects on the {101□2} twin boundary in magnesium: Atomistic and phase-field simulations. *Mechanics of Materials*, **2020**, 143, 103314	3.3	9
67	Mobility of dislocations in aluminum: The role of non-Schmid stress state. *Acta Materialia*, **2020**, 185, 420-432	8.4	9

66	Simultaneous twinning and microband formation under dynamic compression in a high entropy alloy with a complex energetic landscape. *Acta Materialia*, **2020**, 200, 1-11	8.4	20
65	Role of grain boundaries and substrate in plastic deformation of core□shell nanostructures. *Journal of Materials Science*, **2020**, 55, 16990-16999	4.3	
64	Mechanical properties of stabilized nanocrystalline FCC metals. *Journal of Applied Physics*, **2019**, 126, 110901	2.5	5
63	Void collapse and subsequent spallation in Cu50Zr50 metallic glass under shock loading by molecular dynamics simulations. *Journal of Applied Physics*, **2019**, 125, 215903	2.5	7
62	Atomistic Simulation Techniques to Model Hydrogen Segregation and Hydrogen Embrittlement in Metallic Materials **2019**, 357-390		
61	Fracture mechanics of multi-layer molybdenum disulfide. *Engineering Fracture Mechanics*, **2019**, 212, 1-12	4.2	9
60	Grain size effects on Ni/Al nanolaminate combustion. *Journal of Materials Research*, **2019**, 34, 2229-2238	2.5	6
59	Integrating in situ TEM experiments and atomistic simulations for defect mechanics. *Current Opinion in Solid State and Materials Science*, **2019**, 23, 117-128	12	11
58	Mobility of dislocations in Aluminum: Faceting and asymmetry during nanoscale dislocation shear loop expansion. *Acta Materialia*, **2019**, 168, 426-435	8.4	23
57	Transient-State Rheological Behavior of Poly(ethylene glycol) Diacrylate Hydrogels at High Shear Strain Rates. *Macromolecules*, **2019**, 52, 5860-5871	5.5	7
56	Shear-driven motion of Mg {101□2} twin boundaries via disconnection terrace nucleation, growth, and coalescence. *Physical Review Materials*, **2019**, 3,	3.2	10
55	An embedded-atom method potential parameterized for sulfur-induced embrittlement of nickel. *Modelling and Simulation in Materials Science and Engineering*, **2019**, 27, 085016	2	4
54	Effect of water concentration on the shock response of polyethylene glycol diacrylate (PEGDA) hydrogels: A molecular dynamics study. *Journal of the Mechanical Behavior of Biomedical Materials*, **2019**, 90, 30-39	4.1	12
53	Thermodynamics-based stability criteria for constitutive equations of isotropic hyperelastic solids. *Journal of the Mechanics and Physics of Solids*, **2019**, 124, 115-142	5	16
52	Pressure Dependence of the Peierls Stress in Aluminum. *Jom*, **2018**, 70, 1094-1099	2.1	8
51	Shock compression of Cu x Zr100□ metallic glasses from molecular dynamics simulations. *Journal of Materials Science*, **2018**, 53, 5719-5732	4.3	13
50	Influence of vacancy defect concentration on the combustion of reactive Ni/Al nanolaminates. *Journal of Applied Physics*, **2018**, 124, 045105	2.5	10
49	Physical vapor deposition of multiphase materials with phase nucleation via a coupled phase-field approach. *Computational Materials Science*, **2018**, 143, 71-79	3.2	4

48	Atomistic Simulation Techniques to Model Hydrogen Segregation and Hydrogen Embrittlement in Metallic Materials **2018**, 1-34		1
47	Simulation of kinematic Kikuchi diffraction patterns from atomistic structures. *MethodsX*, **2018**, 5, 1187-1203	1.3	3
46	Atomic-level deformation of CuxZr100-x metallic glasses under shock loading. *Journal of Applied Physics*, **2018**, 123, 215101	2.5	14
45	Phase-field simulations of microstructure evolution during physical vapor deposition of single-phase thin films. *Computational Materials Science*, **2017**, 131, 170-177	3.2	14
44	Two-dimensional MoS 2 under ion irradiation: from controlled defect production to electronic structure engineering. *2D Materials*, **2017**, 4, 025078	5.9	99
43	Nanoscale dislocation shear loops at static equilibrium and finite temperature. *Modelling and Simulation in Materials Science and Engineering*, **2017**, 25, 085014	2	14
42	A primer on selecting grain boundary sets for comparison of interfacial fracture properties in molecular dynamics simulations. *Scientific Reports*, **2017**, 7, 8332	4.9	18
41	Traction□eparation relationships for hydrogen induced grain boundary embrittlement in nickel via molecular dynamics simulations. *Materials Science & Engineering A: Structural Materials: Properties, Microstructure and Processing*, **2016**, 650, 354-364	5.3	29
40	Bridging atomistic simulations and experiments via virtual diffraction: understanding homophase grain boundary and heterophase interface structures. *Journal of Materials Science*, **2016**, 51, 1251-1260	4.3	4
39	Phase-field models for simulating physical vapor deposition and grain evolution of isotropic single-phase polycrystalline thin films. *Computational Materials Science*, **2016**, 123, 111-120	3.2	9
38	A molecular dynamics study of dislocation density generation and plastic relaxation during shock of single crystal Cu. *Journal of Applied Physics*, **2016**, 120, 045902	2.5	27
37	Atomistic simulation and virtual diffraction characterization of homophase and heterophase alumina interfaces. *Acta Materialia*, **2015**, 82, 403-413	8.4	9
36	Fracture mechanics of monolayer molybdenum disulfide. *Nanotechnology*, **2015**, 26, 175703	3.4	59
35	A molecular dynamics study of the role of grain size and orientation on compression of nanocrystalline Cu during shock. *Computational Materials Science*, **2015**, 108, 226-232	3.2	22
34	The effect of synthetic driving force on the atomic mechanisms associated with grain boundary motion below the interface roughening temperature. *Computational Materials Science*, **2014**, 86, 38-42	3.2	14
33	A Computational Algorithm to Produce Virtual X-ray and Electron Diffraction Patterns from Atomistic Simulations. *Jom*, **2014**, 66, 408-416	2.1	29
32	Algorithm Development in Computational Materials Science. *Jom*, **2014**, 66, 397-398	2.1	1
31	Atomistic simulation and virtual diffraction characterization of stable and metastable alumina surfaces. *Acta Materialia*, **2014**, 78, 354-368	8.4	8

30	Molecular dynamics simulation of O2 diffusion in polydimethylsiloxane (PDMS) and end-linked PDMS networks. *Molecular Simulation*, **2014**, 40, 976-986	2	8
29	Insights on slip transmission at grain boundaries from atomistic simulations. *Current Opinion in Solid State and Materials Science*, **2014**, 18, 188-195	12	77
28	Effect of point and grain boundary defects on the mechanical behavior of monolayer MoS2 under tension via atomistic simulations. *Journal of Applied Physics*, **2014**, 116, 013508	2.5	54
27	Performance Improvement and Workflow Development of Virtual Diffraction Calculations **2014**,		4
26	Phase transformation in monolayer molybdenum disulphide (MoS2) under tension predicted by molecular dynamics simulations. *Scripta Materialia*, **2014**, 76, 41-44	5.6	32
25	Molecular Dynamics Simulations of Diffusion of O2 and N2 Penetrants in Polydimethylsiloxane-Based Nanocomposites. *Journal of Engineering Materials and Technology, Transactions of the ASME*, **2012**, 134,	1.8	10
24	Foreword: Modeling, Simulation, and Theory of Nanomechanical Materials Behavior. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2011**, 42, 3867-3867	2.3	
23	Molecular dynamics simulation of diffusion of small atmospheric penetratesin polydimethylsiloxane. *Molecular Simulation*, **2011**, 37, 115-122	2	11
22	Melting of Ni and Fe nanoparticles: a molecular dynamics study with application to carbon nanotube synthesis. *Journal of Nanoscience and Nanotechnology*, **2010**, 10, 5587-93	1.3	10
21	Plastic deformation of nanocrystalline copper-antimony alloys. *Journal of Materials Research*, **2010**, 25, 411-421	2.5	27
20	Behavior of dopant-modified interfaces in metallic nanocrystalline materials. *Jom*, **2010**, 62, 70-74	2.1	6
19	Molecular Dynamics Simulations of Dislocation Activity in Single-Crystal and Nanocrystalline Copper Doped with Antimony. *Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science*, **2010**, 41, 854-860	2.3	14
18	Microstructural stability of copper with antimony dopants at grain boundaries: experiments and molecular dynamics simulations. *Journal of Materials Science*, **2010**, 45, 6707-6718	4.3	25
17	Molecular dynamics simulation of nanoconfinement induced organization of n-decane. *Langmuir*, **2009**, 25, 7553-60	4	24
16	Interatomic potential for copper–antimony in dilute solid–solution alloys and application to single crystal dislocation nucleation. *Computational Materials Science*, **2009**, 44, 1258-1264	3.2	8
15	Atomistic Modeling of Grain Boundaries and Dislocation Processes in Metallic Polycrystalline Materials. *Journal of Engineering Materials and Technology, Transactions of the ASME*, **2009**, 131,	1.8	35
14	Heterogeneous dislocation nucleation in single crystal copper–antimony solid-solution alloys. *Modelling and Simulation in Materials Science and Engineering*, **2009**, 17, 055001	2	18
13	On the elastic tensile deformation of <100> bicrystal interfaces in copper. *Computational Materials Science*, **2008**, 42, 57-67	3.2	26

12	Influence of Grain Boundary Structure on Dislocation Nucleation in FCC Metals. *Dislocations in Solids*, **2008**, 14, 43-139		46
11	Microstructure stability of nanocrystalline materials using dopants. *Molecular Simulation*, **2008**, 34, 35-40	2	12
10	Evolution of the E structural unit during uniaxial and constrained tensile deformation. *Mechanics Research Communications*, **2008**, 35, 81-88	2.2	29
9	Tensile strength of <1 0 0> and <1 1 0> tilt bicrystal copper interfaces. *Acta Materialia*, **2007**, 55, 705-714	8.4	192
8	Dislocation nucleation from bicrystal interfaces and grain boundary ledges: Relationship to nanocrystalline deformation. *Journal of the Mechanics and Physics of Solids*, **2007**, 55, 2300-2327	5	104
7	Dislocation nucleation from bicrystal interfaces with dissociated structure. *International Journal of Plasticity*, **2007**, 23, 143-160	7.6	139
6	Atomistic simulations of homogeneous dislocation nucleation in single crystal copper. *Modelling and Simulation in Materials Science and Engineering*, **2007**, 15, 693-709	2	104
5	Effect of deformation path sequence on the behavior of nanoscale copper bicrystal interfaces. *Journal of Engineering Materials and Technology, Transactions of the ASME*, **2005**, 127, 374-382	1.8	19
4	Molecular Dynamics Simulations of Dislocation Nucleation From Bicrystal Interfaces in FCC Metals **2005**, 505		1
3	Nucleation of dislocations from [001] bicrystal interfaces in aluminum. *Acta Materialia*, **2005**, 53, 3579-3589	8.4	177
2	Non-local separation constitutive laws for interfaces and their relation to nanoscale simulations. *Mechanics of Materials*, **2004**, 36, 825-847	3.3	75
1	Mobility of dislocations in FeNiCrCoCu high entropy alloys. *Modelling and Simulation in Materials Science and Engineering*,	2	3