

# Mark A Tschopp

## List of Publications by Year in descending order

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94  
papers

5,294  
citations

87843

38  
h-index

85498

71  
g-index

102  
all docs

102  
docs citations

102  
times ranked

4116  
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular dynamics simulations of deformation mechanisms of amorphous polyethylene. <i>Polymer</i> , 2010, 51, 6071-6083.	1.8	365
2	Probing grain boundary sink strength at the nanoscale: Energetics and length scales of vacancy and interstitial absorption by grain boundaries in $\alpha$ -Fe. <i>Physical Review B</i> , 2012, 85, .	1.1	285
3	Asymmetric tilt grain boundary structure and energy in copper and aluminium. <i>Philosophical Magazine</i> , 2007, 87, 3871-3892.	0.7	237
4	Structures and energies of $\Sigma$ 3 asymmetric tilt grain boundaries in copper and aluminium. <i>Philosophical Magazine</i> , 2007, 87, 3147-3173.	0.7	224
5	Tensile strength of $\Sigma$ 100 and $\Sigma$ 110 tilt bicrystal copper interfaces. <i>Acta Materialia</i> , 2007, 55, 705-714.	1.4	217
6	Effect of grain boundaries on texture formation during dynamic recrystallization of magnesium alloys. <i>Acta Materialia</i> , 2017, 128, 270-283.	3.8	194
7	Porosity prediction: Supervised-learning of thermal history for direct laser deposition. <i>Journal of Manufacturing Systems</i> , 2018, 47, 69-82.	7.6	191
8	Influence of single crystal orientation on homogeneous dislocation nucleation under uniaxial loading. <i>Journal of the Mechanics and Physics of Solids</i> , 2008, 56, 1806-1830.	2.3	167
9	In-situ monitoring of melt pool images for porosity prediction in directed energy deposition processes. <i>IJSE Transactions</i> , 2019, 51, 437-455.	1.6	157
10	Symmetric and asymmetric tilt grain boundary structure and energy in Cu and Al (and transferability) <i>Journal of Applied Physics</i> , 2007, 102, 122301.	1.2	122
11	Atomistic simulations of homogeneous dislocation nucleation in single crystal copper. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2007, 15, 693-709.	0.8	114
12	Dislocation nucleation in $\Sigma$ 3 asymmetric tilt grain boundaries. <i>International Journal of Plasticity</i> , 2008, 24, 191-217.	4.1	111
13	Breakdown of the Schmid law in homogeneous and heterogeneous nucleation events of slip and twinning in magnesium. <i>Journal of the Mechanics and Physics of Solids</i> , 2012, 60, 2084-2099.	2.3	111
14	Mitigating grain growth in binary nanocrystalline alloys through solute selection based on thermodynamic stability maps. <i>Computational Materials Science</i> , 2014, 84, 255-266.	1.4	111
15	Microstructure and mechanical properties of bulk nanostructured Cu-Ta alloys consolidated by equal channel angular extrusion. <i>Acta Materialia</i> , 2014, 76, 168-185.	3.8	108
16	Structure and free volume of $\Sigma$ 110 symmetric tilt grain boundaries with the E structural unit. <i>Acta Materialia</i> , 2007, 55, 3959-3969.	3.8	107
17	Atomic-scale analysis of liquid-gallium embrittlement of aluminum grain boundaries. <i>Acta Materialia</i> , 2014, 73, 312-325.	3.8	105
18	An internal state variable material model for predicting the time, thermomechanical, and stress state dependence of amorphous glassy polymers under large deformation. <i>International Journal of Plasticity</i> , 2013, 42, 168-193.	4.1	100

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19	Atomistic simulations of tension-compression asymmetry in dislocation nucleation for copper grain boundaries. <i>Computational Materials Science</i> , 2008, 44, 351-362.	1.4	91
20	Grain boundary dislocation sources in nanocrystalline copper. <i>Scripta Materialia</i> , 2008, 58, 299-302.	2.6	89
21	Atomistic Investigation of the Role of Grain Boundary Structure on Hydrogen Segregation and Embrittlement in $\alpha$ -Fe. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2013, 44, 1365-1375.	1.1	89
22	Structural, elastic, and thermal properties of cementite ( $\text{Fe}_3\text{C}$ ) calculated using a modified embedded atom method. <i>Physical Review B</i> , 2014, 89, .	1.1	81
23	Evolution of structure and free volume in symmetric tilt grain boundaries during dislocation nucleation. <i>Acta Materialia</i> , 2010, 58, 6464-6473.	3.8	79
24	Grain Boundary Segregation of Interstitial and Substitutional Impurity Atoms in Alpha-Iron. <i>Jom</i> , 2014, 66, 129-138.	0.9	78
25	Microstructure-Dependent Local Strain Behavior in Polycrystals through In-Situ Scanning Electron Microscope Tensile Experiments. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2009, 40, 2363-2368.	1.1	74
26	Energetic driving force for preferential binding of self-interstitial atoms to Fe grain boundaries over vacancies. <i>Scripta Materialia</i> , 2011, 64, 908-911.	2.6	69
27	Solid State Porous Metal Production: A Review of the Capabilities, Characteristics, and Challenges. <i>Advanced Engineering Materials</i> , 2018, 20, 1700766.	1.6	68
28	Tension-compression asymmetry in homogeneous dislocation nucleation in single crystal copper. <i>Applied Physics Letters</i> , 2007, 90, 121916.	1.5	64
29	Effect of resistance spot welding parameters on weld pool properties in a DP600 dual-phase steel: A parametric study using thermomechanically-coupled finite element analysis. <i>Materials &amp; Design</i> , 2014, 56, 387-397.	5.1	64
30	A multiscale model of grain boundary structure and energy: From atomistics to a continuum description. <i>Acta Materialia</i> , 2015, 82, 513-529.	3.8	60
31	Dual process monitoring of metal-based additive manufacturing using tensor decomposition of thermal image streams. <i>Additive Manufacturing</i> , 2018, 23, 443-456.	1.7	60
32	Influence of Grain Boundary Structure on Dislocation Nucleation in FCC Metals. <i>Dislocations in Solids</i> , 2008, 14, 43-139.	1.6	57
33	Enhancing grain refinement in polycrystalline materials using surface mechanical attrition treatment at cryogenic temperatures. <i>Scripta Materialia</i> , 2013, 69, 461-464.	2.6	54
34	Unraveling Recrystallization Mechanisms Governing Texture Development from Rare-Earth Element Additions to Magnesium. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2018, 49, 1809-1829.	1.1	53
35	Quantifying the energetics and length scales of carbon segregation to $\alpha$ -Fe symmetric tilt grain boundaries using atomistic simulations. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2013, 21, 035009.	0.8	47
36	Influence of Mn solute content on grain size reduction and improved strength in mechanically alloyed Al-Mn alloys. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2014, 589, 57-65.	2.6	44

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37	An interatomic potential for saturated hydrocarbons based on the modified embedded-atom method. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 6233-6249.	1.3	41
38	Structural unit and faceting description of $\Sigma$ 3 asymmetric tilt grain boundaries. <i>Journal of Materials Science</i> , 2007, 42, 7806-7811.	1.7	39
39	The candidacy of shuffle and shear during compound twinning in hexagonal close-packed structures. <i>Acta Materialia</i> , 2013, 61, 7646-7659.	3.8	39
40	Characterizing the Local Primary Dendrite Arm Spacing in Directionally Solidified Dendritic Microstructures. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2014, 45, 426-437.	1.1	37
41	The role of Ta on twinnability in nanocrystalline Cu-Ta alloys. <i>Materials Research Letters</i> , 2017, 5, 48-54.	4.1	37
42	Structure and mechanical properties of Fe-Ni-Zr oxide-dispersion-strengthened (ODS) alloys. <i>Journal of Nuclear Materials</i> , 2015, 467, 205-213.	1.3	35
43	Quantification of damage evolution in a 7075 aluminum alloy using an acoustic emission technique. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2011, 528, 6708-6714.	2.6	33
44	Investigating Damage Evolution at the Nanoscale: Molecular Dynamics Simulations of Nanovoid Growth in Single-Crystal Aluminum. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2013, 44, 617-626.	1.1	32
45	Binding energetics of substitutional and interstitial helium and di-helium defects with grain boundary structure in $\Sigma$ -Fe. <i>Journal of Applied Physics</i> , 2014, 115, .	1.1	31
46	Automated analysis of twins in hexagonal close-packed metals using molecular dynamics. <i>Scripta Materialia</i> , 2012, 66, 666-669.	2.6	30
47	Finite element analysis of occupant head injuries: Parametric effects of the side curtain airbag deployment interaction with a dummy head in a side impact crash. <i>Accident Analysis and Prevention</i> , 2013, 55, 232-241.	3.0	30
48	Orientation and rate dependence of dislocation nucleation stress computed using molecular dynamics. <i>Scripta Materialia</i> , 2009, 60, 675-678.	2.6	29
49	Shock wave propagation and spall failure of nanocrystalline Cu/Ta alloys: Effect of Ta in solid-solution. <i>Journal of Applied Physics</i> , 2017, 122, .	1.1	29
50	Multi-scale characterization of orthotropic microstructures. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2008, 16, 065009.	0.8	28
51	Microstructure and damage evolution during tensile loading in a wrought magnesium alloy. <i>Scripta Materialia</i> , 2011, 64, 912-915.	2.6	27
52	He-V cluster nucleation and growth in $\Sigma$ -Fe grain boundaries. <i>Acta Materialia</i> , 2017, 124, 544-555.	3.8	27
53	Role of nanoscale Cu/Ta interfaces on the shock compression and spall failure of nanocrystalline Cu/Ta systems at the atomic scales. <i>Journal of Materials Science</i> , 2018, 53, 5745-5765.	1.7	27
54	The role of grain boundary structure and crystal orientation on crack growth asymmetry in aluminum. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2014, 618, 345-354.	2.6	26

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55	Atomic scale investigation of grain boundary structure role on intergranular deformation in aluminium. <i>Philosophical Magazine</i> , 2014, 94, 3445-3466.	0.7	25
56	Comparison of reconstructed spatial microstructure images using different statistical descriptors. <i>Computational Materials Science</i> , 2012, 51, 437-444.	1.4	24
57	Structure and thermal decomposition of a nanocrystalline mechanically alloyed supersaturated Cu-Ta solid solution. <i>MRS Communications</i> , 2015, 5, 333-339.	0.8	24
58	Effect of vacancy defects on generalized stacking fault energy of fcc metals. <i>Journal of Physics Condensed Matter</i> , 2014, 26, 115404.	0.7	21
59	An efficient Monte Carlo algorithm for determining the minimum energy structures of metallic grain boundaries. <i>Computational Materials Science</i> , 2018, 155, 466-475.	1.4	21
60	Generalized framework for interatomic potential design: Application to Fe-He system. <i>Journal of Nuclear Materials</i> , 2012, 425, 22-32.	1.3	20
61	Mechanical properties of amorphous cellulose using molecular dynamics simulations with a reactive force field. <i>International Journal of Modelling, Identification and Control</i> , 2013, 18, 211.	0.2	20
62	Using Similarity Metrics to Quantify Differences in High-Throughput Data Sets: Application to X-ray Diffraction Patterns. <i>ACS Combinatorial Science</i> , 2017, 19, 25-36.	3.8	20
63	Investigating occupant safety through simulating the interaction between side curtain airbag deployment and an out-of-position occupant. <i>Accident Analysis and Prevention</i> , 2012, 49, 392-403.	3.0	19
64	Machine learning to predict aluminum segregation to magnesium grain boundaries. <i>Scripta Materialia</i> , 2021, 204, 114150.	2.6	18
65	Integrating computational modeling and first-principles calculations to predict stacking fault energy of dilute multicomponent Ni-base alloys. <i>Computational Materials Science</i> , 2014, 91, 50-55.	1.4	17
66	Towards Reaching the Theoretical Limit of Porosity in Solid State Metal Foams: Intraparticle Expansion as A Primary and Additive Means to Create Porosity. <i>Advanced Engineering Materials</i> , 2014, 16, 190-195.	1.6	17
67	Binding of He <sub>n</sub> V clusters to $\pm$ -Fe grain boundaries. <i>Journal of Applied Physics</i> , 2014, 115, .	1.1	16
68	Solid-State Foaming by Oxide Reduction and Expansion: Tailoring the Foamed Metal Microstructure in the Cu-CuO System with Oxide Content and Annealing Conditions. <i>Advanced Engineering Materials</i> , 2016, 18, 83-95.	1.6	16
69	Beyond initial twin nucleation in hcp metals: Micromechanical formulation for determining twin spacing during deformation. <i>Acta Materialia</i> , 2017, 133, 134-146.	3.8	15
70	Simulations of tensile bond rupture in single alkane molecules using reactive interatomic potentials. <i>Chemical Physics Letters</i> , 2015, 635, 278-284.	1.2	14
71	A Review on Capturing Twin Nucleation in Crystal Plasticity for Hexagonal Metals. <i>Metals</i> , 2021, 11, 1373.	1.0	14
72	Evaluating Local Primary Dendrite Arm Spacing Characterization Techniques Using Synthetic Directionally Solidified Dendritic Microstructures. <i>Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science</i> , 2015, 46, 4610-4628.	1.1	13

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73	Challenges of Engineering Grain Boundaries in Boron-Based Armor Ceramics. <i>Jom</i> , 2016, 68, 1605-1615.	0.9	13
74	Symmetry-based automated extraction of microstructural features: Application to dendritic cores in single-crystal Ni-based superalloys. <i>Scripta Materialia</i> , 2010, 62, 357-360.	2.6	12
75	Effect of magnetic fields on microstructure evolution. <i>Computational Materials Science</i> , 2018, 150, 464-474.	1.4	12
76	Property mapping of friction stir welded Al-2139 T8 plate using site specific shear punch testing. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2017, 682, 192-201.	2.6	11
77	Measurement of $\text{Ni}_3\text{Al}$ precipitates in a nickel-based superalloy using energy-filtered transmission electron microscopy coupled with automated segmenting techniques. <i>Micron</i> , 2010, 41, 641-647.	1.1	10
78	Synthesis, characterization and quantitative analysis of porous metal microstructures: Application to microporous copper produced by solid state foaming. <i>AIMS Materials Science</i> , 2016, 3, 573-590.	0.7	10
79	Multi-scale characterization of inhomogeneous morphologically textured microstructures. <i>Materials Science &amp; Engineering A: Structural Materials: Properties, Microstructure and Processing</i> , 2010, 527, 883-889.	2.6	9
80	Automated extraction of symmetric microstructure features in serial sectioning images. <i>Materials Characterization</i> , 2010, 61, 1406-1417.	1.9	8
81	Molecular Dynamics Simulations of the Glass Transition Temperature of Amorphous Cellulose. <i>Applied Mechanics and Materials</i> , 0, 214, 7-11.	0.2	7
82	Automated detection and characterization of microstructural features: application to eutectic particles in single crystal Ni-based superalloys. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2010, 18, 025014.	0.8	6
83	Bridging atomistic simulations and experiments via virtual diffraction: understanding homophase grain boundary and heterophase interface structures. <i>Journal of Materials Science</i> , 2016, 51, 1251-1260.	1.7	6
84	Automated identification and characterisation of secondary and tertiary $\text{Ni}_3\text{Al}$ precipitates in nickel-based superalloys. <i>Materials Science and Technology</i> , 2010, 26, 1414-1422.	0.8	4
85	Quantifying Parameter Sensitivity and Uncertainty for Interatomic Potential Design: Application to Saturated Hydrocarbons. <i>ASCE-ASME Journal of Risk and Uncertainty in Engineering Systems, Part B: Mechanical Engineering</i> , 2018, 4, .	0.7	4
86	Correlating deformation mechanisms with X-ray diffraction phenomena in nanocrystalline metals using atomistic simulations. <i>Computational Materials Science</i> , 2018, 154, 178-186.	1.4	3
87	Transition of deformation mechanisms in nanotwinned single crystalline SiC. <i>Philosophical Magazine</i> , 2019, 99, 2636-2660.	0.7	3
88	Effect of Processing Parameters on the Microstructure of Mechanically Alloyed Nanostructured Al-Mn Alloys. , 2015, , 3-11.		3
89	Algorithm Development in Computational Materials Science. <i>Jom</i> , 2014, 66, 397-398.	0.9	1
90	Rebuttal comments on "Mitigating grain growth in binary nanocrystalline alloys through solute selection based on thermodynamic stability maps". <i>Computational Materials Science</i> , 2015, 107, 238-242.	1.4	1

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91	A thermodynamic and kinetic-based grain growth model for nanocrystalline materials: Parameter sensitivity analysis and model extension. Computational Materials Science, 2017, 131, 250-265.	1.4	1
92	Multiscale Characterization of Spatial Heterogeneity in Multiphase Composite Microstructures. Journal of Engineering Materials and Technology, Transactions of the ASME, 2011, 133, .	0.8	0
93	Integrating exploratory data analytics into ReaxFF parameterization. MRS Communications, 2018, 8, 1300-1310.	0.8	0
94	Enhancing Mechanical Properties of Hot Wrought Steel by Microalloying and Optimizing Heat Treatments. Journal of Materials Engineering and Performance, 2020, 29, 5374-5387.	1.2	0