Enrique Martinez

List of Publications by Citations

94 papers	1,985 citations	23 h-index	41 g-index
102 ext. papers	2,410 ext. citations	4.3 avg, IF	5.2 L-index

#	Paper	IF	Citations
94	Outstanding radiation resistance of tungsten-based high-entropy alloys. *Science Advances*, **2019**, 5, eaav2002	4.9	174
93	Scalable parallel Monte Carlo algorithm for atomistic simulations of precipitation in alloys. *Physical Review B*, **2012**, 85,	3.3	159
92	The relationship between grain boundary structure, defect mobility, and grain boundary sink efficiency. *Scientific Reports*, **2015**, 5, 9095	4.9	104
91	Atomistically informed dislocation dynamics in fcc crystals. *Journal of the Mechanics and Physics of Solids*, **2008**, 56, 869-895	5	97
90	Synchronous parallel kinetic Monte Carlo for continuum diffusion-reaction systems. *Journal of Computational Physics*, **2008**, 227, 3804-3823	4.1	70
89	Properties of Helium bubbles in Fe and FeCr alloys. *Journal of Nuclear Materials*, **2011**, 418, 261-268	3.3	64
88	Modeling radiation induced segregation in iron□chromium alloys. *Acta Materialia*, **2016**, 103, 1-11	8.4	59
87	Loop and void damage during heavy ion irradiation on nanocrystalline and coarse grained tungsten: Microstructure, effect of dpa rate, temperature, and grain size. *Acta Materialia*, **2018**, 149, 206-219	8.4	57
86	Decomposition kinetics of Fe-Cr solid solutions during thermal aging. *Physical Review B*, **2012**, 86,	3.3	52
85	Simple concentration-dependent pair interaction model for large-scale simulations of Fe-Cr alloys. *Physical Review B*, **2011**, 84,	3.3	51
84	Atomistic simulations of the decomposition kinetics in Fe□Cr alloys: Influence of magnetism. *Acta Materialia*, **2014**, 73, 97-106	8.4	43
83	Helium bubble precipitation at dislocation networks. *Scripta Materialia*, **2012**, 66, 17-20	5.6	38
82	A dislocation dynamics study of the strength of stacking fault tetrahedra. Part I: interactions with screw dislocations. *Philosophical Magazine*, **2008**, 88, 809-840	1.6	38
81	An atomistic investigation of the interaction of dislocations with Guinier-Preston zones in Al-Cu alloys. *Acta Materialia*, **2019**, 162, 189-201	8.4	38
80	Radiation induced effects on mechanical properties of nanoporous gold foams. *Applied Physics Letters*, **2014**, 104, 233109	3.4	36
79	Mobility and coalescence of stacking fault tetrahedra in Cu. *Scientific Reports*, **2015**, 5, 9084	4.9	35
78	Spatially resolved stochastic cluster dynamics for radiation damage evolution in nanostructured metals. *Journal of Nuclear Materials*, **2013**, 443, 128-139	3.3	34

77	Unprecedented irradiation resistance of nanocrystalline tungsten with equiaxed nanocrystalline grains to dislocation loop accumulation. *Acta Materialia*, **2019**, 165, 118-128	8.4	34
76	Billion-atom synchronous parallel kinetic Monte Carlo simulations of critical 3D Ising systems. *Journal of Computational Physics*, **2011**, 230, 1359-1369	4.1	33
75	Micro/meso-scale computational study of dislocation-stacking-fault tetrahedron interactions in copper. *Journal of Materials Research*, **2009**, 24, 3628-3635	2.5	33
74	A rate theory study of helium bubble formation and retention in CuNb nanocomposites. *Journal of Nuclear Materials*, **2013**, 435, 141-152	3.3	27
73	Liquid-phase thermodynamics and structures in the CuNb binary system. *Modelling and Simulation in Materials Science and Engineering*, **2013**, 21, 025005	2	25
72	Cr interactions with He and vacancies in dilute Fe-Cr alloys from first principles. *Physical Review B*, **2011**, 84,	3.3	25
71	Interaction of small mobile stacking fault tetrahedra with free surfaces, dislocations, and interfaces in Cu and Cu-Nb. *Physical Review B*, **2016**, 93,	3.3	23
70	Identification of dominant damage accumulation processes at grain boundaries during irradiation in nanocrystalline Fe: A statistical study. *Acta Materialia*, **2016**, 110, 306-323	8.4	22
69	Deformation mechanisms of irradiated metallic nanofoams. *Applied Physics Letters*, **2013**, 103, 031909	3.4	22
68	Atomistic modeling of long-term evolution of twist boundaries under vacancy supersaturation. *Physical Review B*, **2012**, 86,	3.3	22
67	A dislocation dynamics study of the strength of stacking fault tetrahedra. Part II: interactions with mixed and edge dislocations. *Philosophical Magazine*, **2008**, 88, 841-863	1.6	22
66	Atomistic modeling of defect-induced plasticity in CuNb nanocomposites. *Physical Review B*, **2014**, 90,	3.3	21
65	Helium bubble growth at BCC twist grain boundaries. *Journal of Nuclear Materials*, **2011**, 419, 201-207	3.3	21
64	Thermostating extended Lagrangian Born-Oppenheimer molecular dynamics. *Journal of Chemical Physics*, **2015**, 142, 154120	3.9	20
63	Helium segregation to screw and edge dislocations in ron and their yield strength. *Acta Materialia*, **2015**, 84, 208-214	8.4	19
62	Solute effects on edge dislocation pinning in complex alpha-Fe alloys. *Journal of Nuclear Materials*, **2017**, 494, 311-321	3.3	19
61	Modal analysis of dislocation vibration and reaction attempt frequency. *Acta Materialia*, **2017**, 134, 203-210	8.4	18
60	Defect Distributions and Transport in Nanocomposites: A Theoretical Perspective. *Materials Research Letters*, **2013**, 1, 193-199	7.4	18

59	Thermal activation of dislocations in large scale obstacle bypass. *Journal of the Mechanics and Physics of Solids*, **2017**, 105, 150-160	5	17
58	Structure of a 2? (010) Cu twist boundary interface and the segregation of vacancies and He atoms. *Physical Review B*, **2012**, 85,	3.3	17
57	Role of Sink Density in Nonequilibrium Chemical Redistribution in Alloys. *Physical Review Letters*, **2018**, 120, 106101	7.4	16
56	Effect of Li on the deformation mechanisms of nanocrystalline hexagonal close packed magnesium. *Computational Materials Science*, **2017**, 126, 252-264	3.2	16
55	The capillarity equation at the nanoscale: Gas bubbles in metals. *Acta Materialia*, **2015**, 89, 14-21	8.4	16
54	Nodal effects in □ron dislocation mobility in the presence of helium bubbles. *Physical Review B*, **2013**, 87,	3.3	15
53	Influence of the stress state on the cross-slip free energy barrier in Al: An atomistic investigation. *Acta Materialia*, **2020**, 184, 109-119	8.4	15
52	Chemical short-range order in derivative Cr-Ta-Ti-V-W high entropy alloys from the first-principles thermodynamic study. *Physical Chemistry Chemical Physics*, **2020**, 22, 23929-23951	3.6	15
51	Atomistic modeling of helium segregation to grain boundaries in tungsten and its effect on de-cohesion. *Nuclear Fusion*, **2017**, 57, 086044	3.3	14
50	Basal dislocation/precipitate interactions in Mg□l alloys: an atomistic investigation. *Modelling and Simulation in Materials Science and Engineering*, **2019**, 27, 075003	2	13
49	Structure of nanoscale gas bubbles in metals. *Applied Physics Letters*, **2013**, 103, 213115	3.4	13
48	Probing ultrafast shock-induced chemistry in liquids using broad-band mid-infrared absorption spectroscopy. *Journal of Chemical Physics*, **2019**, 150, 204503	3.9	12
47	Multiscale modeling of Radiation Induced Segregation in iron based alloys. *Computational Materials Science*, **2018**, 149, 324-335	3.2	12
46	Synchronous parallel spatially resolved stochastic cluster dynamics. *Computational Materials Science*, **2016**, 120, 43-52	3.2	12
45	On the analytic calculation of critical size for alpha prime precipitation in FeCr. *Journal of Nuclear Materials*, **2013**, 439, 180-184	3.3	12
44	Solute precipitation on a screw dislocation and its effects on dislocation mobility in bcc Fe. *Journal of Nuclear Materials*, **2019**, 519, 265-273	3.3	11
43	Strengthening of Al□u alloys by Guinier□Preston zones: Predictions from atomistic simulations. *Journal of the Mechanics and Physics of Solids*, **2019**, 132, 103675	5	11
42	Simulations of Decomposition Kinetics of Fe-Cr Solid Solutions during Thermal Aging. *Solid State Phenomena*, **2011**, 172-174, 1016-1021	0.4	11

41	Prediction of the Al-rich part of the Al-Cu phase diagram using cluster expansion and statistical mechanics. *Acta Materialia*, **2020**, 195, 317-326	8.4	11
40	Reaction Rates in Nitromethane under High Pressure from Density Functional Tight Binding Molecular Dynamics Simulations. *Journal of Physical Chemistry A*, **2020**, 124, 3314-3328	2.8	10
39	Discovering mechanisms relevant for radiation damage evolution. *Computational Materials Science*, **2018**, 147, 282-292	3.2	10
38	Parallel replica dynamics simulations of reactions in shock compressed liquid benzene. *Journal of Chemical Physics*, **2019**, 150, 244108	3.9	10
37	Radiation-induced segregation in W-Re: from kinetic Monte Carlo simulations to atom probe tomography experiments. *European Physical Journal B*, **2019**, 92, 1	1.2	9
36	formation kinetics and radiation induced segregation in neutron irradiated 14YWT nanostructured ferritic alloys. *Scientific Reports*, **2019**, 9, 8345	4.9	9
35	On the mobility of carriers at semi-coherent oxide heterointerfaces. *Physical Chemistry Chemical Physics*, **2017**, 19, 23122-23130	3.6	9
34	Temperature threshold for preferential bubble formation on grain boundaries in tungsten under in-situ helium irradiation. *Scripta Materialia*, **2020**, 180, 6-10	5.6	8
33	Sublattice parallel replica dynamics. *Physical Review E*, **2014**, 89, 063308	2.4	8
32	Perspectives on multiscale modelling and experiments to accelerate materials development for fusion. *Journal of Nuclear Materials*, **2021**, 554, 153113	3.3	7
31	Helium implantation damage resistance in nanocrystalline W-Ta-V-Cr high entropy alloys. *Materials Today Energy*, **2021**, 19, 100599	7	6
30	Atomic-Scale Studies of Defect Interactions with Homo- and Heterophase Interfaces. *Jom*, **2016**, 68, 1616-1624	2.1	6
29	Coherent phase decomposition in the Pd H system. *Journal of Materials Science*, **2020**, 55, 4864-4882	4.3	5
28	Atomistic modeling of the reordering process of disordered particles in Ni-Al alloys. *Journal of Nuclear Materials*, **2016**, 478, 207-214	3.3	4
27	How relative defect migration energies drive contrasting temperature-dependent microstructural evolution in irradiated ceramics. *Physical Review Materials*, **2018**, 2,	3.2	4
26	Does sink efficiency unequivocally characterize how grain boundaries impact radiation damage?. *Physical Review Materials*, **2018**, 2,	3.2	4
25	A pathway to synthesizing single-crystal Fe and FeCr films. *Surface and Coatings Technology*, **2020**, 403, 126346	4.4	4
24	Influence of Chemistry and Misfit Dislocation Structure on Dopant Segregation at Complex Oxide Heterointerfaces. *Advanced Theory and Simulations*, **2019**, 2, 1800095	3.5	4

23	Kinetic Monte Carlo Algorithms for Nuclear Materials Applications **2018**, 1-22		4
22	Dissociated vacancies and screw dislocations in MgO and UO: atomistic modeling and linear elasticity analysis. *Scientific Reports*, **2019**, 9, 6499	4.9	3
21	Structure and Mobility of Dissociated Vacancies at Twist Grain Boundaries and Screw Dislocations in Ionic Rocksalt Compounds. *Chemistry of Materials*, **2018**, 30, 1980-1988	9.6	3
20	Thermally Induced Interdiffusion and Precipitation in a Ni/Ni3Al System. *Materials Research Letters*, **2015**, 3, 169-176	7.4	3
19	Atomistic analysis of the {101⃗2} twin stability and growth in ⃗Ti. *Physical Review Materials*, **2018**, 2,	3.2	3
18	Screw-dislocation constrictions in face-centered cubic crystals. *Physical Review B*, **2014**, 90,	3.3	2
17	DFT-Parameterized Object Kinetic Monte Carlo Simulations of Radiation Damage **2018**, 1-32		2
16	Development of a solute and defect concentration dependant Ising model for the study of transmutation induced segregation in neutron irradiated W-(Re, Os) systems. *Journal of Physics Condensed Matter*, **2021**, 33,	1.8	2
15	Non-orthogonal computational grids for studying dislocation motion in phase field approaches. *Computational Materials Science*, **2021**, 200, 110834	3.2	2
14	Point defect evolution under irradiation: Finite size effects and spatio-temporal correlations. *Journal of Nuclear Materials*, **2020**, 539, 152233	3.3	1
13	Thermal gradient effect on helium and self-interstitial transport in tungsten. *Journal of Applied Physics*, **2021**, 130, 215904	2.5	1
12	Accelerated Molecular Dynamics Methods in a Massively Parallel World **2020**, 1-28		1
11	DFT-Parameterized Object Kinetic Monte Carlo Simulations of Radiation Damage **2020**, 2457-2488		1
10	On the cross-slip of screw dislocations in zirconium. *Acta Materialia*, **2021**, 208, 116764	8.4	1
9	Accelerated Molecular Dynamics Methods in a Massively Parallel World **2018**, 1-28		1
8	Interaction of transmutation products with precipitates, dislocations and grain boundaries in neutron irradiated W. *Materialia*, **2022**, 22, 101370	3.2	1
7	Accelerated Molecular Dynamics Methods in a Massively Parallel World **2020**, 745-772		0
6	A stochastic solver based on the residence time algorithm for crystal plasticity models. *Computational Mechanics*,1	4	0

5	Atomistic and machine learning studies of solute segregation in metastable grain boundaries.. *Scientific Reports*, **2022**, 12, 6673	4.9	0
4	Accelerated Molecular Dynamics Simulations of Shock-Induced Chemistry: Application to Liquid Benzene. *Challenges and Advances in Computational Chemistry and Physics*, **2019**, 53-70	0.7	
3	Analytical model of the effect of misfit dislocation character on the bubble-to-void transition in metals. *Journal of Nuclear Materials*, **2016**, 469, 106-111	3.3	
2	L□lliage fer-chrome et ses surfaces : des calculs ab initio aux isothermes de s□gr□gation. *Revue De Metallurgie*, **2011**, 108, 21-25		
1	Kinetic Monte Carlo Algorithms for Nuclear Materials Applications **2020**, 2193-2214		