Sergei Dudarev

List of Publications by Year
in descending order

115	18,354	53751 45	22147 113
papers	citations	h-index	g-index

116	116	116	17711
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Electron-energy-loss spectra and the structural stability of nickel oxide:â€,â€,An LSDA+U study. Physical Review B, 1998, 57, 1505-1509.	1.1	10,657
2	Recent progress in research on tungsten materials for nuclear fusion applications in Europe. Journal of Nuclear Materials, 2013, 432, 482-500.	1.3	610
3	Multiscale modeling of crowdion and vacancy defects in body-centered-cubic transition metals. Physical Review B, 2007, 76, .	1.1	396
4	Self-interstitial atom defects in bcc transition metals: Group-specific trends. Physical Review B, 2006, 73, .	1.1	360
5	Primary radiation damage: A review of current understanding and models. Journal of Nuclear Materials, 2018, 512, 450-479.	1.3	358
6	Effect of Mott-Hubbard correlations on the electronic structure and structural stability of uranium dioxide. The Philosophical Magazine: Physics of Condensed Matter B, Statistical Mechanics, Electronic, Optical and Magnetic Properties, 1997, 75, 613-628.	0.6	278
7	Improving atomic displacement and replacement calculations with physically realistic damage models. Nature Communications, 2018, 9, 1084.	5.8	241
8	An integrated model for materials in a fusion power plant: transmutation, gas production, and helium embrittlement under neutron irradiation. Nuclear Fusion, 2012, 52, 083019.	1.6	228
9	Developing structural, high-heat flux and plasma facing materials for a near-term DEMO fusion power plant: The EU assessment. Journal of Nuclear Materials, 2014, 455, 277-291.	1.3	210
10	Interatomic potentials for modelling radiation defects and dislocations in tungsten. Journal of Physics Condensed Matter, 2013, 25, 395502.	0.7	192
11	Effect of the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi><mml:mo>â^'</mml:mo><mml:mi>Î³</mml:mi></mml:math>Phase Transition on the Stability of Dislocation Loops in bcc Iron. Physical Review Letters, 2008, 100, 135503.	2.9	187
12	High-energy collision cascades in tungsten: Dislocation loops structure and clustering scaling laws. Europhysics Letters, 2013, 103, 46003.	0.7	174
13	Review on the EFDA programme on tungsten materials technology and science. Journal of Nuclear Materials, 2011, 417, 463-467.	1.3	157
14	Phase stability, point defects, and elastic properties of W-V and W-Ta alloys. Physical Review B, 2011, 84, .	1.1	139
15	Large-scale simulation of the spin-lattice dynamics in ferromagnetic iron. Physical Review B, 2008, 78, .	1.1	138
16	Lattice swelling and modulus change in a helium-implanted tungsten alloy: X-ray micro-diffraction, surface acoustic wave measurements, and multiscale modelling. Acta Materialia, 2015, 89, 352-363.	3.8	123
17	Neutron-induced dpa, transmutations, gas production, and helium embrittlement of fusion materials. Journal of Nuclear Materials, 2013, 442, S755-S760.	1.3	122
18	Monte Carlo study of thermodynamic properties and clustering in the bcc Fe-Cr system. Physical Review B, 2007, 75, .	1.1	121

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19	Phase stability of ternary fcc and bcc Fe-Cr-Ni alloys. Physical Review B, 2015, 91, .	1.1	114
20	Recent advances in modeling and simulation of the exposure and response of tungsten to fusion energy conditions. Nuclear Fusion, 2017, 57, 092008.	1.6	113
21	Magnetic cluster expansion model for bcc-fcc transitions in Fe and Fe-Cr alloys. Physical Review B, 2010, 81, .	1.1	111
22	Elastic trapping of dislocation loops in cascades in ion-irradiated tungsten foils. Journal of Physics Condensed Matter, 2014, 26, 375701.	0.7	111
23	Direct observation of size scaling and elastic interaction between nano-scale defects in collision cascades. Europhysics Letters, 2015, 110, 36001.	0.7	102
24	Density Functional Theory Models for Radiation Damage. Annual Review of Materials Research, 2013, 43, 35-61.	4.3	101
25	Understanding STM images and EELS spectra of oxides with strongly correlated electrons: a comparison of nickel and uranium oxides. Micron, 2000, 31, 363-372.	1.1	96
26	Ab initioscaling laws for the formation energy of nanosized interstitial defect clusters in iron, tungsten, and vanadium. Physical Review B, 2016, 94, .	1.1	84
27	Radiation damage production in massive cascades initiated by fusion neutrons in tungsten. Journal of Nuclear Materials, 2014, 455, 207-211.	1.3	79
28	Coherent motion of interstitial defects in a crystalline material. Philosophical Magazine, 2003, 83, 3577-3597.	0.7	78
29	Structure and metastability of mesoscopic vacancy and interstitial loop defects in iron and tungsten. Journal of Physics Condensed Matter, 2008, 20, 345214.	0.7	78
30	Non-Contact Measurement of Thermal Diffusivity in Ion-Implanted Nuclear Materials. Scientific Reports, 2015, 5, 16042.	1.6	78
31	Lambda transitions in materials science: Recent advances in CALPHAD and firstâ€principles modelling. Physica Status Solidi (B): Basic Research, 2014, 251, 53-80.	0.7	75
32	The EU programme for modelling radiation effects in fusion reactor materials: An overview of recent advances and future goals. Journal of Nuclear Materials, 2009, 386-388, 1-7.	1.3	68
33	Constrained density functional for noncollinear magnetism. Physical Review B, 2015, 91, .	1.1	68
34	Langevin model for real-time Brownian dynamics of interacting nanodefects in irradiated metals. Physical Review B, 2010, 81, .	1.1	65
35	Theory and simulation of the diffusion of kinks on dislocations in bcc metals. Physical Review B, 2013, 87, .	1.1	62
36	A multi-scale model for stresses, strains and swelling of reactor components under irradiation. Nuclear Fusion, 2018, 58, 126002.	1.6	61

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37	The Feâ€“Cr system: atomistic modelling of thermodynamics and kinetics of phase transformations. Comptes Rendus Physique, 2008, 9, 379-388.	0.3	60
38	Spatial ordering of nano-dislocation loops in ion-irradiated materials. Journal of Nuclear Materials, 2014, 455, 16-20.	1.3	58
39	Fast, vacancy-free climb of prismatic dislocation loops in bcc metals. Scientific Reports, 2016, 6, 30596.	1.6	56
40	Cascade fragmentation: deviation from power law in primary radiation damage. Materials Research Letters, 2017, 5, 357-363.	4.1	56
41	Spin-lattice-electron dynamics simulations of magnetic materials. Physical Review B, 2012, 85, .	1.1	54
42	Universality of point defect structure in body-centered cubic metals. Physical Review Materials, 2019, 3, .	0.9	53
43	The non-Arrhenius migration of interstitial defects in bcc transition metals. Comptes Rendus Physique, 2008, 9, 409-417.	0.3	52
44	European materials development: Results and perspective. Fusion Engineering and Design, 2019, 146, 1300-1307.	1.0	50
45	A first-principles model for anomalous segregation in dilute ternary tungsten-rhenium-vacancy alloys. Journal of Physics Condensed Matter, 2017, 29, 145403.	0.7	49
46	Elastic fields, dipole tensors, and interaction between self-interstitial atom defects in bcc transition metals. Physical Review Materials, 2018, 2, .	0.9	47
47	Trapping of He clusters by inert-gas impurities in tungsten: First-principles predictions and experimental validation. Nuclear Instruments & Methods in Physics Research B, 2015, 352, 86-91.	0.6	45
48	Low temperature diffusivity of self-interstitial defects in tungsten. New Journal of Physics, 2017, 19, 073024.	1.2	45
49	Microscopic structure of a heavily irradiated material. Physical Review Materials, 2020, 4, .	0.9	45
50	Surface structure and bonding in the strongly correlated metal oxides NiO and UO2. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1998, 16, 1055-1058.	0.9	44
51	Magnetic cluster expansion simulations of FeCr alloys. Journal of Nuclear Materials, 2009, 386-388, 22-25.	1.3	43
52	Elastic interactions between nano-scale defects in irradiated materials. Acta Materialia, 2017, 125, 425-430.	3.8	43
53	Optimization of the magnetic potential for Î±-Fe. Journal of Physics Condensed Matter, 2011, 23, 206001.	0.7	40
54	Multiscale modelling of the interaction of hydrogen with interstitial defects and dislocations in BCC tungsten. Nuclear Fusion, 2018, 58, 016006.	1.6	40

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55	Magnetic origin of nano-clustering and point defect interaction in Feâ€“Cr alloys: an ab-initio study. Journal of Computer-Aided Materials Design, 2007, 14, 159-169.	0.7	39
56	Effects of elastic interactions on post-cascade radiation damage evolution in kinetic Monte Carlo simulations. Philosophical Magazine, 2005, 85, 661-675.	0.7	38
57	Subcascade formation and defect cluster size scaling in high-energy collision events in metals. Europhysics Letters, 2016, 115, 26001.	0.7	38
58	Observation of Transient and Asymptotic Driven Structural States of Tungsten Exposed to Radiation. Physical Review Letters, 2020, 125, 225503.	2.9	38
59	Perspectives on multiscale modelling and experiments to accelerate materials development for fusion. Journal of Nuclear Materials, 2021, 554, 153113.	1.3	37
60	Simulations of weak-beam diffraction contrast images of dislocation loops by the many-beam Howieâ€“Basinski equations. Philosophical Magazine, 2006, 86, 4851-4881.	0.7	36
61	Dynamic simulation of structural phase transitions in magnetic iron. Physical Review B, 2017, 96, .	1.1	36
62	Systematic group-specific trends for point defects in bcc transition metals: An ab initio study. Journal of Nuclear Materials, 2007, 367-370, 257-262.	1.3	35
63	Phonon drag force acting on a mobile crystal defect: Full treatment of discreteness and nonlinearity. Physical Review B, 2015, 92, .	1.1	35
64	Relaxation volumes of microscopic and mesoscopic irradiation-induced defects in tungsten. Journal of Applied Physics, 2019, 126, .	1.1	35
65	Parametrization of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>LSDA</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math> for noncollinear magnetic configurations: Multipolar magnetism in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>UO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> Physical Review Materials, 2019, 3, .	0.9	35
66	Simulating dislocation loop internal dynamics and collective diffusion using stochastic differential equations. Physical Review B, 2011, 84, .	1.1	34
67	Direct observation of the spatial distribution of primary cascade damage in tungsten. Acta Materialia, 2018, 144, 905-917.	3.8	33
68	Spatial heterogeneity of tungsten transmutation in a fusion device. Nuclear Fusion, 2017, 57, 044002.	1.6	31
69	Effect of stress on vacancy formation and migration in body-centered-cubic metals. Physical Review Materials, 2019, 3, .	0.9	31
70	Model many-body Stoner Hamiltonian for binary FeCr alloys. Physical Review B, 2009, 80, .	1.1	29
71	SPILADY: A parallel CPU and GPU code for spinâ€“lattice magnetic molecular dynamics simulations. Computer Physics Communications, 2016, 207, 350-361.	3.0	29
72	Interatomic potentials for materials with interacting electrons. Journal of Computer-Aided Materials Design, 2007, 14, 129-140.	0.7	28

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73	Symmetry-broken self-interstitial defects in chromium, molybdenum, and tungsten. Physical Review Materials, 2019, 3, .	0.9	28
74	Heterogeneous void swelling near grain boundaries in irradiated materials. Physical Review B, 2003, 67, .	1.1	27
75	The non-degenerate core structure of a Â½âŸ¨111âŸ© screw dislocation in bcc transition metals modelled using Finnisâ€“Sinclair potentials: The necessary and sufficient conditions. Philosophical Magazine, 2009, 89, 3235-3243.	0.7	27
76	First-principles models for phase stability and radiation defects in structural materials for future fusion power-plant applications. Journal of Materials Science, 2012, 47, 7385-7398.	1.7	26
77	Hubbard-like Hamiltonians for interacting electrons in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>s</mml:mi><mml:mo>,</mml:mo><mml:mi>p</mml:mi></mml:math>, and<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>d</mml:mi></mml:math>orbitals. Physical Review B, 2016, 93, .	1.1	26
78	Parameter-free quantitative simulation of high-dose microstructure and hydrogen retention in ion-irradiated tungsten. Physical Review Materials, 2021, 5, .	0.9	26
79	Discrete stochastic model of point defect-dislocation interaction for simulating dislocation climb. International Journal of Plasticity, 2021, 136, 102848.	4.1	24
80	Elastic dipole tensors and relaxation volumes of point defects in concentrated random magnetic Fe-Cr alloys. Computational Materials Science, 2021, 194, 110435.	1.4	24
81	High-temperature dynamics of surface magnetism in iron thin films. Philosophical Magazine, 2009, 89, 2921-2933.	0.7	23
82	Materials for in-vessel components. Fusion Engineering and Design, 2022, 174, 112994.	1.0	23
83	Ab initio multi-string Frenkelâ€“Kontorova model for a b =a/2[111] screw dislocation in bcc iron. Philosophical Magazine, 2010, 90, 1035-1061.	0.7	22
84	Driven mobility of self-interstitial defects under electron irradiation. Nuclear Instruments & Methods in Physics Research B, 2007, 256, 253-259.	0.6	20
85	Classical Mobility of Highly Mobile Crystal Defects. Physical Review Letters, 2014, 113, 215501.	2.9	20
86	Quantum de-trapping and transport of heavy defects in tungsten. Nature Materials, 2020, 19, 508-511.	13.3	20
87	Diffusion and interaction of prismatic dislocation loops simulated by stochastic discrete dislocation dynamics. Physical Review Materials, 2019, 3, .	0.9	20
88	Non-local model for diffusion-mediated dislocation climb and cavity growth. Journal of the Mechanics and Physics of Solids, 2017, 103, 121-141.	2.3	19
89	Multiscale analysis of dislocation loops and voids in tungsten. Physical Review Materials, 2020, 4, .	0.9	17
90	Comparative Assessment of Material Performance in DEMO Fusion Reactors. Fusion Science and Technology, 2014, 66, 9-17.	0.6	16

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91	Dynamics of magnetism in Fe-Cr alloys with Cr clustering. Physical Review B, 2019, 99, .	1.1	16
92	Comparative study of deuterium retention and vacancy content of self-ion irradiated tungsten. Journal of Nuclear Materials, 2022, 558, 153373.	1.3	16
93	Hydrogen accumulation around dislocation loops and edge dislocations: from atomistic to mesoscopic scales in BCC tungsten. Physica Scripta, 2017, T170, 014073.	1.2	15
94	Atomistic-object kinetic Monte Carlo simulations of irradiation damage in tungsten. Modelling and Simulation in Materials Science and Engineering, 2019, 27, 055003.	0.8	15
95	Nonuniversal structure of point defects in face-centered cubic metals. Physical Review Materials, 2021, 5, .	0.9	14
96	Atomistic-to-continuum description of edge dislocation core: Unification of the Peierls-Nabarro model with linear elasticity. Physical Review Materials, 2018, 2, .	0.9	14
97	CALANIE: Anisotropic elastic correction to the total energy, to mitigate the effect of periodic boundary conditions. Computer Physics Communications, 2020, 252, 107130.	3.0	13
98	Multiscale modelling for fusion and fission materials: The M4F project. Nuclear Materials and Energy, 2021, 29, 101051.	0.6	12
99	Macroscopic elastic stress and strain produced by irradiation. Nuclear Fusion, 0, , .	1.6	11
100	Dislocation dynamics simulation of thermal annealing of a dislocation loop microstructure. Journal of Nuclear Materials, 2022, 562, 153552.	1.3	11
101	Experimental observation of the number of visible defects produced in individual primary damage cascades in irradiated tungsten. Europhysics Letters, 2018, 122, 66001.	0.7	10
102	Kink-limited Orowan strengthening explains the brittle to ductile transition of irradiated and unirradiated bcc metals. Physical Review Materials, 2018, 2, .	0.9	9
103	Statistical model for diffusion-mediated recovery of dislocation and point-defect microstructure. Physical Review E, 2018, 98, .	0.8	8
104	Ultraviolet catastrophe of a fluctuating curved dislocation line. Physical Review Research, 2020, 2, .	1.3	8
105	First-principles model for voids decorated by transmutation solutes: Short-range order effects and application to neutron irradiated tungsten. Physical Review Materials, 2021, 5, .	0.9	7
106	Spin-lattice dynamics model for magnon-phonon-electron heat transfer on a million atom scale. Journal of Applied Physics, 2012, 111, 07D114.	1.1	6
107	Continuum model for the core of a straight mixed dislocation. Physical Review Materials, 2019, 3, .	0.9	5
108	Microstructural complexity and dimensional changes in heavily irradiated zirconium. Physical Review Materials, 2021, 5, .	0.9	5

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109	Spin-Lattice Dynamics Simulations of Ferromagnetic Iron. AIP Conference Proceedings, 2008, , .	0.3	4
110	The microscopic Einstein-de Haas effect. Journal of Chemical Physics, 2019, 150, 224109.	1.2	4
111	Volume of a dislocation network. Physical Review Materials, 2022, 6, .	0.9	3
112	Atomistic Spin-Lattice Dynamics. , 2020, , 1017-1035.		2
113	Elastic dipole tensor of a defect at a finite temperature: Definition and properties. Physical Review Materials, 2021, 5, .	0.9	2
114	Statistical mechanics of kinks on a gliding screw dislocation. Physical Review Research, 2020, 2, .	1.3	2
115	Atomistic Spin-Lattice Dynamics. , 2018, , 1-19.		0