

# Sergei Dudarev

## List of Publications by Year in descending order

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115  
papers

18,354  
citations

53794

45  
h-index

22166

113  
g-index

116  
all docs

116  
docs citations

116  
times ranked

17711  
citing authors

#	ARTICLE	IF	CITATIONS
1	Comparative study of deuterium retention and vacancy content of self-ion irradiated tungsten. Journal of Nuclear Materials, 2022, 558, 153373.	2.7	16
2	Materials for in-vessel components. Fusion Engineering and Design, 2022, 174, 112994.	1.9	23
3	Dislocation dynamics simulation of thermal annealing of a dislocation loop microstructure. Journal of Nuclear Materials, 2022, 562, 153552.	2.7	11
4	Volume of a dislocation network. Physical Review Materials, 2022, 6, .	2.4	3
5	Discrete stochastic model of point defect-dislocation interaction for simulating dislocation climb. International Journal of Plasticity, 2021, 136, 102848.	8.8	24
6	Elastic dipole tensors and relaxation volumes of point defects in concentrated random magnetic Fe-Cr alloys. Computational Materials Science, 2021, 194, 110435.	3.0	24
7	First-principles model for voids decorated by transmutation solutes: Short-range order effects and application to neutron irradiated tungsten. Physical Review Materials, 2021, 5, .	2.4	7
8	Elastic dipole tensor of a defect at a finite temperature: Definition and properties. Physical Review Materials, 2021, 5, .	2.4	2
9	Multiscale modelling for fusion and fission materials: The M4F project. Nuclear Materials and Energy, 2021, 29, 101051.	1.3	12
10	Parameter-free quantitative simulation of high-dose microstructure and hydrogen retention in ion-irradiated tungsten. Physical Review Materials, 2021, 5, .	2.4	26
11	Perspectives on multiscale modelling and experiments to accelerate materials development for fusion. Journal of Nuclear Materials, 2021, 554, 153113.	2.7	37
12	Nonuniversal structure of point defects in face-centered cubic metals. Physical Review Materials, 2021, 5, .	2.4	14
13	Microstructural complexity and dimensional changes in heavily irradiated zirconium. Physical Review Materials, 2021, 5, .	2.4	5
14	CALANIE: Anisotropic elastic correction to the total energy, to mitigate the effect of periodic boundary conditions. Computer Physics Communications, 2020, 252, 107130.	7.5	13
15	Observation of Transient and Asymptotic Driven Structural States of Tungsten Exposed to Radiation. Physical Review Letters, 2020, 125, 225503.	7.8	38
16	Quantum de-trapping and transport of heavy defects in tungsten. Nature Materials, 2020, 19, 508-511.	27.5	20
17	Atomistic Spin-Lattice Dynamics. , 2020, , 1017-1035.		2
18	Microscopic structure of a heavily irradiated material. Physical Review Materials, 2020, 4, .	2.4	45

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19	Multiscale analysis of dislocation loops and voids in tungsten. <i>Physical Review Materials</i> , 2020, 4, .	2.4	17
20	Ultraviolet catastrophe of a fluctuating curved dislocation line. <i>Physical Review Research</i> , 2020, 2, .	3.6	8
21	Statistical mechanics of kinks on a gliding screw dislocation. <i>Physical Review Research</i> , 2020, 2, .	3.6	2
22	Relaxation volumes of microscopic and mesoscopic irradiation-induced defects in tungsten. <i>Journal of Applied Physics</i> , 2019, 126, .	2.5	35
23	The microscopic Einstein-de Haas effect. <i>Journal of Chemical Physics</i> , 2019, 150, 224109.	3.0	4
24	Atomistic-object kinetic Monte Carlo simulations of irradiation damage in tungsten. <i>Modelling and Simulation in Materials Science and Engineering</i> , 2019, 27, 055003.	2.0	15
25	Dynamics of magnetism in Fe-Cr alloys with Cr clustering. <i>Physical Review B</i> , 2019, 99, .	3.2	16
26	European materials development: Results and perspective. <i>Fusion Engineering and Design</i> , 2019, 146, 1300-1307.	1.9	50
27	Universality of point defect structure in body-centered cubic metals. <i>Physical Review Materials</i> , 2019, 3, .	2.4	53
28	Symmetry-broken self-interstitial defects in chromium, molybdenum, and tungsten. <i>Physical Review Materials</i> , 2019, 3, .	2.4	28
29	Effect of stress on vacancy formation and migration in body-centered-cubic metals. <i>Physical Review Materials</i> , 2019, 3, .	2.4	31
30	Diffusion and interaction of prismatic dislocation loops simulated by stochastic discrete dislocation dynamics. <i>Physical Review Materials</i> , 2019, 3, .	2.4	20
31	Parametrization of $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{LSDA} \langle \text{mml:mi} \rangle \langle \text{mml:mo} \rangle + \langle \text{mml:mo} \rangle \langle \text{mml:mi} \rangle \text{U} \langle \text{mml:mi} \rangle$ for noncollinear magnetic configurations: Multipolar magnetism in $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{UO} \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 2 \langle \text{mml:mn} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mi} \rangle$ <i>Physical Review Materials</i> , 2019, 3, .	2.4	35
32	Continuum model for the core of a straight mixed dislocation. <i>Physical Review Materials</i> , 2019, 3, .	2.4	5
33	Improving atomic displacement and replacement calculations with physically realistic damage models. <i>Nature Communications</i> , 2018, 9, 1084.	12.8	241
34	Multiscale modelling of the interaction of hydrogen with interstitial defects and dislocations in BCC tungsten. <i>Nuclear Fusion</i> , 2018, 58, 016006.	3.5	40
35	Direct observation of the spatial distribution of primary cascade damage in tungsten. <i>Acta Materialia</i> , 2018, 144, 905-917.	7.9	33
36	Atomistic Spin-Lattice Dynamics. , 2018, , 1-19.		0

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37	Statistical model for diffusion-mediated recovery of dislocation and point-defect microstructure. <i>Physical Review E</i> , 2018, 98, .	2.1	8
38	Primary radiation damage: A review of current understanding and models. <i>Journal of Nuclear Materials</i> , 2018, 512, 450-479.	2.7	358
39	Experimental observation of the number of visible defects produced in individual primary damage cascades in irradiated tungsten. <i>Europhysics Letters</i> , 2018, 122, 66001.	2.0	10
40	A multi-scale model for stresses, strains and swelling of reactor components under irradiation. <i>Nuclear Fusion</i> , 2018, 58, 126002.	3.5	61
41	Elastic fields, dipole tensors, and interaction between self-interstitial atom defects in bcc transition metals. <i>Physical Review Materials</i> , 2018, 2, .	2.4	47
42	Kink-limited Orowan strengthening explains the brittle to ductile transition of irradiated and unirradiated bcc metals. <i>Physical Review Materials</i> , 2018, 2, .	2.4	9
43	Atomistic-to-continuum description of edge dislocation core: Unification of the Peierls-Nabarro model with linear elasticity. <i>Physical Review Materials</i> , 2018, 2, .	2.4	14
44	A first-principles model for anomalous segregation in dilute ternary tungsten-rhenium-vacancy alloys. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 145403.	1.8	49
45	Spatial heterogeneity of tungsten transmutation in a fusion device. <i>Nuclear Fusion</i> , 2017, 57, 044002.	3.5	31
46	Recent advances in modeling and simulation of the exposure and response of tungsten to fusion energy conditions. <i>Nuclear Fusion</i> , 2017, 57, 092008.	3.5	113
47	Non-local model for diffusion-mediated dislocation climb and cavity growth. <i>Journal of the Mechanics and Physics of Solids</i> , 2017, 103, 121-141.	4.8	19
48	Elastic interactions between nano-scale defects in irradiated materials. <i>Acta Materialia</i> , 2017, 125, 425-430.	7.9	43
49	Low temperature diffusivity of self-interstitial defects in tungsten. <i>New Journal of Physics</i> , 2017, 19, 073024.	2.9	45
50	Dynamic simulation of structural phase transitions in magnetic iron. <i>Physical Review B</i> , 2017, 96, .	3.2	36
51	Cascade fragmentation: deviation from power law in primary radiation damage. <i>Materials Research Letters</i> , 2017, 5, 357-363.	8.7	56
52	Hydrogen accumulation around dislocation loops and edge dislocations: from atomistic to mesoscopic scales in BCC tungsten. <i>Physica Scripta</i> , 2017, T170, 014073.	2.5	15
53	Ab initio scaling laws for the formation energy of nanosized interstitial defect clusters in iron, tungsten, and vanadium. <i>Physical Review B</i> , 2016, 94, .	3.2	84
54	Subcascade formation and defect cluster size scaling in high-energy collision events in metals. <i>Europhysics Letters</i> , 2016, 115, 26001.	2.0	38

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55	Fast, vacancy-free climb of prismatic dislocation loops in bcc metals. Scientific Reports, 2016, 6, 30596.	3.3	56
56	SPLADY: A parallel CPU and GPU code for spin-lattice magnetic molecular dynamics simulations. Computer Physics Communications, 2016, 207, 350-361.	7.5	29
57	Hubbard-like Hamiltonians for interacting electrons in $s$ and $d$ orbitals. Physical Review B, 2016, 93, .	3.2	26
58	Phonon drag force acting on a mobile crystal defect: Full treatment of discreteness and nonlinearity. Physical Review B, 2015, 92, .	3.2	35
59	Non-Contact Measurement of Thermal Diffusivity in Ion-Implanted Nuclear Materials. Scientific Reports, 2015, 5, 16042.	3.3	78
60	Direct observation of size scaling and elastic interaction between nano-scale defects in collision cascades. Europhysics Letters, 2015, 110, 36001.	2.0	102
61	Phase stability of ternary fcc and bcc Fe-Cr-Ni alloys. Physical Review B, 2015, 91, .	3.2	114
62	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.	7.9	123
63	Constrained density functional for noncollinear magnetism. Physical Review B, 2015, 91, .	3.2	68
64	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.	1.4	45
65	Elastic trapping of dislocation loops in cascades in ion-irradiated tungsten foils. Journal of Physics Condensed Matter, 2014, 26, 375701.	1.8	111
66	Spatial ordering of nano-dislocation loops in ion-irradiated materials. Journal of Nuclear Materials, 2014, 455, 16-20.	2.7	58
67	Classical Mobility of Highly Mobile Crystal Defects. Physical Review Letters, 2014, 113, 215501.	7.8	20
68	Radiation damage production in massive cascades initiated by fusion neutrons in tungsten. Journal of Nuclear Materials, 2014, 455, 207-211.	2.7	79
69	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.	2.7	210
70	Lambda transitions in materials science: Recent advances in CALPHAD and first-principles modelling. Physica Status Solidi (B): Basic Research, 2014, 251, 53-80.	1.5	75
71	Comparative Assessment of Material Performance in DEMO Fusion Reactors. Fusion Science and Technology, 2014, 66, 9-17.	1.1	16
72	Density Functional Theory Models for Radiation Damage. Annual Review of Materials Research, 2013, 43, 35-61.	9.3	101

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73	Neutron-induced dpa, transmutations, gas production, and helium embrittlement of fusion materials. <i>Journal of Nuclear Materials</i> , 2013, 442, S755-S760.	2.7	122
74	Theory and simulation of the diffusion of kinks on dislocations in bcc metals. <i>Physical Review B</i> , 2013, 87, .	3.2	62
75	Recent progress in research on tungsten materials for nuclear fusion applications in Europe. <i>Journal of Nuclear Materials</i> , 2013, 432, 482-500.	2.7	610
76	Interatomic potentials for modelling radiation defects and dislocations in tungsten. <i>Journal of Physics Condensed Matter</i> , 2013, 25, 395502.	1.8	192
77	High-energy collision cascades in tungsten: Dislocation loops structure and clustering scaling laws. <i>Europhysics Letters</i> , 2013, 103, 46003.	2.0	174
78	Spin-lattice dynamics model for magnon-phonon-electron heat transfer on a million atom scale. <i>Journal of Applied Physics</i> , 2012, 111, 07D114.	2.5	6
79	An integrated model for materials in a fusion power plant: transmutation, gas production, and helium embrittlement under neutron irradiation. <i>Nuclear Fusion</i> , 2012, 52, 083019.	3.5	228
80	First-principles models for phase stability and radiation defects in structural materials for future fusion power-plant applications. <i>Journal of Materials Science</i> , 2012, 47, 7385-7398.	3.7	26
81	Spin-lattice-electron dynamics simulations of magnetic materials. <i>Physical Review B</i> , 2012, 85, .	3.2	54
82	Phase stability, point defects, and elastic properties of W-V and W-Ta alloys. <i>Physical Review B</i> , 2011, 84, .	3.2	139
83	Simulating dislocation loop internal dynamics and collective diffusion using stochastic differential equations. <i>Physical Review B</i> , 2011, 84, .	3.2	34
84	Optimization of the magnetic potential for $\hat{\pm}$ -Fe. <i>Journal of Physics Condensed Matter</i> , 2011, 23, 206001.	1.8	40
85	Review on the EFDA programme on tungsten materials technology and science. <i>Journal of Nuclear Materials</i> , 2011, 417, 463-467.	2.7	157
86	<i>Ab initio</i> multi-string Frenkel-Kontorova model for a $b = a/2[111]$ screw dislocation in bcc iron. <i>Philosophical Magazine</i> , 2010, 90, 1035-1061.	1.6	22
87	Langevin model for real-time Brownian dynamics of interacting nanodefects in irradiated metals. <i>Physical Review B</i> , 2010, 81, .	3.2	65
88	Magnetic cluster expansion model for bcc-fcc transitions in Fe and Fe-Cr alloys. <i>Physical Review B</i> , 2010, 81, .	3.2	111
89	High-temperature dynamics of surface magnetism in iron thin films. <i>Philosophical Magazine</i> , 2009, 89, 2921-2933.	1.6	23
90	Magnetic cluster expansion simulations of FeCr alloys. <i>Journal of Nuclear Materials</i> , 2009, 386-388, 22-25.	2.7	43

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91	The EU programme for modelling radiation effects in fusion reactor materials: An overview of recent advances and future goals. <i>Journal of Nuclear Materials</i> , 2009, 386-388, 1-7.	2.7	68
92	Model many-body Stoner Hamiltonian for binary FeCr alloys. <i>Physical Review B</i> , 2009, 80, .	3.2	29
93	The non-degenerate core structure of a $\frac{1}{2}\langle 111 \rangle$ screw dislocation in bcc transition metals modelled using Finnisâ€“Sinclair potentials: The necessary and sufficient conditions. <i>Philosophical Magazine</i> , 2009, 89, 3235-3243.	1.6	27
94	The non-Arrhenius migration of interstitial defects in bcc transition metals. <i>Comptes Rendus Physique</i> , 2008, 9, 409-417.	0.9	52
95	The Feâ€“Cr system: atomistic modelling of thermodynamics and kinetics of phase transformations. <i>Comptes Rendus Physique</i> , 2008, 9, 379-388.	0.9	60
96	Effect of the $\langle 111 \rangle$ Phase Transition on the Stability of Dislocation Loops in bcc Iron. <i>Physical Review Letters</i> , 2008, 100, 135503.	7.8	187
97	Structure and metastability of mesoscopic vacancy and interstitial loop defects in iron and tungsten. <i>Journal of Physics Condensed Matter</i> , 2008, 20, 345214.	1.8	78
98	Spin-Lattice Dynamics Simulations of Ferromagnetic Iron. <i>AIP Conference Proceedings</i> , 2008, , .	0.4	4
99	Large-scale simulation of the spin-lattice dynamics in ferromagnetic iron. <i>Physical Review B</i> , 2008, 78, .	3.2	138
100	Monte Carlo study of thermodynamic properties and clustering in the bcc Fe-Cr system. <i>Physical Review B</i> , 2007, 75, .	3.2	121
101	Driven mobility of self-interstitial defects under electron irradiation. <i>Nuclear Instruments &amp; Methods in Physics Research B</i> , 2007, 256, 253-259.	1.4	20
102	Systematic group-specific trends for point defects in bcc transition metals: An ab initio study. <i>Journal of Nuclear Materials</i> , 2007, 367-370, 257-262.	2.7	35
103	Multiscale modeling of crowdion and vacancy defects in body-centered-cubic transition metals. <i>Physical Review B</i> , 2007, 76, .	3.2	396
104	Interatomic potentials for materials with interacting electrons. <i>Journal of Computer-Aided Materials Design</i> , 2007, 14, 129-140.	0.7	28
105	Magnetic origin of nano-clustering and point defect interaction in Feâ€“Cr alloys: an ab-initio study. <i>Journal of Computer-Aided Materials Design</i> , 2007, 14, 159-169.	0.7	39
106	Self-interstitial atom defects in bcc transition metals: Group-specific trends. <i>Physical Review B</i> , 2006, 73, .	3.2	360
107	Simulations of weak-beam diffraction contrast images of dislocation loops by the many-beam Howieâ€“Basinski equations. <i>Philosophical Magazine</i> , 2006, 86, 4851-4881.	1.6	36
108	Effects of elastic interactions on post-cascade radiation damage evolution in kinetic Monte Carlo simulations. <i>Philosophical Magazine</i> , 2005, 85, 661-675.	1.6	38

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109	Heterogeneous void swelling near grain boundaries in irradiated materials. Physical Review B, 2003, 67, .	3.2	27
110	Coherent motion of interstitial defects in a crystalline material. Philosophical Magazine, 2003, 83, 3577-3597.	1.6	78
111	Understanding STM images and EELS spectra of oxides with strongly correlated electrons: a comparison of nickel and uranium oxides. Micron, 2000, 31, 363-372.	2.2	96
112	Electron-energy-loss spectra and the structural stability of nickel oxide: An LSDA+U study. Physical Review B, 1998, 57, 1505-1509.	3.2	10,657
113	Surface structure and bonding in the strongly correlated metal oxides NiO and UO <sub>2</sub> . Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 1998, 16, 1055-1058.	2.1	44
114	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
115	Macroscopic elastic stress and strain produced by irradiation. Nuclear Fusion, 0, , .	3.5	11