

# Avinash Parashar

## List of Publications by Citations

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75  
papers

1,362  
citations

21  
h-index

34  
g-index

79  
ext. papers

1,744  
ext. citations

3.1  
avg, IF

5.95  
L-index

#	Paper	IF	Citations
75	Effect of Point and Line Defects on Mechanical and Thermal Properties of Graphene: A Review. <i>Critical Reviews in Solid State and Materials Sciences</i> , <b>2016</b> , 41, 47-71	10.1	90
74	Atomistic modeling of graphene/hexagonal boron nitride polymer nanocomposites: a review. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2018</b> , 8, e1346	7.9	63
73	Atomistic modeling of BN nanofillers for mechanical and thermal properties: a review. <i>Nanoscale</i> , <b>2016</b> , 8, 22-49	7.7	61
72	Representative volume element to estimate buckling behavior of graphene/polymer nanocomposite. <i>Nanoscale Research Letters</i> , <b>2012</b> , 7, 515	5	59
71	Experimental and Computational Studies to Analyze the Effect of h-BN Nanosheets on Mechanical Behavior of h-BN/Polyethylene Nanocomposites. <i>Journal of Physical Chemistry C</i> , <b>2019</b> , 123, 20059-20070	3.8	51
70	Enhanced thermal transport across a bi-crystalline graphene-polymer interface: an atomistic approach. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 6229-6237	3.6	49
69	Tersoff potential with improved accuracy for simulating graphene in molecular dynamics environment. <i>Materials Research Express</i> , <b>2016</b> , 3, 035011	1.7	49
68	Effect of grain boundaries on the interfacial behaviour of graphene-polyethylene nanocomposite. <i>Applied Surface Science</i> , <b>2019</b> , 470, 1085-1092	6.7	49
67	The effect of STW defects on the mechanical properties and fracture toughness of pristine and hydrogenated graphene. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 16023-16037	3.6	47
66	Molecular dynamics based simulations to study failure morphology of hydroxyl and epoxide functionalised graphene. <i>Computational Materials Science</i> , <b>2018</b> , 143, 15-26	3.2	47
65	Molecular dynamics based simulations to study the fracture strength of monolayer graphene oxide. <i>Nanotechnology</i> , <b>2018</b> , 29, 115706	3.4	44
64	Optimised cut-off function for Tersoff-like potentials for a BN nanosheet: a molecular dynamics study. <i>Nanotechnology</i> , <b>2016</b> , 27, 085706	3.4	44
63	Tailoring the failure morphology of 2D bicrystalline graphene oxide. <i>Journal of Applied Physics</i> , <b>2018</b> , 124, 015102	2.5	39
62	Adhesively bonded composite tubular joints: Review. <i>International Journal of Adhesion and Adhesives</i> , <b>2012</b> , 38, 58-68	3.4	36
61	Effects of Different Hydrogenation Regimes on Mechanical Properties of h-BN: A Reactive Force Field Study. <i>Journal of Physical Chemistry C</i> , <b>2016</b> , 120, 21932-21938	3.8	32
60	Structural and chemical insights into thermal transport for strained functionalised graphene: a molecular dynamics study. <i>Materials Research Express</i> , <b>2018</b> , 5, 115605	1.7	29
59	A molecular dynamics based study to estimate the point defects formation energies in graphene containing STW defects. <i>Materials Research Express</i> , <b>2019</b> , 6, 015606	1.7	26

58	A review on thermo-mechanical properties of bi-crystalline and polycrystalline 2D nanomaterials. <i>Critical Reviews in Solid State and Materials Sciences</i> , <b>2020</b> , 45, 134-170	10.1	26
57	Atomistic simulations to study crack tip behaviour in single crystal of bcc niobium and hcp zirconium. <i>Current Applied Physics</i> , <b>2019</b> , 19, 37-43	2.6	25
56	Enhancement of fracture toughness of graphene via crack bridging with stone-thrower-wales defects. <i>Diamond and Related Materials</i> , <b>2017</b> , 74, 90-99	3.5	24
55	Reactive force field based atomistic simulations to study fracture toughness of bicrystalline graphene functionalised with oxide groups. <i>Diamond and Related Materials</i> , <b>2018</b> , 88, 193-203	3.5	23
54	Fracture toughness enhancement of h-BN monolayers via hydrogen passivation of a crack edge. <i>Nanotechnology</i> , <b>2017</b> , 28, 165702	3.4	21
53	Effect of geometrical defects and functionalization on the interfacial strength of h-BN/polyethylene based nanocomposite. <i>Polymer</i> , <b>2018</b> , 146, 82-90	3.9	20
52	Mechanical and fracture behavior of water submerged graphene. <i>Journal of Applied Physics</i> , <b>2019</b> , 125, 215107	2.5	19
51	Molecular dynamics study on the mechanical response and failure behaviour of graphene: performance enhancement via 5778 defects. <i>RSC Advances</i> , <b>2016</b> , 6, 26361-26373	3.7	19
50	Surface Modification Techniques for the Preparation of Different Novel Biofibers for Composites <b>2020</b> , 1-34		19
49	Atomistic simulations to study the effect of water molecules on the mechanical behavior of functionalized and non-functionalized boron nitride nanosheets. <i>Computational Materials Science</i> , <b>2019</b> , 169, 109092	3.2	18
48	Atomistic simulations to study the effect of grain boundaries and hydrogen functionalization on the fracture toughness of bi-crystalline h-BN nanosheets. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 13116-13125	3.6	16
47	Effect of symmetric and asymmetric tilt grain boundaries on the tensile behaviour of bcc-Niobium. <i>Computational Materials Science</i> , <b>2018</b> , 143, 126-132	3.2	16
46	Dislocation assisted crack healing in h-BN nanosheets. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 21739-21747	3.6	15
45	Molecular dynamics based study of an irradiated single crystal of niobium. <i>Computational Materials Science</i> , <b>2017</b> , 131, 48-54	3.2	14
44	Role of Chemical Adatoms in Fracture Mechanics of Graphene Nanolayer. <i>Materials Today: Proceedings</i> , <b>2019</b> , 11, 920-924	1.4	14
43	Multiscale Model to Study of Fracture Toughening in Graphene/Polymer Nanocomposite. <i>International Journal of Fracture</i> , <b>2013</b> , 179, 221-228	2.3	14
42	Multiscale model to investigate the effect of graphene on the fracture characteristics of graphene/polymer nanocomposites. <i>Nanoscale Research Letters</i> , <b>2012</b> , 7, 595	5	14
41	Mechanical and fracture behaviour of hydroxyl functionalized h-BN nanosheets. <i>Journal of Materials Science</i> , <b>2020</b> , 55, 3228-3242	4.3	14

40	Effect of symmetrical and asymmetrical tilt grain boundaries on the tensile deformation of zirconium bicrystals: a MD-based study. <i>Journal of Materials Science</i> , <b>2019</b> , 54, 3082-3095	4.3	14
39	Inter-granular fracture toughness of bi-crystalline graphene nanosheets. <i>Diamond and Related Materials</i> , <b>2020</b> , 102, 107667	3.5	13
38	Defect formation dynamics in dry and water submerged graphene nanosheets. <i>Materials Research Express</i> , <b>2019</b> , 6, 075063	1.7	11
37	Effect of Hexagonal Boron Nitride Nanoplatelet on Crystal Nucleation, Mechanical Behavior, and Thermal Stability of High-Density Polyethylene-Based Nanocomposites. <i>Macromolecular Materials and Engineering</i> , <b>2020</b> , 305, 2000248	3.9	11
36	Mechanical strength of a nanoporous bicrystalline h-BN nanomembrane in a water submerged state. <i>Physical Chemistry Chemical Physics</i> , <b>2020</b> , 22, 20453-20465	3.6	11
35	Characterization of 2D Nanomaterials for Energy Storage. <i>Lecture Notes in Mechanical Engineering</i> , <b>2020</b> , 221-226	0.4	10
34	Effect of symmetrical and asymmetrical tilt grain boundaries on radiation-induced defects in zirconium. <i>Journal Physics D: Applied Physics</i> , <b>2018</b> , 51, 265301	3	10
33	Anisotropic compressive response of Stone-Thrower-Wales defects in graphene: A molecular dynamics study. <i>Materials Research Express</i> , <b>2016</b> , 3, 095015	1.7	9
32	Molecular dynamics-based simulations to study crack tip interaction with symmetrical and asymmetrical tilt grain boundaries in Zr. <i>Journal of Nuclear Materials</i> , <b>2019</b> , 526, 151739	3.3	9
31	Study of Mode I Fracture of Graphene Sheets Using Atomistic Based Finite Element Modeling and Virtual Crack Closure Technique. <i>International Journal of Fracture</i> , <b>2012</b> , 176, 119-126	2.3	9
30	Lifecycle Assessment of Thermoplastic and Thermosetting Bamboo Composites <b>2021</b> , 235-246		9
29	Defect dynamics and uniaxial tensile deformation of equi and non-equi-atomic configuration of multi-elemental alloys. <i>Materials Chemistry and Physics</i> , <b>2021</b> , 266, 124549	4.4	9
28	Finite Element Analysis to Study the Effect of Dimensional and Geometrical Parameters on the Stability of Graphene Sheets. <i>Journal of Computational and Theoretical Nanoscience</i> , <b>2013</b> , 10, 292-298	0.3	8
27	Polymer-based nanocomposites for impact loading: A review. <i>Mechanics of Advanced Materials and Structures</i> , 1-26	1.8	8
26	Effect of van der Waals interaction on the mode I fracture characteristics of graphene sheet. <i>Solid State Communications</i> , <b>2013</b> , 173, 56-60	1.6	7
25	Effect of non-bonded interactions on failure morphology of a defective graphene sheet. <i>Materials Research Express</i> , <b>2016</b> , 3, 045009	1.7	7
24	Atomistic simulations to study crack tip behaviour in multi-elemental alloys. <i>Engineering Fracture Mechanics</i> , <b>2021</b> , 243, 107536	4.2	7
23	Displacement thresholds and knock-on cross sections for hydrogenated h-BN monolayers. <i>Computational Materials Science</i> , <b>2018</b> , 142, 82-88	3.2	6

22	Experimental and atomistic insight on the thermal transport properties of h-BN/high density polyethylene nanocomposite. <i>International Journal of Heat and Mass Transfer</i> , <b>2021</b> , 170, 121039	4.9	6
21	Effect of Nb precipitate on defect formation and migration energies in bi-crystalline Zr. <i>Materials Chemistry and Physics</i> , <b>2019</b> , 235, 121729	4.4	4
20	Effect of topological defects on mechanical properties of graphene sheets: a molecular dynamics study. <i>Materials Today: Proceedings</i> , <b>2018</b> , 5, 6780-6788	1.4	4
19	Atomistic simulations to study the effect of helium nanobubble on the shear deformation of nickel crystal. <i>Journal of Nuclear Materials</i> , <b>2021</b> , 557, 153245	3.3	4
18	Molecular Dynamics Study of Anisotropic Shock Response in Mono- and Bicrystalline Boron Nitride Nanosheets: Implications for Shock-Resistant Solid-State Devices. <i>ACS Applied Nano Materials</i> , <b>2022</b> , 5, 2787-2800	5.6	4
17	Atomistic simulations to study the effect of Nb precipitate on fracture properties of bi-crystalline Zr. <i>Journal Physics D: Applied Physics</i> , <b>2019</b> , 52, 355304	3	3
16	Fracture behaviour of pristine and defective form of water submerged h-BN nanosheets. <i>Journal Physics D: Applied Physics</i> , <b>2021</b> , 54, 035306	3	3
15	Enhancement in Mechanical Properties of Polyethylene Using h-BN Nanofiller. <i>Lecture Notes in Mechanical Engineering</i> , <b>2021</b> , 127-133	0.4	3
14	Inter-granular fracture behaviour in bicrystalline boron nitride nanosheets using atomistic and continuum mechanics-based approaches. <i>Journal of Materials Science</i> , <b>2021</b> , 56, 6235-6250	4.3	3
13	Sequential multiscale model to study crack tip behavior in bi-crystalline graphene. <i>Journal of Applied Physics</i> , <b>2020</b> , 127, 225103	2.5	2
12	Effect of BNNR on mechanical properties of polyethylene nanocomposites. <i>Materials Today: Proceedings</i> , <b>2021</b> , 47, 2875-2875	1.4	2
11	Effect of lattice distortion and nanovoids on the shock compression behavior of (Co-Cr-Cu-Fe-Ni) high entropy alloy. <i>Computational Materials Science</i> , <b>2022</b> , 209, 111402	3.2	2
10	Effect of Crack on the Tensile Strength of a Bicrystal Zr - A MD Based Evaluation. <i>Materials Science Forum</i> , <b>2020</b> , 978, 487-491	0.4	1
9	Atomistic simulations to study point defect dynamics in bi-crystalline niobium. <i>Materials Chemistry and Physics</i> , <b>2020</b> , 255, 123628	4.4	1
8	Evaluation of Interfacial Shear Strength of h-BN/PE Nanocomposites Using Molecular Dynamics. <i>Lecture Notes in Mechanical Engineering</i> , <b>2021</b> , 105-113	0.4	1
7	An atomistic approach to study the dynamic and structural response in 2D nanofiller reinforced polyethylene nanocomposites under ultra-short shock pulse loading. <i>Mechanics of Materials</i> , <b>2022</b> , 169, 104305	3.3	1
6	Deformation dynamics of h-BN reinforced polyethylene nanocomposite under shock/impact loading. <i>International Journal of Mechanical Sciences</i> , <b>2022</b> , 107379	5.5	1
5	A Comparison between $\beta$ Asymmetrical Tilt Grain Boundary Energies in Niobium Obtained Analytically and through Molecular Dynamics Based Simulations. <i>Materials Science Forum</i> , <b>2020</b> , 998, 179-184	0.4	0

4	Fracture Toughness Enhancement of Boron Nitride Nanosheets via Crack Edge Passivation Using Various Radicals. <i>Lecture Notes in Mechanical Engineering</i> , <b>2021</b> , 111-117	0.4	o
3	Effect of symmetrical tilt grain boundary on dislocation nucleation and growth in Niobium bi-crystal. <i>Materials Today: Proceedings</i> , <b>2019</b> , 11, 925-928	1.4	
2	Effect of defects and functionalization on mechanical and fracture properties of two-dimensional nanomaterials <b>2021</b> , 543-567		
1	Enhanced Mechanical Properties of h-BN Nanosheets via Edge Passivation Using Various Radicals. <i>Lecture Notes in Mechanical Engineering</i> , <b>2021</b> , 97-103	0.4	