AVINASH PARASHAR

(Professional Engineer-APEGA, Canada)

14/2 Niti Nagar Roorkee (India) 247667 avinash.parashar@me.iitr.ac.in +91-1332-284801

Education

Ph.D., Mechanical Engineering, University of Alberta, Canada

 (GPA- 4.0/4.0)

 Masters, Mechanical Engineering, Concordia University, Canada

 (GPA-3.93)

 B.E., Mechanical Engineering, N.I.T., Bhopal, India
 1998 - 2002

Professional Experience

(79.5 % - Distinction with honors)

Faculty
Department of Mechanical & Industrial Engineering, IIT Roorkee

June, 2014- cont.

Attached Scientist May, 2013-May, 2014
Atomic Energy of Canada Limited, Chalk River Laboratories, Canada

Postdoctoral Researcher
 Dec, 2012-Mar,2013

 Department of Civil Engineering, John Hopkins University, USA

Executive Engineer Sept 2004- Sept 2006
National Thermal Power Corporation Ltd.

Engineer Oct 2003-Jul 2004
Honda Siel Cars India Ltd

➢ Graduate Engineer Trainee LML Ltd
July 2002-Oct, 2003

Funded Research Projects

Project Area	Sponsoring Agency	Amount (Lacs)	Status
Tailoring polymer properties	MHRD-IIT Roorkee	10.00	Completed
Atomistic study of nanocomposites	Nanomission, DST	24.09	Completed
Irradiation effect on Zr-Nb alloys	BRNS, DAE	22.79	Completed
2D nanosheets for water desalination	CSIR	15.88	Completed
PEGDA Hydrogels	SERB (CRG)	20.57	Completed
Polymer nanocomposites	VSSC, ISRO	20.79	Completed
High entropy alloys	SERB (MATRICS)	6.60	Completed

Awards & Honours

Award	Amount
Best performing project, VSSC, ISRO	-
Best Paper Award, International conference on design and manufacturing technologies	-
3rd Prize, International Conference on Processing and Characterisation of Materials	-
Institute Research Fellow (IIT Roorkee)	Rs.9,00,000/-
Excellent grades for executing research project, DST	-
Shortlisted for Policy Maker Position, Canada (NSERC Fellow)	-
Atomic Energy of Canada Limited postdoctoral fellowship	\$57200/-
NSERC (Visiting postdoctoral fellowship)	\$47234.
NSERC postgraduate scholarship	\$63000/-
Alberta innovates graduate scholarship in nanotechnology	\$1,23000/-
Ontario graduate scholarship	\$45000/-
Presidents doctoral prize of distinction	\$20,200/-
ASME OMAE Calgary graduate scholarship	\$39,000/-
Tuition fees waiver	\$1500/-
University of Toronto fellowship	\$9,000/-
Best Newcome Engineer, Honda Siel Cars India Ltd.	
President Scout	-

Supervision of PhD Thesis

Candidate	Status	Outreach	
Rajasekaran G	Awarded (2014-2017)	o Assistant Professor, NIT Trichy	
Daiach Vyman	Awarded (2015-2018)	o DST Travel Grant	
		o University of Connecticut, USA (Postdoctoral fellow)	
Rajesh Kumar		 Assistant Professor, NIT Hamirpur 	
		 Assistant Professor, NIT Kurukshetra 	
	Awarded (2016-2019)	o Shortlisted for excellence in doctoral thesis award (2020)	
Divya Singh		o John Hopkins University, USA (Postdoctoral fellow)	
		o University of California, Irvine USA (Postdoctoral fellow)	
		 Assistant Professor, Utah Tech University, USA 	
Akarsh Verma	Awarded (2016-2020)	o Fulbright Indo –US fellowship	
		o Awarded best doctoral thesis award, IIT Roorkee (2020)	
		○ JSPS postdoctoral fellow (University of Osaka)	
	Awarded (2017-2021)	o IISc Bengaluru (Postdoctoral fellow)	
Bharat B Sharma		o Shortlisted for excellence in doctoral thesis award (2021)	
		 Assistant Professor, GATI SHAKTI University 	
Ankur Chaurasia	Awarded	 Assistant Professor, PDEU, Gandhinagar, Gujrat 	
Ankur Chaurasia	(2018-2022)	 Assistant Professor, NIT Patna 	
Sandeep Kr Singh	Awarded (2019-2022)	o University of Tokyo, Japan (Postdoctoral fellow)	
Saurabh S Sharma	Awarded (2019-2023)	o Commander, Indian Navy	
Raju Kumar	Awarded (2021-2025)	o Linkoping University, Sweden (Postdoctoral fellow)	

Supervision of M.Tech Thesis

Candidate	Status	Placement
Anand Kumar	Awarded	L&T
Vikas Tiwari	Awarded	NTPC Ltd.
Sanchit Tamrakar	Awarded	Bajaj Auto
Kaung Satt Lin	Awarded	Myanmar Air Force
Abhinav Kumar Sharma	Awarded	EATON, India
Prince Verma	Awarded	EATON, India
Saurabh S Sharma	Awarded	Commander, Indian Navy
Prashant Sharma	Awarded	KBR, INC
Pankaj Sharma	Awarded	Siemens, India
Mukesh Kumar	Awarded	Heavy Engineering Corporation
Rohit Kumar	Awarded	DAAD Fellow, EATON, India
Anil Kumar Gautam	Awarded	A.E. Irrigation, UP Govt.

Administration duties (IIT Roorkee)

- 1. Chairman Hindi Cell (September 2024 Till date)
- 2. Coordinator course allocation policy MIED
- 3. Timetable committee
- 4. Deputy superintendent examination
- 5. Coordinator Lab based project (MIN-399)
- 6. Coordinator Training and Placement Seminar (MIN-499)
- 7. Coordinator BTP (Design)
- 8. Faculty Coordinator Industrial Tour
- 9. Faculty Coordinator MIESS
- 10. Founding member SPARK
- 11. Member DAPC, DAC, DRC and space committees

Publications

Journal (Published/accepted)

1. Sanjay Patil, **Avinash Parashar** (2025) Effect of intra- and intergranular hydride precipitation on phonon thermal transport behavior of zirconium: A molecular dynamics study. **Journal of nuclear materials** (in **Print**)

- Sanjay Patil, Avinash Parashar (2025) Atomistic study on the effects of hydride precipitation on shock behavior of single crystal zirconium. <u>Mechanics of materials</u>, 210, 105456.
- Raju Kumar, Jenish Patel, Avinash Parashar, Ankur Chaurasia (2025) Tribo-Mechanical and Antibacterial Performance of 3D-Printed hBN/PEGDA Nanocomposites for Load-Bearing Tissue Engineering Applications. <u>ACS applied bio materials</u>, 8,6439-6454.
- Lalit Kumar, S.P.Harsha, Avinash Parashar (2025) Crack tip behaviour in a non-equiatomic configurations of multiple elemental alloys: A MD based study. Physica scripta, 100, 045938
- 6. Kaushlendra Kumar, Ankur Chaurasia, S P Harsha, **Avinash Parashar** (2025) Functionalised h-BN nanosheets with bonded interface for enhanced compressive strength of HDPE nanocomposite. **Journal of materials science**, 60, 6121-6137.
- Lalit Kumar, Raju Kumar, Sandeep Kumar Singh, Saurabh S Sharma, S.P.Harsha,
 Avinash Parashar (2025) A review of atomistic simulations to study the multipleelemental alloys. <u>Materials today communications</u>, 43, 111823.
- 8. Lalit Kumar, S.P.Harsha, Anand Gupta, **Avinash Parashar** (2025) Effect of lattice distortion on the mechanical behaviour of non-equi-atomic configurations of multiple elemental alloys. **Physica B: Condensed Mater**, 696, 416667
- 9. Raju Kumar, Abhishek Tewari, Avinash Parashar (2024) An atomistic and experimental approach to study the effect of water and nanofillers on the compressive strength of PEGDA hydrogels for cartilage replacement. <u>Mechanics of materials</u>, 199,105161.
- Ashutosh Mittal, Avinash Parashar, (2024) Effect of degree of polymerization, crystallinity and sulfonation on the thermal behaviour of PEEK: a molecular dynamics based study. <u>PCCP</u>, 26, 23335.
- Sanjay Patil, Avinash Parashar (2024) Effects of intergranular hydride precipitation on the mechanical behavior of bi-crystalline zirconium: a Molecular dynamics-based study. <u>Mechanics of materials</u>, 198, 105124.
- Sanjay Patil, Avinash Parashar (2024) Mechanical behavior of zirconium hydride phases: insights from molecular dynamics based simulations. <u>Journal of physics D:</u> <u>applied physics</u>, 57, 505302.
- 13. Saurabh S Sharma, **Avinash Parashar** (**2024**) A review of atomistic simulations to study the effect of helium bubble formation in metal crystals. **Physica Scripta**, 99,102001.

- Raju Kumar, Abhishek Tewari, Avinash Parashar (2024) Experimental and atomistic insight on the mechanical behaviour of h-BN reinforced PEGDA hydrogel for biomedical applications. <u>International journal of mechanical sciences</u>, 277, 109397
- Raju Kumar, Abhishek Tewari, Avinash Parashar (2024) Thermal transport phenomena in PEGDA based nanocomposites hydrogel using atomistic and experimental technique. <u>The journal of physical chemistry B</u>,128, 5254–5267
- Kaushlendra Kumar, S.P. Harsha, Avinash Parashar (2024) Molecular dynamics-based simulations to study the diffusion of gases in medium and high-density polyethylene. <u>ACS</u> <u>Applied Nano Materials</u>, 7, 1978-1985.
- 17. Ankur Chaurasia, Kaushlenrda Kumar, S.P.Harsha, **Avinash Parashar** (**2023**) Covalently functionalized interface in h-BN/PE nanocomposites for enhanced mechanical and thermal properties. **PCCP**, 25, 31396-31409
- Saurabh S Sharma, Avinash Parashar (2024) Effect of helium on the thermal transport properties in single and bi crystals of Ni: a MD based study. <u>Journal of physics D:</u> <u>applied physics</u>, 57,055304.
- 19. Sandeep Kumar Singh, **Avinash Parashar** (2023) Effect of Frenkel pairs on the tensile and shock compression strength of multi-elemental alloys. **Physica Scripta**, 98,095939
- Raju Kumar, Avinash Parashar (2023) Effect of degree of polymerization and water content on the thermal transport phenomena in PEGDA hydrogel: A Molecular Dynamics Based Study. PCCP, 25, 18960-18972
- 21. Saurabh S Sharma, **Avinash Parashar** (2023) Effect of Symmetrical and asymmetrical tilt grain boundaries with <001> as the tilt axis on the shock response of bi-crystalline Ni. **Materials chemistry and physics**, 308, 128298
- Raju Kumar, Avinash Parashar (2023) Atomistic simulations of nanocomposite- based hydrogels: a review. <u>Wires Computational molecular science</u>, 2023;13:e1655 (<u>Top cited article</u>)
- 23. Sandeep Kumar Singh, **Avinash Parashar** (2022) Effect of lattice distortion and grain size on the crack tip behaviour in Co-Cr-Cu-Fe-Ni under mode-I and mode-II loading. **Engineering fracture mechanics**, 274C, 108809.
- 24. Sandeep Kumar Singh, **Avinash Parashar** (2022) Shock resistance capability of multiprincipal elemental alloys as a function of lattice distortion and grain size. **Journal of applied physics**, 132, 095903.
- 25. Saurabh S Sharma, **Avinash Parashar** (2022) Shock resistance capabilities of nickel crystal containing helium nanobubbles. **Journal of applied physics**, 132, 065902.
- Ankur Chaurasia, Rahul S Mulik, Avinash Parashar (2022) Polymer based nanocomposites for impact loading: a review. <u>Mechanics of advanced materials and</u> structures, 29, 2581-2606.
- 27. Ankur Chaurasia, **Avinash Parashar** (2022) Deformation dynamics of h-BN reinforced polyethylene nanocomposites under shock/impact loading. <u>International journal of mechanical sciences</u>, 225, 107379.

- 28. Ankur Chaurasia, **Avinash Parashar** (2022) Anisotropic shock response in mono and bicrystalline boron nitride nanosheets. **ACS Applied nano materials**, 5, 2787-2800.
- 29. Ankur Chaurasia, **Avinash Parashar** (2022) An atomistic approach to study the dynamic and structural response in 2D reinforced (mono and bi-crystalline) polyethylene nanocomposites under ultra-short shock pulse loading. **Mechanics of materials**, 169,104305.
- 30. Sandeep Kumar Singh, **Avinash Parashar** (2022) Effect of lattice distortion on the shock compression behaviour of Co-Cr-Cu-Fe-Ni high entropy alloy using molecular dynamics based simulations. **Computational materials science**, 209,111402.
- 31. Abhinav Kumar Sharma, Saurabh S Sharma, Sandeep Kumar Singh, **Avinash Parashar** (2021) Atomisitic simulations to study the effect of helium nanobubble on the shear deformation of nickel crystal. **Journal of nuclear materials**, 557, 153245.
- 32. Saurabh S Sharma, **Avinash Parashar** (2021) Atomistic simulations to study the effect of helium bubble on the crack tip behaviour in single crystal Ni. **Journal of physics D:** applied physics, 54,365305.
- 33. Sandeep Kumar Singh, **Avinash Parashar** (2021)Defect dynamics and uniaxial tensile deformation of equi and non-equi-atomic configuration of multi elemental alloys. **Materials chemistry and physics**, 266,124549.
- 34. Ankur Chaurasia, **Avinash Parashar** (2021) Effect of grain boundary configuration on the interfacial thermal transport properties in BNNS/PE nanocomposite. **International journal of heat and mass transfer**, 170,121039.
- 35. Sandeep Kumar Singh, **Avinash Parashar** (2021) Atomistic simulations to study crack tip behaviour in multi-elemental alloys. **Engineering fracture mechanics**,243,107536.
- 36. Bharat Bhushan Sharma, **Avinash Parashar** (2021) Inter-granular fracture behavior in bicrystalline boron nitride nanosheets using atomistic and continuum mechanics based approaches. **Journal of materials science**, 56, 6235-6250.
- 37. Bharat Bhushan Sharma, **Avinash Parashar** (2021) Fracture behaviour of pristine and defective form of water submerged h-BN nanosheets. **Journal of physics D: applied physics**, 54, 035306.
- 38. Bharat Bhushan Sharma, **Avinash Parashar** (2020) Mechanical strength of nanoporous bicrystalline h-BN nanomembrane under water submerged state. **PCCP**, 22, 20453-20465. (Listed as HOT article 2020)
- 39. Divya Singh, Prashant Sharma, **Avinash Parashar** (2020) Molecular dynamics based simulations to study the effect of tilt grain boundaries on defect formation and migration energies in niobium. **Materials chemistry and physics**, 255, 123628.
- 40. Prince Verma, **Avinash Parashar** (**2020**) Sequential multi scale model to study the crack tip behaviour in bi-crystalline graphene. **Journal of applied physics**, 127, 225103.
- 41. Ankur Chaurasia, **Avinash Parashar**, Rahul S Mulik, (2020) Effect of hexagonal boron nitride nanoplatelet on crystal nucleation, mechanical behaviour and thermal stability of

- high density polyethylene based nanocomposites. <u>Macromolecular materials and engineering</u>, 305, 2000248.
- 42. Prince Bharat Verma. Bhushan Sharma, Ankur Chaurasia, Avinash Parashar (2020) Intergranular fracture toughness of bi-crystalline graphene nanosheets. Diamond and related materials, 102,107667.
- 43. Bharat Bhushan Sharma, **Avinash Parashar**, (**2020**) A review on thermo-mechanical properties of bi-crystalline and polycrystalline 2D nanomaterials. **Critical reviews in solid state and materials sciences**, 45,134-170.
- 44. Bharat Bhushan Sharma, **Avinash Parashar** (2020) Mechanical and Fracture Behaviour of hydroxyl functionalised h-BN nanosheets. <u>Journal of Materials science</u>, 55,3228-3242.
- 45. Ankur Chaurasia, Akarsh Verma, **Avinash Parashar**, Rahul S Mulik, **(2019)** An Experimental and Computational Study to Analyse the Effect of h-BN Nanosheets on Mechanical Behaviour of h-BN/Polyethylene Nanocomposite. **The Journal of physical chemistry C**, 123, 20059-20070.
- 46. Divya Singh, **Avinash Parashar**, Rajeev Kapoor, Apu Sarkar, A. Kedharnath (**2019**), Molecular dynamics-based simulations to study crack tip interaction with symmetrical and asymmetrical tilt grain boundaries in zirconium. **Journal of nuclear materials**, 526,151739.
- 47. Bharat Bhushan Sharma, **Avinash Parashar** (2019) Atomistic simulations to study the effect of water molecules on the mechanical behavior of functionalized and nonfunctionalized h-BN .**Computational materials science**, 169, 109092.
- 48. Bharat Bhushan Sharma, **Avinash Parashar** (2019) Atomisite simulations to study the effect of grain boundaries and hydrogen functionalisation on the fracture toughness of bicrystalline h-BN nanosheets. **PCCP**, 21, 13116-13125.
- 49. Divya Singh, **Avinash Parashar** (**2019**) Effect of Nb precipitate on defect formation and migration energies in bi-crystalline Zr. **Materials chemistry and physics**, 235, 121729.
- 50. Saurabh S Sharma, Bharat Bhushan Sharma, **Avinash Parashar** (**2019**) Defect formation dynamics in dry and water submerged graphene nanosheets. **Materials research express**, 6, 075063.
- 51. Saurabh S Sharma, Bharat Bhushan Sharma, **Avinash Parashar** (**2019**) Mechanical and fracture behaviour of water submerged graphene. **Journal of applied physics**, 125, 215107.
- 52. Divya Singh, **Avinash Parashar** (2019) Atomistic simulations to study the effect of Nb precipitate on fracture properties of bi-crystalline Zr. **Journal of physics D: applied physics**, 52,355304.
- 53. Akarsh Verma, Rajesh Kumar, **Avinash Parashar** (2019) Enhanced thermal transport across bi-crystalline graphene-polymer interface: An atomistic approach. <u>PCCP</u>, 21, 6229-6237.

- 54. Akarsh Verma, **Avinash Parashar**, Muthukumaran Packirisamy (**2019**), Effect of grain boundaries on the interfacial behaviour of graphene-polyethylene nanocomposite. **Applied surface science**, 470, 1085-1092.
- 55. Divya Singh, **Avinash Parashar**, Rajeev Kapoor, Apu Sarkar, A. Kedharnath (**2019**), Effect of symmetrical and asymmetrical tilt grain boundaries on the tensile deformation of zirconium bi-crystals: a MD based study. **Journal of Materials science**, 54, 3082-3095.
- 56. Vibhor Singla, Akarsh Verma, Avinash Parashar (2019), A molecular dynamics based study to estimate the point defects formation energies in graphene containing STW defects. <u>Materials research express</u>, 6,015606 (<u>SPARK INTRENSHIP WORK</u>).
- 57. Divya Singh, Pankaj Sharma, Sahil Jindal, Prince Kumar, Piyush Kumar, **Avinash Parashar** (2018): Atomistic simulations to study crack tip behaviour in single crystal of bcc Niobium and hcp Zirconium. **Current applied physics** 19,37-43.
- 58. Akarsh Verma, **Avinash Parashar** (2018) Structural and Chemical Insights into Thermal Transport for Strained Functionalised Graphene: A Molecular Dynamics Study. <u>Materials research express</u>, 5,116505.
- 59. Akarsh Verma, **Avinash Parashar** (**2018**) Tailoring the failure morphology of bicrystalline graphene oxide. **Journal of Applied Physics**, 124, 015102.
- 60. Akarsh Verma, **Avinash Parashar** (2018) Reactive force field based atomistic simulations to study fracture toughness of bicrystalline graphene functionalised with oxide groups. **Diamond and Related Materials**, 88, 193-203.
- 61. Divya Singh, **Avinash Parashar** (2018) Effect of symmetrical and asymmetrical tilt grain boundaries on radiation induced defects in zirconium. **Journal of Physics D: Applied physics**, 51,265301.
- 62. Rajesh Kumar, **Avinash Parashar** (2018) Effect of geometrical defects and functionalization on the interfacial strength of h-BN / polyethylene based nanocomposite. **Polymer**, 146, 82-90.
- 63. Akarsh Verma, **Avinash Parashar** (**2018**) Molecular dynamics based simulations to study the fracture strength of monolayer graphene oxide. **Nanotechnology** 29,115706.
- 64. Divya Singh, **Avinash Parasha**r (**2018**) Effect of symmetric and asymmetric tilt grain boundaries on the tensile behaviour of bcc-Niobium. **Computational materials science**, **143**, 126-132.
- 65. Akarsh Verma, **Avinash Parashar** (2018) Molecular dynamics based simulations to study failure morphology of hydroxyl and epoxide functionalised graphene. **Computational materials science**. 143, 15-26.
- 66. Akarsh Verma, **Avinash Parashar**, Muthukumaran Packirisamy (**2018**) Atomistic modeling of graphene/h-BN polymer nanocomposites: A review. **Wires Computational molecular science**, 3,1-50.

- 67. Rajesh Kumar, **Avinash Parashar**, Pierre Martiny (**2018**) Displacement thresholds and knock-on cross sections for hydrogenated h-BN monolayers. **Computational materials science**, 142,82-88.
- 68. Rajesh Kumar, **Avinash Parashar**, (**2017**) Dislocation assisted crack healing in h-BN nanosheets. **PCCP**,19, 21739-21747.
- 69. Akarsh Verma, **Avinash Parashar**,(**2017**) Effect of STW defects on mechanical properties and fracture toughness of pristine and hydrogenated graphene. **PCCP**, 19, 16023 6037.
- 70. Rajesh Kumar, **Avinash Parashar**, (2017)Fracture toughness enhancement of h-BN monolayers via hydrogen-passivation of crack surface. **Nanotechnology**, 28,165702.
- 71. Rajasekaran G., **Avinash Parashar**, (2017) Enhancement of Fracture Toughness of Graphene via Crack Bridging with Stone-Thrower-Wales Defects. <u>Diamond and related materials</u>. 74,90-99.
- 72. **Avinash Parashar**, Divya Singh, (**2017**) Molecular dynamics based study of an irradiated single crystal of niobium. **Computational materials science**.131,48-54.
- 73. Rajasekaran G., **Avinash Parashar**, (2016) Anisotropic compressive response of Stone-Thrower-Wales defects in graphene: A molecular dynamics study. **Materials research express**, 9 095015.
- 74. Rajesh Kumar, Pierre Pertiny, **Avinash Parashar**, (**2016**) Effects of Different Hydrogenation Regimes on Mechanical Properties of h-BN: A Reactive Force Field Study: A Reactive Force Field Study. **The Journal of physical chemistry C**. *120*, 21932–21938.
- 75. Muse Degefe, **Avinash Parashar**, **(2016)** Effect of non-bonded interactions on failure morphology of defective graphene. **Materials research express**, 4, 045009.
- 76. Rajasekaran G., **Avinash Parashar**, (2016) Molecular Dynamics Study on Mechanical Response and Failure Behaviour of Graphene: Performance Enhancement via 5-7-7-5 Defects. **RSC Advances**, 6, 26361-26373.
- 77. Rajasekaran G., **Avinash Parashar**, (2016) Molecular dynamics based simulations to study the effect of modified cut-off function for Tersoff potential on estimating mechanical properties of graphene. **Material research express**, 3, 035011.
- 78. Rajesh Kumar, Rajasekaran G, **Avinash Parashar**, (**2016**), Optimised cut-off function for Tersoff like potentials for BN nanosheet: A molecular dynamics study. **Nanotechnology**, 27,085706.
- 79. Rajesh Kumar, **Avinash Parashar**, (**2016**), Atomistic modelling of mechanical and thermal properties of BN nanofillers: a review. **Nanoscale**, 8,22-49.
- 80. Rajasekaran G., **Avinash Parashar** (2016) Effect of point and line defects on the properties of graphene. <u>Critical reviews in solid state and materials sciences</u>. 41,46-70. (Listed as highly cited and read article)

- 81. **Avinash Parashar**, Pierre Mertiny, (2013) Effect of van der Waals interaction on the fracture characteristics of graphene sheet. **Solid State Communication**. 173, 56-60.
- 82. **Avinash Parashar**, Pierre Mertiny, (**2013**) Effect of van der Waals forces on the buckling strength of multiple graphene sheets. **Computational and theoretical nanoscience**, 10, 2626-2630.
- 83. **Avinash Parashar**, Pierre Mertiny (2013) Multiscale model to study fracture toughening in graphene/polymer nanocomposites, <u>International journal of fracture</u>, 179, 221-228.
- 84. **Avinash Parashar**, Pierre Mertiny, (2013) Failure mechanism in adhesively bonded FRP pipe sections with different fibre architecture, **Composite part B**, 47, 102-106.
- 85. **Avinash Parashar**, Pierre Mertiny, (2013) Finite element analysis to study the effect of dimensional and geometrical parameters on the stability of graphene sheets. **Journal of computational and theoretical nanoscience**, 10, 292-296.
- 86. Avinash Parashar, Pierre Mertiny, (2012) Representative volume element to estimate buckling behavior of graphene/polymer nanocomposite. <a href="Manage-Parashar-
- 87. Avinash Parashar, Pierre Mertiny, (2012) Multiscale model to investigate the effect of graphene on the fracture characteristics of graphene/polymer nanocomposite, Nanoscale research letters, 7, 595. (In Oct 2012 was listed among the top 20 downloaded papers)
- 88. **Avinash Parashar**, Pierre Mertiny, (2012) Effect of FRP pipe scaling on its adhesive bonding strength. **Journal of adhesion**, 88, 866-880.
- 89. **Avinash Parashar**, Pierre Mertiny, (2012) Study of mode I fracture of graphene sheets using atomistic based finite element modeling and virtual crack closure technique. **International journal of fracture**, 176,119-126.
- 90. **Avinash Parashar**, Pierre Mertiny, **(2012)** Adhesively bonded composite tubular joints: Review. **International journal of adhesion and adhesives**, 38, 58-68. **(In Oct 2012 was listed among the top 5 downloaded papers)**
- 91. Jasjit Singh Mann, **Avinash Parashar**, Ankur Shah, N.R.Sivakumar, **(2010)** Numerical and experimental analysis of nanosecond pulsed laser drilling with dual frequency. **International journal of abrasion technology**, 3, 141-156.
- 92. Ankur Shah, **Avinash Parashar**, Jasjit Singh Mann, N.R. Sivakumar, (**2009**) Interference assisted laser induced forward transfer for structured patterning. **The open applied physics**, 2, 49-52.
- 93. **Avinash Parashar**, Jasjit Singh Mann, Ankur Shah, N.R.Sivakumar, (**2009**) Numerical and experimental study of interference based micromachining of stainless steel. **Journal** of laser micro/nano engineering, 4, 124-127.
- 94. Jasjit Singh Mann, **Avinash Parashar**, Ankur Shah, N.R.Sivakumar, (**2009**) Optical setup with high power transmission for creating gratings at the focusing length. **Journal of modern optics**, 56, 1341-1347.

- 95. **Avinash Parashar**, Jasjit Singh Mann, Ankur Shah, N.R.Sivakumar, (**2009**) Interference based marking method for toric contact eye lens inserts. **Journal of modern optics**, 56, 855-862.
- 96. Avinash Parashar, Ankur Shah, Muthukumaran Packirisamy, N.R.Sivakumar, (2007) Three cavity tunable MEMS Fabry Perot interferometer. <u>Journal of sensors</u>, 7, 3071-3083. (Published in special issue on modeling, testing and reliability issues in MEMS engineering)

Book Chapter

- 97. Ankur Chaurasia, SandeepKumar Singh, Akarsh Verma, Avinash Parashar. (2024) Effect of reinforcing nanomaterials on the glass transient temperature and viscoelastic properties of polymer composites. *In book: Dynamic Mechanical and Creep-Recovery Behavior of Polymer-Based Composites*.
- 98. Akarsh Verma, **Avinash Parashar** and Adri C.T. van Duin. (2022) "Graphene-reinforced polymeric membranes for water desalination and gas separation/barrier applications" in the book titled "Innovations in Graphene-based Polymer Composites" published by the *Elsevier (Woodhead Publishing)*, Chapter 6, pp.133-165.
- 99. Akarsh Verma, **Avinash Parashar**, Sandeep Kumar Singh, Naman Jain, Sanjay MR and Suchart Siengchin. (2020) "Modeling and Simulation in Polymer Coatings" in the book titled "Polymer Coatings: Technologies and Applications" published by the *Taylor & Francis Group (CRC Press)*, *Boca Raton*, Chapter 16, pp.309-324.
- 100. Akarsh Verma, Naman Jain, **Avinash Parashar**, Amit Gaur, Sanjay MR and Suchart Siengchin. (2020) "Lifecycle Assessment of Thermoplastic and Thermosetting Bamboo Composites" in the book titled "Bamboo Fiber Composites Processing, Properties and Applications" published by the *Springer Nature*, *Singapore*, Chapter 13, pp.235-246.
- 101. Akarsh Verma, Naman Jain, Avinash Parashar, VK Singh, Sanjay MR and Suchart Siengchin. (2020) "Lightweight Graphene Composite materials" in the book titled "Lightweight Polymer Composite Structures: Design and Manufacturing Techniques" published by the *Taylor & Francis Group (CRC Press)*, *Boca Raton*, Chapter 1, pp.1-20.
- 102. Akarsh Verma, Naman Jain, **Avinash Parashar**, VK Singh, Sanjay MR and Suchart Siengchin. (2020) "Design and Modeling of Lightweight Polymer Composite Structures" in the book titled "Lightweight Polymer Composite Structures: Design and Manufacturing Techniques" published by the *Taylor & Francis Group (CRC Press)*, *Boca Raton*, Chapter 7, pp.193-224.

- 103. Akarsh Verma and **Avinash Parashar**. (2020) "Characterization of 2D Nanomaterials for Energy Storage" in the book titled "Recent Advances in Theoretical, Applied, Computational and Experimental Mechanics" published by the *Springer Nature*, *Singapore*, Chapter 18, pp.221-226.
- 104.Akarsh Verma, **Avinash Parashar**, Naman Jain, VK Singh, Sanjay MR and Suchart Siengchin. (2020) "Surface Modification Techniques for the Preparation of Different Novel Biofibers for Composites" in the book titled "Biofibers and Biopolymers for Biocomposites: Synthesis, Characterization and Properties" published by the *Springer Nature*, *Switzerland*, Chapter 1, pp.1-34.
- 105. Bharat Bhushan Sharma, **Avinash Parashar** (2021) Effect of defects and functionalization on the mechanical and fracture properties of 2D nanomaterials. In book: Fundamentals and Properties of Multifunctional Nanomaterials. Elsevier.
- 106. Chaurasia A, Singh S K, **Parashar A** (2022) Reinforcing potential of 2D nanofiller in polyethylene: a molecular dynamics approach Forcefields for Atomistic-Scale Simulations:Materials and Applications (Springer, Singapore).
- 107. Chaurasia A, Singh S K, Kumar P, **Parashar A** (2023), Strain Rate Dependent Characterization of Soft Materials: A Review, Proceeding Book of the ICRAM 2022, ISBN number: 978-93-91355-76-0.

Conference proceeding

- 1. Kaushlendra Kumar, S. P. Harsha, **Avinash Parashar**, *Diffusion of gases in high-density polyethylene: An atomistic simulation*. Proceedings of the XVIII Vibration Engineering & Technology of Machinery Conference (2023).
- Sanchit Tamrakar, Vikash Tiwari Avinash Parashar, FEM based Simulation for Studying High Strain Rate Deformation in Nano-composites. Proceedings of the XVIII Vibration Engineering & Technology of Machinery Conference (2023).
- 3. Raju Kumar, Ankur Chaurasia, Abhishek Tewari, **Avinash Parashar**, *Deformation governing mechanism of PEGDA hydrogel subjected to tensile deformation using Molecular Dynamics*. Proceedings of the XVIII Vibration Engineering & Technology of Machinery Conference (2023).
- Ankur Chaurasia, Raju Kumar, Avinash Parashar, Compressive behavior of BNNS/PE nanocomposites: A Molecular Dynamics approach. Proceedings of the XVIII Vibration Engineering & Technology of Machinery Conference (2023).
- 5. **Avinash Parashar**, Ankur Chaurasia, *Mechanical behaviour of h-BN reinforced PE based nanocomposites with modified interface*. FEMS EUROMAT, September 3-7, 2023 Frankfurt am Main.

- 6. Saurabh S Sharma, **Avinash Parashar**, *Molecular dynamics study of effects of helium configurations on the crack tip performance in nickel*. FEMS EUROMAT, September 3-7, 2023 Frankfurt am Main.
- 7. Sandeep Kumar Singh, Ankur Chaurasia, **Avinash Parashar**, *Atomistic insights to study the effects of nano-voids on compression behaviour of single and bicrystal nickel*, The 13th International Symposium on Plasticity and Impact Mechanics (IMPLAST 2022), IIT Madras.
- 8. Sandeep Kumar Singh, Ankur Chaurasia, **Avinash Parashar**, *Atomistic simulations to study shock and ultrashort pulse response of high entropy alloy*, Conference on Advancement and Futuristic Trends in Mechanical and Materials Engineering (AFTMME, IIT Ropar, 2021)
- 9. Sandeep Kumar Singh, **Avinash Parashar**, *Molecular dynamics simulations to explore cracktip behaviour in High entropy alloys*, 2021 MRS Fall Meeting and Exhibit (MRS, Boston, USA)
- Ankur Chaurasia, Sandeep Kumar Singh, Makhan Singh, Avinash Parashar, Shock compression of multilayered BNNS reinforced PE nanocomposites, The 13th International Symposium on Plasticity and Impact Mechanics (IMPLAST 2022), IIT Madras.
- 11. Ankur Chaurasia, Sandeep Kumar Singh, **Avinash Parashar**, *Atomistic scale insight to investigate the strain rate effect on mechanical response of boron nitride nanosheet reinforced nanocomposites*, Conference on Advancement and Futuristic Trends in Mechanical and Materials Engineering (AFTMME, IIT Ropar, 2021)
- 12. Ankur Chaurasia, **Avinash Parashar**, Rahul S Mulik. *Effect of aspect ratio and orientation of rectangular h-BN nanosheets on tensile strength of h-BN/PE nanocomposites- A molecular dynamics study*.6th International Conference on Advanced Nanomaterials and Nanotechnology (ICANN2019), IIT Guwahati.
- 13. Ankur Chaurasia, **Avinash Parashar**, Rahul S Mulik, *Enhancement in mechanical properties of polyethylene using h-BN nanofiller*. 43rd National Systems Conference on Innovative and Emerging Trends in Engineering Systems (NSC 2019), IIT Roorkee.
- 14. Bharat B Sharma, **Avinash Parashar**, *Fracture toughness enhancement of boron nitride nanosheets via crack edge passivation using various radicals*. 43rd National Systems Conference on Innovative and Emerging Trends in Engineering Systems (NSC 2019), IIT Roorkee.
- 15. Bharat B Sharma, **Avinash Parashar**, *Thermal properties of bicrystalline and polycrystalline graphene: A review*. 7th International Congress on Computational Mechanics and Simulation (ICCMS 2019), IIT Mandi.

- 16. Bharat B Sharma, **Avinash Parashar**, *Structural stability of dry and water submerged h-BN nanosheets*. 6th International Conference on Advanced Nanomaterials and Nanotechnology (ICANN2019), IIT Guwahati.
- Bharat Bhushan Sharma, Avinash Parashar, Enhanced Mechanical Properties of h-BN Nanosheets via Edge Passivation Using Various Radicals. International Conference on Innovative Engineering Design (ICoIED 2020), IIT Roorkee, NIT Uttarakhand and IEI Dehradun.
- 18. Divya Singh, **Avinash Parashar**, A comparison between ∑3 asymmetrical tilt grain boundary energies in Niobium obtained analytically and through molecular dynamics based simulations. ICMSET, 2019, Singapore.
- 19. Akarsh Verma, Avinash Parashar, "Topology Influence of Hydroxyl and Epoxide Functional Groups on the Mechanical and Fracture Behavior of Graphene Domain", Poster Presentation at 2020 MRS Spring/Fall Meeting & Exhibit (MRS), organized by the Materials Research Society (MRS), Boston, USA, November 27 - December 4, 2020.
- 20. Akarsh Verma, **Avinash Parashar** "Anomalous Characteristics of Functionalized Grain Boundaries in Graphene—A Nano-Mechanics Study", Poster Presentation at 2020 MRS Spring/Fall Meeting & Exhibit (MRS), organized by the Materials Research Society (MRS), Boston, USA, November 27 December 4, 2020.
- 21. Akarsh Verma, **Avinash Parashar**, M. Packirisamy, "Fracture characterization of polycrystalline graphene for energy storage", Poster Presentation at International Meeting on Energy Storage Devices (IMESD), organized by IIT Roorkee, India, December 10-12, 2018.
- 22. Akarsh Verma, **Avinash Parashar**, M. Packirisamy, "Role of chemical species in fracture mechanics of graphene nanolayer", Oral Presentation at International Multi-Conference on Computing, Communication, Electrical & Nanotechnology (I2CN-2K18), organized by Mangalam College of Engineering, Kerala, India, April 26-27, 2018.
- 23. Akarsh Verma, **Avinash Parashar**, M. Packirisamy, "Molecular mechanics of oxidation on strained 2D nanomaterial: A ReaxFF study", Oral Presentation at International Conference on Advances in Construction Materials and Structures (ACMS), organized by IIT Roorkee, India, March 7-8, 2018.
- 24. Akarsh Verma, **Avinash Parashar**, "Strength and fracture investigation of polycrystalline graphene with tilt grain boundaries", Oral Presentation at International Conference on Advances in Construction Materials and Structures (ACMS), organized by IIT Roorkee, India, March 7-8, 2018.
- 25. Akarsh Verma, **Avinash Parashar**, "Characterization of 2D Nanomaterials for Energy Storage", Oral Presentation at 7th International Conference on Theoretical, Applied, Computational and Experimental Mechanics (ICTACEM), organized by IIT Kharagpur, India, December 28-30, 2017.
- 26. Akarsh Verma, **Avinash Parashar**, "Effect of hydrogen functionalisation on 2D nanomaterials", Oral Presentation at 7th International Conference on Theoretical, Applied, Computational and Experimental Mechanics (ICTACEM), organized by IIT Kharagpur, India, December 28-30, 2017.
- 27. Akarsh Verma, **Avinash Parashar**, "Mechanics of plasticity in epoxide functionalized nanographene", Oral Presentation at International Conference on Advances in

- Materials & Processing: Challenges & Opportunities (AMPCO), organized by IIT Roorkee, India, November 30 December 2, 2017.
- 28. Akarsh Verma, **Avinash Parashar**, "Molecular insights on 2D nanomaterials for hydrogen storage", Oral Presentation at International Conference on Advances in Materials & Processing: Challenges & Opportunities (AMPCO), organized by IIT Roorkee, India, November 30 December 2, 2017.
- 29. Akarsh Verma, **Avinash Parashar**, "Effect of hydrogenation on mechanical and fracture properties of graphene", Oral Presentation at 3rd Indian Conference on Applied Mechanics (INCAM), organized by Motilal Nehru National Institute of Technology (MNNIT) Allahabad and Indian Society for Applied Mechanics (ISAM), India, July 5-7, 2017. (Presenter)
- 30. Divya Singh, **Avinash Parashar**, Estimation of vacancy migration energy and mean energy path in a single crystal hcp zirconium by MD simulations. AMEST, 2019, NEHU, Shillong.
- 31. Saurabh S Sharma, **Avinash Parashar**, Effect of water on structural and fracture behavior of graphene nanosheet. ICANM 2019, Montreal Aug 12-14, 2019.
- 32. Divya Singh, **Avinash Parashar**, Effect of symmetrical tilt grain boundary on dislocation nucleation and growth in Niobium bi-crystal. International Multi-Conference on Computing, Communication, Electrical & Nanotechnology, 2018, Mangalam College of Engineering, Kottayam, Kerala. (Published in Materials Today: Proceedings, 11 (3), 925-928.
- 33. Divya Singh, **Avinash Parashar**, Effect of crack on tensile strength of a bi-crystal Zr- a MD based evaluation, 2018, ICPCM, NIT Rourkela. (accepted in Trans Tech Publications periodical)
- 34. Divya Singh, **Avinash Parashar**, Molecular dynamics based simulations to study grain boundaries in niobium. 2017, INCAM 2017, MNNIT Allahabad.
- 35. Rajasekaran G, **Avinash Parashar**, Effect of topological defects mechanical properties of graphene sheets: a molecular dynamics study. 2017; Materials today proceedings.
- 36. **Avinash Parashar**, Pierre Mertiny. Impact of scaling on fracture strength of adhesively bonded fibre reinforced polymer piping. Procedia Engineering. 2011; 10: 455-459.
- 37. **Avinash Parashar**, Pierre Mertiny. Challenges in joining thermoset composite piping. International pipeline conference.2010 Calgary -IPC2010-31297.
- 38. Pierre Mertiny, Mohamed T. Bashar, **Avinash Parashar**, Kulwinder Juss. Technological advances for improved performance and operation of fiber reinforced polymer piping. ASME Pressure Vessels & Piping Conference 2010
- 39. **Avinash Parashar**, Ankur Shah, N.R.Sivakumar. Laser micromachining for biomedical applications. International Conference LPM.2008 Quebec.