

Publications 2012 — 2019

Total number submitted, published, or accepted: 344

* Joint publications between CMEDE consortium and ARL researchers

Ceramics

2018

- 1 Cereceda Senas, D. Kats, D. Daphalapurkar, N. and Brady, L. (2018) "A micro-mechanical modeling approach for dynamic fragmentation in brittle multi-phase materials." *International Journal of Solids and Structures*, 134, 116-129. doi: <https://doi.org/10.1016/j.ijsolstr.2017.10.026>.
- 2 Cil, M. B. Hurley, R. and Brady, L. (2018) "A breakage model for granular materials considering the impacts of breakage and relative density on critical state." *International Journal for Numerical and Analytical Methods in Geomechanics*, Submitted.
- 3 Hwang, C. Ornek, M. Reddy, M. Domnich, V. Miller, S. Hemker, K. and Haber, R. (2018) "Effect of synthesis conditions of BCNO on the formation and structural ordering of BN at 1200 °C and 1 GPa." *Diamond and Related Materials*, 87, 156-162. doi: <https://doi.org/10.1016/j.diamond.2018.06.002>.
- 4 Hwang, C. Yang, Q. Xiang, S. Domnich, V. Khan, A. Xie, K. Hemker, K. and Haber, R. (2018) "Fabrication of Dense B4C-Preceramic Polymer Derived SiC Composite." *Journal of European Ceramic Society*, Submitted.
- 5 *Hwang, C. DiPietro, S. Xie, K. Yang, Q. Celik, A. M. Khan, A. Domnich, V. Walck, S. Hemker, K. and Haber, R. (2018) "Incorporating TiB₂ into B4C through sputter deposition and hot pressing." *Journal of the American Ceramic Society*, Submitted.
- 6 *Khan, A. Etzold, A. Yang, X. Domnich, V. Xie, K. Hwang, C. Behler, K. Chen, M. An, Q. LaSalvia, J. Hemker, K. Goddard, W. and Haber, R. (2018) "Locating Si atoms in Si-doped boron carbide: A route to understand amorphization mitigation mechanism." *Acta Materialia*, 187, 106-113. doi: <https://doi.org/10.1016/j.actamat.2018.07.021>.

2017

- 1 An, Q. and Goddard, W. (2017) "Ductility in Crystalline Boron Subphosphide (B₁₂P₂) for Large Strain Indentation." *J. Phys. Chem. C*, 121(30), 16644-16649. doi: <https://doi.org/10.1021/acs.jpcc.7b05429>.

- 2 An, Q. and Goddard, W. (2017) "Improved Ductility of B₁₂ Icosahedra-based Superhard Materials through Icosahedral Slip." *J. Phys. Chem. C*, 121(21), 11831-11838. doi: <https://doi.org/10.1021/acs.jpcc.7b01761>.
- 3 An, Q. Reddy, M. Xie, K. Hemker, K. and Goddard, W. (2017) "Erratum: New Ground-State Crystal Structure of Elemental Boron [Phys. Rev. Lett. 117, 085501 (2016)]." *Phys. Rev. Lett.*, 118(15), 59902-59902. doi: <http://doi.org/10.1103/PhysRevLett.118.159902>.
- 4 An, Q. and Goddard, W. (2017) "Nanotwins soften boron-rich boron carbide (B₁₃C₂)."*Applied Physics Letters*, 110(11), 11902-11902. doi: <http://dx.doi.org/10.1063/1.4978644>.
- 5 An, Q. Reddy, M. Xie, K. Hemker, K. and Goddard, W. (2017) "An et al. Reply." *Phys. Rev. Lett.*, 118(8), 89602-89602. doi: <https://doi.org/10.1103/PhysRevLett.118.089602>.
- 6 Cereceda Senas, D. Brady, L. and Daphalapurkar, N. (2017) "Modeling dynamic fragmentation of heterogeneous brittle materials." *International Journal of Impact Engineering*, 99, 85-101. doi: <https://doi.org/10.1016/j.ijimpeng.2016.09.012>.
- 7 Farbaniec, L. Hogan, J. Xie, K. Shaeffer, M. Hemker, K. and Ramesh, K. (2017) "Damage evolution of hot-pressed boron carbide under confined dynamic compression." *International Journal of Impact Engineering*, 99, 75-84. doi: <https://doi.org/10.1016/j.ijimpeng.2016.09.008>.
- 8 Hernández-Rivera, E. Coleman, S. and Tschopp, M. (2017) "Using Similarity Metrics to Quantify Differences in High-Throughput Data Sets: Application to X-ray Diffraction Patterns." *ACS Combinatorial Science*, 19(1), 25-36. doi: <http://dx.doi.org/10.1021/acscombsci.6b00142>.
- 9 *Hogan, J. Farbaniec, L. Mallick, D. Domnich, V. Kuwelkar, K. Sano, T. McCauley, J. W. and Ramesh, K. (2017) "Fragmentation of an advanced ceramic under ballistic impact: Mechanisms and microstructure." *International*

- Journal of Impact Engineering, 102, 47-54. doi: <https://doi.org/10.1016/j.ijimpeng.2016.12.008>.
- 10 Khan, A. Domnich, V. and Haber, R. (2017) "Boron carbide based ceramics: Problems and possible solutions." ACerS Bulletin, 96(6), 30-35. doi: <http://ceramics.org/publications-and-resources/the-bulletin/bulletin-archives>.
 - 11 Ramesh, K. Stickle, A. and Kimberley, J. (2017) "Rocks, Shocks and Asteroids, and Some Interesting Research Directions in Mechanics." Experimental Mechanics, 57(8), 1149-1159. doi: <http://dx.doi.org/10.1007/s11340-017-0324-9>.
 - 12 Swab, J. Meredith, C. Casem, D. and Gamble, W. (2017) "Static and dynamic compression strength of hot-pressed boron carbide using a dumbbell-shaped specimen." Journal of Materials Science, 52(17), 10073-10084. doi: <http://dx.doi.org/10.1007/s10853-017-1210-7>.
 - 13 Taylor, D. (2017) "Convergence acceleration of molecular dynamics methods for shocked materials using velocity scaling." Molecular Physics, 115(5), 603-617. doi: <http://dx.doi.org/10.1080/00268976.2016.1241905>.
 - 14 Taylor, D. (2017) "Molecular dynamics simulation of the Hugoniot states of boron suboxide." Materials Letters, 188, 331-333. doi: <https://doi.org/10.1016/j.matlet.2016.11.118>.
 - 15 Toksoy, M. Rafaniello, B. Xie, K. Ma, L. Hemker, K. and Haber, R. (2017) "Densification and characterization of rapid carbothermal synthesized boron carbide." International Journal of Applied Ceramic Technology, 14(3), 443-453. doi: <http://dx.doi.org/10.1111/ijac.12654>.
 - 16 *Tonge, A. and Ramesh, K. (2017) "Corrigendum to: Multi-scale defect interactions in high-rate brittle material failure. Part I: Model formulation and application to AION." Journal of the Mechanics and Physics of Solids, 106, 313-314. doi: <https://doi.org/10.1016/j.jmps.2017.05.020>.
 - 17 Xie, K. Domnich, V. Farbaniec, L. Chen, B. Kuwelkar, K. Ma, L. McCauley, J. W. Haber, R. Ramesh, K. and Chen, M. (2017) "Microstructural Characterization of Boron-rich Boron Carbide." Acta Materialia, 136, 202-214. doi: <http://dx.doi.org/10.1016/j.actamat.2017.06.063>.
- 2016**
- 1 An, Q. Reddy, M. Xie, K. Hemker, K. and Goddard, W. (2016) "New Ground-State Crystal Structure of Elemental Boron." Phys. Rev. Lett., 117(8), 85501-85501. doi: <https://doi.org/10.1103/PhysRevLett.117.085501>.
 - 2 An, Q. Reddy, M. Qian, J. Hemker, K. Chen, M. and Goddard, W. (2016) "Nucleation of amorphous shear bands at nanotwins in boron suboxide." Nature Communications, 7, 1-7. doi: <https://doi.org/10.1038/ncomms11001>.
 - 3 An, Q. Samwer, K. Demetrou, M. Floyd, M. Duggins, D. Johnson, W. and Goddard, W. (2016) "How the toughness in metallic glasses depends on topological and chemical heterogeneity." Proceedings of the National Academy of Sciences, 113(26), 7053-7058. doi: <http://dx.doi.org/10.1073/pnas.1607506113>.
 - 4 An, Q. Reddy, M. Dong, H. Chen, M. Oganov, A. and Goddard, W. (2016) "Nanotwinned Boron Suboxide (B₆O): New Ground State of B₆O." Nano Letters, 16(7), 4236-4242. doi: <http://dx.doi.org/10.1021/acs.nanolett.6b01204>.
 - 5 An, Q. Goddard, W. Xie, K. Sim, G. Hemker, K. Munhollon, T. Toksoy, M. and Haber, R. (2016) "Superstrength through Nanotwinning." Nano Letters, 16(12), 7573-7579. doi: <http://pubs.acs.org/doi/abs/10.1021/acs.nanolett.6b03414>.
 - 6 Coleman, S. Hernandez, E. Behler, K. Synowczynski-Dunn, J. and Tschoop, M. (2016) "Challenges of Engineering Grain Boundaries in Boron-Based Armor Ceramics." JOM, 68(6), 1605-1615. doi: <http://dx.doi.org/10.1007/s11837-016-1856-7>.
 - 7 Farbaniec, L. Hogan, J. McCauley, J. W. and Ramesh, K. (2016) "Anisotropy of Mechanical Properties in a Hot-Pressed Boron Carbide." International Journal of Applied Ceramic Technology, 13(6), 1008-1016. doi: <http://dx.doi.org/10.1111/ijac.12585>.
 - 8 Gao, H. Etzold, A. Munhollon, T. Goddard, W. and Haber, R. (2016) "Processing factors influencing the free carbon contents in boron carbide powder by rapid carbothermal reduction." Diamond and Related Materials, 61, 14-20. doi: <https://doi.org/10.1016/j.diamond.2015.11.005>.
 - 9 *Hilton, C. McCauley, J. W. Swab, J. Shanholtz, E. and Chen, M. (2016) "Using Hardness Tests to Quantify Bulk Plasticity and Predict Transition Velocities in SiC Materials." International Journal of Applied Ceramic Technology, 10(1), 114-122. doi: <http://dx.doi.org/10.1111/j.1744-7402.2012.02817.x>.
 - 10 Hogan, J. Farbaniec, L. Daphalapurkar, N. and Ramesh, K. (2016) "On Compressive Brittle Fragmentation." Journal of the American Ceramic Society, 99(6), 2159-2169. doi:

- [https://doi.org/10.1111/jace.14171.](https://doi.org/10.1111/jace.14171)
- 11 *Hogan, J. Farbaniec, L. Sano, T. Shaeffer, M. and Ramesh, K. (2016) "The effects of defects on the uniaxial compressive strength and failure of an advanced ceramic." *Acta Materialia*, 102, 263-272. doi: <https://doi.org/10.1016/j.actamat.2015.09.028>.
 - 12 Huq, F. Brannon, R. and Brady, L. (2016) "An efficient binning scheme with application to statistical crack mechanics." *International Journal for Numerical Methods in Engineering*, 105(1), 33-62. doi: <http://dx.doi.org/10.1002/nme.4959>.
 - 13 Li, G. An, Q. Goddard, W. Hanus, R. Zhai, P. Zhang, Q. and Snyder, G. (2016) "Atomistic explanation of brittle failure of thermoelectric skutterudite CoSb 3." *Acta Materialia*, 103, 775-780. doi: <https://doi.org/10.1016/j.actamat.2015.11.021>.
 - 14 Liu, J. and Brady, L. (2016) "Effective anisotropic compliance relationships for wing-cracked brittle materials under compression." *International Journal of Solids and Structures*, 100, 151-168. doi: <http://dx.doi.org/10.1016/j.ijsolstr.2016.08.012>.
 - 15 Liu, J. and Brady, L. (2016) "Perturbation-based surrogate models for dynamic failure of brittle materials in a multiscale and probabilistic context." *International Journal for Multiscale Computational Engineering*, 14(3), 273-290. doi: <https://doi.org/10.1615/IntJMultCompEng.2016015857>.
 - 16 McDonald, J. and Satapathy, S. (2016) "Surface waves and their influence on cone cracking in brittle materials." *International Journal of Impact Engineering*, 93, 144-152. doi: <https://doi.org/10.1016/j.ijimpeng.2016.03.003>.
 - 17 *Reddy, M. Hwang, C. Ornek, M. Lavenstein, S. Goddard, W. Burgess, A. Haber, R. and Doherty, K. (2016) "Observations of nanocrystalline cubic boron nitride formed with plasma spraying." *Acta Materialia*, 116, 155-165. doi: <https://doi.org/10.1016/j.actamat.2016.06.038>.
 - 18 *Tonge, A. Ramesh, K. and Barnouin, O. (2016) "A model for impact-induced lineament formation and porosity growth on Eros." *Icarus*, 266, 76-87. doi: <https://doi.org/10.1016/j.icarus.2015.11.018>.
 - 19 *Tonge, A. and Ramesh, K. (2016) "Multi-scale defect interactions in high-rate brittle material failure. Part I: Model formulation and application to design of protection materials." *Journal of the Mechanics and Physics of Solids*, 86, 117-149. doi: <https://doi.org/10.1016/j.jmps.2015.10.007>.
 - 20 *Tonge, A. and Ramesh, K. (2016) "Multi-scale defect interactions in high-rate failure of brittle materials, Part II: Application to design of protection materials." *Journal of the Mechanics and Physics of Solids*, 86, 237-258. doi: <https://doi.org/10.1016/j.jmps.2015.10.006>.
 - 21 Xie, K. An, Q. Sato, T. Breen, A. Ringer, S. Goddard, W. Cairney, J. and Hemker, K. (2016) "Breaking the icosahedra in boron carbide." *Proceedings of the National Academy of Sciences*, 113(43), 12012-12016. doi: <https://doi.org/10.1073/pnas.1607980113>.
 - 22 *Xie, K. Kuwelkar, K. Haber, R. LaSalvia, J. and Doherty, K. (2016) "Microstructural Characterization of a Commercial Hot-Pressed Boron Carbide Armor Plate." *Journal of the American Ceramic Society*, 99(8), 2834-2841. doi: <http://dx.doi.org/10.1111/jace.14295>.
 - 23 *Zhao, S. Kad, B. Remington, B. LaSalvia, J. Wehrenberg, C. Behler, K. and Meyers, M. (2016) "Directional amorphization of boron carbide subjected to laser shock compression." *Proceedings of the National Academy of Sciences*, 113(43), 12088-12093. doi: <http://dx.doi.org/10.1073/pnas.1604613113>.

2015

- 1 An, Q. and Goddard, W. (2015) "Atomistic Origin of Brittle Failure of Boron Carbide from Large-Scale Reactive Dynamics Simulations: Suggestions toward Improved Ductility." *Phys. Rev. Lett.*, 115, 5501-5506. doi: <http://dx.doi.org/10.1103/PhysRevLett.115.105501>.
- 2 Aydelotte, B. and Schuster, B. (2015) "Impact and Penetration of SiC: The Role of Rod Strength in the Transition from Dwell to Penetration." *Procedia Engineering*, 103, 19-26. doi: <https://doi.org/10.1016/j.proeng.2015.04.004>.
- 3 Beaudet, T. Smith, J. and Adams, J. (2015) "Surface energy and relaxation in boron carbide (101?1) from first principles." *Solid State Communications*, 219, 43-47. doi: <https://doi.org/10.1016/j.ssc.2015.06.021>.
- 4 Brady, L. Katcoff, Z. Mayercsik, N. and Kurtis, K. (2015) "Micromechanical Model and Associated Validation for Dynamic Failure of Brittle Materials Containing Pores and Slit-Like Flaws." *Journal of Engineering Mechanics*, 141(10), 5-10. doi: [https://doi.org/10.1061/\(ASCE\)EM.1943-7889.0000927#sthash.xrzgreal.dpuf](https://doi.org/10.1061/(ASCE)EM.1943-7889.0000927#sthash.xrzgreal.dpuf).

- 5 Cao, B. Daphalapurkar, N. and Ramesh, K. (2015) "Ultra-high-strain-rate shearing and deformation twinning in nanocrystalline aluminum." *Meccanica*, 50(2), 561-574. doi: <http://dx.doi.org/10.1007/s11012-014-9952-7>.
- 6 Casem, D. Dwivedi, A. Swab, J. Wright, J. and Mondal, A. (2015) "Analysis of a Three-Bar Kolsky Apparatus for High-Rate Three-Point Flexure." *Journal of Dynamic Behavior of Materials*, 1(1), 75-93. doi: <http://dx.doi.org/10.1007/s40870-014-0002-2>.
- 7 Clayton, J. and Tonge, A. (2015) "A nonlinear anisotropic elastic-inelastic constitutive model for polycrystalline ceramics and minerals with application to boron carbide." *International Journal of Solids and Structures*, 64, 191-207. doi: <https://doi.org/10.1016/j.ijsolstr.2015.03.024>.
- 8 Clayton, J. (2015) "Penetration resistance of armor ceramics: Dimensional analysis and property correlations." *International Journal of Impact Engineering*, 85, 124-131. doi: <https://doi.org/10.1016/j.ijimpeng.2015.06.025>.
- 9 Farbaniec, L. Hogan, J. and Ramesh, K. (2015) "Micromechanisms associated with the dynamic compressive failure of hot-pressed boron carbide." *Scripta Materialia*, 106, 52-56. doi: <http://dx.doi.org/10.1016/j.scriptamat.2015.05.004>.
- 10 Gao, Y. Rafaniello, B. Toksoy, M. Munhollon, T. and Haber, R. (2015) "Improvement of crystallization and particle size distribution of boric acid in the processing of a boron carbide precursor." *RSC Adv.*, 5(25), 19067-19073. doi: <http://dx.doi.org/10.1039/C4RA16279J>.
- 11 *Hogan, J. Farbaniec, L. Bratcher, M. and Ramesh, K. (2015) "The Effects of Microstructure and Confinement on the Compressive Fragmentation of an Advanced Ceramic." *Journal of the American Ceramic Society*, 98(3), 902-912. doi: <http://dx.doi.org/10.1111/jace.13353>.
- 12 Holland, C. Gamble, E. Zok, F. Deshp, V. and McMeeking, B. (2015) "Effect of design on the performance of steel-alumina bilayers and trilayers subject to ballistic impact." *Mechanics of Materials*, 91, 241-251. doi: <http://dx.doi.org/10.1016/j.mechmat.2015.05.002>.
- 13 Hu, G. Liu, J. Brady, L. and Ramesh, K. (2015) "A 3D mechanistic model for brittle materials containing evolving flaw distributions under dynamic multiaxial loading." *Journal of the Mechanics and Physics of Solids*, 78, 269-297. doi: <http://dx.doi.org/10.1016/j.jmps.2015.02.014>.
- 14 Klinsmann, M. Rosato, D. Kamlah, M. McMeeking, R. and McMeeking, B. (2015) "An assessment of the phase field formulation for crack growth." *Computer Methods in Applied Mechanics and Engineering*, 294, 313-330. doi: <http://dx.doi.org/10.1016/j.cma.2015.06.009>.
- 15 Ramesh, K. Hogan, J. Kimberley, J. and Stickle, A. (2015) "A review of mechanisms and models for dynamic failure, strength, and fragmentation." *Planetary and Space Science*, 107, 10-23. doi: <http://dx.doi.org/10.1016/j.pss.2014.11.010>.
- 16 Schuster, B. Aydelotte, B. Leavy, B. Satapathy, S. and Zellner, M. (2015) "Concurrent Velocimetry and Flash X-ray Characterization of Impact and Penetration in an Armor Ceramic." *Procedia Engineering*, 103, 553-560. doi: <https://doi.org/10.1016/j.proeng.2015.04.072>.
- 17 Tang, B. An, Q. and Goddard, W. (2015) "Improved Ductility of Boron Carbide by Microalloying with Boron Suboxide." *The Journal of Physical Chemistry C*, 119(43), 24649-24656. doi: <http://dx.doi.org/10.1021/acs.jpcc.5b08086>.
- 18 Taylor, D. (2015) "Shock Compression of Boron Carbide: A Quantum Mechanical Analysis." *Journal of the American Ceramic Society*, 98(10), 3308-3318. doi: <http://dx.doi.org/10.1111/jace.13711>.
- 19 *Tonge, A. Leavy, B. LaSalvia, J. Ramesh, K. and Brannon, R. (2015) "A Quantitative Approach to Comparing High Velocity Impact Experiments and Simulations Using XCT Data." *Procedia Engineering*, 103, 610-617. doi: <https://doi.org/10.1016/j.proeng.2015.04.079>.
- 20 Xie, K. An, Q. Toksoy, M. McCauley, J. W. Haber, R. Goddard, W. and Hemker, K. (2015) "Atomic-Level Understanding of "Asymmetric Twins" in Boron Carbide." *Phys. Rev. Lett.*, 115, 1-5. doi: <https://doi.org/10.1103/PhysRevLett.115.175501>.
- 21 Xie, K. Livi, K. McCauley, J. W. and Hemker, K. (2015) "Precipitation of AlN in a commercial hot-pressed boron carbide." *Scripta Materialia*, 101, 95-98. doi: <http://dx.doi.org/10.1016/j.scriptamat.2015.02.002>.

2014

- 1 An, Q. Goddard, W. and Chengcheng, T. (2014) "Atomistic Explanation of Shear-Induced Amorphous Band Formation in Boron Carbide." *Phys. Rev. Lett.*, 113, 95501-95501. doi: <https://link.aps.org/doi/10.1103/PhysRevLett.113.095501>

- 2 An, Q. Goddard, W. Xiao, H. and Cheng, T. (2014) "Deformation Induced Solid–Solid Phase Transitions in Gamma Boron." *Chemistry of Materials*, 26(14), 4289-4298. doi: <http://dx.doi.org/10.1021/cm5020114>.
- 3 *Batyrev, I. Taylor, D. Gazonas, G. and McCauley, J. W. (2014) "Density functional theory and evolution algorithm calculations of elastic properties of AION." *Journal of Applied Physics*, 115(2), 23505-23505. doi: <https://doi.org/10.1063/1.4859435>.
- 4 Daphalapurkar, N. Wilkerson, J. Wright, T. and Ramesh, K. (2014) "Kinetics of a fast moving twin boundary in nickel." *Acta Materialia*, 68, 82-92. doi: <https://doi.org/10.1016/j.actamat.2014.01.010>.
- 5 Katcoff, C. and Brady, L. (2014) "Modeling dynamic brittle behavior of materials with circular flaws or pores." *International Journal of Solids and Structures*, 51(3), 754-766. doi: <http://dx.doi.org/10.1016/j.ijsolstr.2013.11.004>.
- 6 Xie, K. Toksoy, M. Kuwelkar, K. Zhang, B. Krogstad, J. Haber, R. and Hemker, K. (2014) "Effect of Alumina on the Structure and Mechanical Properties of Spark Plasma Sintered Boron Carbide." *Journal of the American Ceramic Society*, 97(11), 3710-3718. doi: <http://dx.doi.org/10.1111/jace.13178>.
- 1 Clayton, J. Kraft, R. and Leavy, B. (2012) "Mesoscale modeling of nonlinear elasticity and fracture in ceramic polycrystals under dynamic shear and compression." *International Journal of Solids and Structures*, 49(18), 2686-2702. doi: <https://doi.org/10.1016/j.ijsolstr.2012.05.035>.
- 2 Clayton, J. (2012) "Towards a nonlinear elastic representation of finite compression and instability of boron carbide ceramic." *Philosophical Magazine*, 92(23), 2860-2893. doi: <http://dx.doi.org/10.1080/14786435.2012.682171>.
- 3 *Reddy, K. Guo, J. Shinoda, Y. Fujita, T. Hirata, A. Singh, J. McCauley, J. W. and Chen, M. (2012) "Enhanced mechanical properties of nanocrystalline boron carbide by nanoporosity and interface phases." *Nature Communications*, 1, 1052-1052. doi: <http://doi.org/10.1038/ncomm2047>
- 4 Swab, J. Wereszczak, A. Strong, K. Danna, D. LaSalvia, J. Ragan, M. and Ritt, P. (2012) "Knoop Hardness–Apparent Yield Stress Relationship in Ceramics." *International Journal of Applied Ceramic Technology*, 9(3), 650-655. doi: <http://dx.doi.org/10.1111/j.1744-7402.2011.02686.x>.
- 5 *Taylor, D. McCauley, J. W. and Wainwright, E. (2012) "The effects of stoichiometry on the mechanical properties of icosahedral boron carbide under loading." *Journal of Physics: Condensed Matter*, 24(50), 505-402. doi: <http://doi.org/10.1088/0953-8984/24/50/505402>.
- 6 *Tonge, A. Kimberley, J. and Ramesh, K. (2012) "The mechanism of compressive unloading failure in single crystal quartz and other brittle solids." *International Journal of Solids and Structures*, 49(26), 3923-3934. doi: <https://doi.org/10.1016/j.ijsolstr.2012.08.021>.
- 7 Wildman, R. and Gazonas, G. (2012) "A perfectly matched layer for peridynamics in two dimensions." *Journal of Mechanics of Materials and Structures*, 7(8), 765-781. doi: <http://dx.doi.org/10.2140/jomms.2012.7.765>.

2013

- 1 Clayton, J. (2013) "Mesoscale modeling of dynamic compression of boron carbide polycrystals." *Mechanics Research Communications*, 49, 57-64. doi: <https://doi.org/10.1016/j.mechrescom.2013.02.005>.
- 2 Kimberley, J. Ramesh, K. and Daphalapurkar, N. (2013) "A scaling law for the dynamic strength of brittle solids." *Acta Materialia*, 61(9), 3509-3521. doi: <https://doi.org/10.1016/j.actamat.2013.02.045>.
- 3 Szlufarska, I. Ramesh, K. and Warner, D. (2013) "Simulating Mechanical Behavior of Ceramics Under Extreme Conditions." *Annual Review of Materials Research*, 43(1), 131-156. doi: <https://doi.org/10.1146/annurev-matsci-071312-121714>.
- 4 *Tonge, A. Kimberley, J. and Ramesh, K. (2013) "A Consistent Scaling Framework for Simulating High Rate Brittle Failure Problems." *Procedia Engineering*, 58, 692-701. doi: <https://doi.org/10.1016/j.proeng.2013.05.080>.

2012

Composites

2018

- 1 Abu-Obaid, A. Ganesh, R. and Gillespie, J. (2018) "Investigation of Axial Compressive Behavior of Kevlar Fibers Using Dynamic Loop Test." *Textile Research Journal*, Submitted.

- 2 An, Q. Tamrakar, S. Gillespie, J. Rider, A. and Thostenson, E. (2018) "Tailored Glass Fiber Interphases via Electrophoretic Deposition of Carbon Nanotubes: Fiber and Interphase Characterization." *Composite Science and Technology*, doi: <https://doi.org/10.1016/j.compscitech.2018.01.003>. Accepted.
- 3 Bhaduri, A. He, Y. Brady, L. and Kirby, R. (2018) "Stochastic collocation approach with adaptive mesh refinement for parametric uncertainty analysis." *Journal of Computational Physics*, 371, 732-750. doi: <https://doi.org/10.1016/j.jcp.2018.06.003>.
- 4 Bhaduri, A. and Brady, L. (2018) "An efficient adaptive sparse grid collocation method through derivative estimation." *Probabilistic Engineering Mechanics*, 51, 11-22. doi: <https://doi.org/10.1016/j.probengmech.2017.11.002>.
- 5 Chowdhury, S. Wise, E. Ganesh, R. and Gillespie, J. (2018) "Effect of Surface Crack on the Mechanical Properties of Silica: A Molecular Dynamics Simulation Study." *Engineering Fracture Mechanics*, Submitted.
- 6 Chowdhury, S. and Gillespie, J. (2018) "A molecular dynamics study of the effects of hydrogen bonds on mechanical properties of Kevlar® crystal." *Computational Material Science*, 148(1), 286-300. doi: <http://doi.org/10.1016/j.commatsci.2018.02.055>.
- 7 Ganesh, R. Sockalingam, S. and Gillespie, J. (2018) "Dynamic effects of a single fiber break in unidirectional glass fiber-reinforced polymer composites: Effects of matrix plasticity." *Journal of Composite Materials*, 52(14), 1873-1886. doi: <http://doi.org/10.1177/0021998317737604>.
- 8 Haque, B. Ali, M. Tamrakar, S. Yen, C. O'Brien, D. and Gillespie, J. (2018) "Stochastic Micromechanical Modeling of Transverse Punch Shear Damage Behavior of Unidirectional Composites." *Journal of Composites Materials*, 1(1), 1-17. doi: <https://doi.org/10.1177/0021998318796174>.
- 9 *Haque, B. Z. Ali, M. Ganesh, R. Tamrakar, S. Gillespie, J. Yen, C. and O'Brien, D. (2018) "Stochastic micromechanical modeling of transverse punch shear damage behavior of unidirectional composites." *Journal of Composite Materials*, doi: <https://doi.org/10.1177/0021998318796174>.
- 10 Li, Z. and Ghosh, S. (2018) "Developing Space-Time Boundary Conditions for Composite RVEs at High Strain-Rates." *International Journal of Solids and Structures*, Submitted.
- 11 Meyer, C. Bonyi, E. Haque, B. O'Brien, D. Aslan, K. and Gillespie, J. (2018) "Ballistic Impact Experiments and Quantitative Assessments of Mesoscale Damage Modes in a Single-layer Woven Composite." *Dynamic Behavior of Materials*, 1, doi: <http://dx.doi.org/10.1007/978-3-319-95089-1>.
- 12 *Meyer, C. Haque, B. Z. O'Brien, D. Getinet, N. Yu, J. Bonyi, E. Aslan, K. and Gillespie, J. (2018) "Mesoscale Ballistic Damage Mechanics of a Single-Ply Woven Glass/Epoxy Composite." *International Journal of Impact Engineering*, 113(1), 118-131. doi: <https://doi.org/10.1016/j.ijimpeng.2017.11.005>.
- 13 *Meyer, C. Gillespie, J. Haque, B. Z. O'Brien, D. Yu, J. Aslan, K. Bonyi, E. and Getinet, N. (2018) "Assessment and Quantification of Ballistic Impact Damage of a Single-Layer Woven Fabric Composite." *International Journal of Damage Mechanics*, 1(1), 1-21. doi: <https://doi.org/10.1177/1056789518758153>.
- 14 Sockalingam, S. Thomas, F. Casem, D. Gillespie, J. and Weerasooriya, T. (2018) "Failure of Dyneema® SK76 single fiber under multiaxial transverse loading." *Textile Research Journal*, 1(1), 1-17. doi: <https://doi.org/10.1177/0040517518798653>.
- 15 Tamrakar, S. Ganesh, R. and Sockalingam, S. (2018) "Rate Dependent Mode II Traction Separation Law for S-2 Glass/Epoxy Interface Using a Microdroplet Test Method." *Composites Part A*, Submitted.
- 16 Tamrakar, S. Ganesh, R. Sockalingam, S. Haque, B. Z. and Gillespie, J. (2018) "Modeling strain rate dependent large deformation inelastic behavior of an epoxy resin." *Journal of Dynamic Behavior of Materials*, Submitted.
- 17 Tamrakar, S. Ganesh, R. Sockalingam, S. Haque, B. Z. and Gillespie, J. (2018) "Experimental Investigation of Strain Rate and Temperature Dependent Response of an Epoxy Resin Undergoing Large Deformation." *Journal of Dynamic Behavior of Materials*, 4(1), 114-128. doi: <https://doi.org/10.1007/s40870-018-0144-8>.
- 18 *Zhang, X. O'Brien, D. and Ghosh, S. (2018) "Parametrically Homogenized Continuum Damage Mechanics (PHCDM) Models for Composites from Micromechanical Analysis." *Computer Methods in Applied Mechanics and Engineering*, Accepted.

2017

- 1 *Chowdhury, S. Elder, R. Sirk, T. van Duin, A. and Gillespie, J. (2017) "Modeling of glycidoxypropyltrimethoxy silane compositions using molecular dynamics simulations." Computational Materials Science, 140, 82-88. doi: <http://dx.doi.org/10.1016/j.commatsci.2017.08.033>.
- 2 Chowdhury, S. and Gillespie, J. (2017) "Silica - silane coupling agent interphase properties using molecular dynamics simulations." Journal of Materials Science, 52, 12981-12988. doi: <http://link.springer.com/article/10.1007/s10853-017-1412-z>.
- 3 *Chu, J. Claus, B. Parab, N. O'Brien, D. Sun, T. Fezzaa, K. and Chen, W. (2017) "Visualization of dynamic fiber-matrix interfacial shear debonding." Journal of Materials Science, 1, 1-15. doi: <http://dx.doi.org/10.1007/s10853-017-1759-1>.
- 4 Ganesh, R. Sockalingam, S. Haque, B. Z. and Gillespie, J. (2017) "Dynamic effects of single fiber break in unidirectional glass fiber-reinforced composites." Journal of Composite Materials, 51(9), 1307-1320. doi: <http://dx.doi.org/10.1177/0021998316669218>.
- 5 Srikanth, A. Vergara, J. Palmese, G. and Abrams, C. (2017) "The effect of alkyl chain length on material properties of fatty-acid-functionalized amidoamine-epoxy systems." Journal, 89, 285-292. doi: <https://doi.org/10.1016/j.eurpolymj.2017.01.037>.
- 6 Tamrakar, S. Sockalingam, S. and Gillespie, J. (2017) "Determination of Mode II traction separation law for S-2 glass/epoxy interface under different loading rates using a microdroplet test method." Composites Part A, Submitted.
- 7 Tamrakar, S. Ganesh, R. Sockalingam, S. Haque, B. Z. and Gillespie, J. (2017) "Thermo-mechanical response of epoxy resin at different rates of loading." Materials and Design, Submitted.
- 8 Yang, J. Srikanth, A. Jang, C. and Abrams, C. (2017) "Relationships between molecular structure and thermomechanical properties of bio-based thermosetting polymers." Journal of Polymer Science Part B: Polymer Physics, 55(3), 285-292. doi: <http://dx.doi.org/10.1002/polb.24270>.
- 9 Yeager, M. Simacek, P. and Advani, S. (2017) "Role of fiber distribution and air evacuation time on capillary driven flow into fiber tows." Composites Part A: Applied Science and Manufacturing, 93, 144-152. doi: <https://doi.org/10.1016/j.compositesa.2016.11.016>.
- ## 2016
- 1 *Advani, S. Reddy, M. Xie, K. Doherty, K. and Goddard, W. (2016) "New Ground-State Crystal Structure of Elemental Boron." Phys. Rev. Lett., 117, 85501-85501. doi: <https://doi.org/10.1103/PhysRevLett.117.085501>.
 - 2 Bain, E. Knorr, D. Richardson, A. Masser, K. Yu, J. and Lenhart, J. (2016) "Failure processes governing high-rate impact resistance of epoxy resins filled with core-shell rubber nanoparticles." Journal of Materials Science, 51(5), 2347-2370. doi: <http://dx.doi.org/10.1007/s10853-015-9544-5>.
 - 3 Chen, W. (2016) "Experimental Methods for Characterizing Dynamic Response of Soft Materials." Journal of Dynamic Behavior of Materials, 2(1), 2-14. doi: <https://link.springer.com/article/10.1007%2Fs40870-016-0047-5>.
 - 4 Chowdhury, S. Haque, B. Z. and Gillespie, J. (2016) "Molecular dynamics simulations of the structure and mechanical properties of silica glass using ReaxFF." Journal of Materials Science, 51(22), 10139-10159. doi: <https://link.springer.com/article/10.1007/s10853-016-0242-8>.
 - 5 Grujicic, M. Ramaswami, S. Snipes, J. Avuthu, V. Yen, C. and Cheeseman, B. (2016) "Application of the materials-by-design approach to armor-grade polymer-matrix composites for enhancement of ballistic-penetration resistance." International Journal of Structural Integrity, 7(1), 142-174. doi: <http://dx.doi.org/10.1108/IJSI-02-2015-0005>.
 - 6 *Guo, S. Casem, D. Hudspeth, M. Farbaniec, L. Sun, J. and Chen, W. (2016) "Transverse compression of two high-performance ballistic fibers." Textile Research Journal, 86(5), 502-511. doi: <http://dx.doi.org/10.1177/0040517515592814>.
 - 7 Jang, C. and Abrams, C. (2016) "Thermal and mechanical properties of thermosetting polymers using coarse-grained simulation." The European Physical Journal Special Topics, 225(8), 1775-1783. doi: <https://link.springer.com/article/10.1140/epjst/e2016-60143-0>.
 - 8 Jang, C. Sharifi, M. Palmese, G. and Abrams, C. (2016) "Toughness enhancement of thermosetting polymers using a novel partially reacted substructure curing protocol: A combined molecular simulation and experimental study." Polymer, 90, 249-255. doi:

- [https://doi.org/10.1016/j.polymer.2016.03.023.](https://doi.org/10.1016/j.polymer.2016.03.023)
- 9 Levine, S. Nie, Y. and Chen, W. (2016) "Dynamic Transverse Debonding of a Single Fiber." *Journal of Dynamic Behavior of Materials*, 2(4), 521-531. doi: <https://link.springer.com/article/10.1007/s40870-016-0086-y>.
 - 10 *Li, Z. Ghosh, S. Getinet, N. and O'Brien, D. (2016) "Micromechanical modeling and characterization of damage evolution in glass fiber epoxy matrix composites." *Mechanics of Materials*, 99, 37-52. doi: <https://doi.org/10.1016/j.mechmat.2016.05.006>.
 - 11 Masser, K. Bain, E. Beyer, F. Savage, A. Yu, J. and Lenhart, J. (2016) "Influence of nano-scale morphology on impact toughness of epoxy blends." *Polymer*, 103, 337-346. doi: <https://doi.org/10.1016/j.polymer.2016.09.076>.
 - 12 Misumi, J. Ganesh, R. Sockalingam, S. and Gillespie, J. (2016) "Experimental characterization of tensile properties of epoxy resin by using micro-fiber specimens." *Journal of Reinforced Plastics and Composites*, 35(24), 1792-1801. doi: <http://dx.doi.org/10.1177/0731684416669248>.
 - 13 Obaid, A. Yarlagadda, S. and Gillespie, J. (2016) "Combined effects of kink bands and hygrothermal conditioning on tensile strength of polyarylate liquid crystal co-polymer and aramid fibers." *Journal of Composite Materials*, 50(3), 339-350. doi: <http://dx.doi.org/10.1177/0021998315574754>.
 - 14 Sun, J. Hudspeth, M. and Chen, W. (2016) "Biaxial shear/tension failure behavior of Spectra single fibers." *Composites Part A: Applied Science and Manufacturing*, 88, 286-294. doi: <https://doi.org/10.1016/j.compositesa.2016.06.009>.
 - 15 Tamrakar, S. Haque, B. Z. and Gillespie, J. (2016) "High rate test method for fiber-matrix interface characterization." *Polymer Testing*, 52, 174-183. doi: <http://dx.doi.org/10.1016/j.polymertesting.2016.04.016>.
 - 16 Tamrakar, S. An, Q. Thostenson, E. Rider, A. and Gillespie, J. (2016) "Tailoring Interfacial Properties by Controlling Carbon Nanotube Coating Thickness on Glass Fibers Using Electrophoretic Deposition." *ACS Applied Materials & Interfaces*, 8(2), 1501-1510. doi: <http://dx.doi.org/10.1021/acsami.5b10903>.
 - 17 Yeager, M. Hwang, W. and Advani, S. (2016) "Prediction of capillary pressure for resin flow between fibers." *Composites Science and Technology*, 126, 130-138. doi: <https://doi.org/10.1016/j.compscitech.2016.02.014>.

2015

- 1 Elder, R. Andzelm, J. and Sirk, T. (2015) "A molecular simulation study of the glass transition of cross-linked poly(dicyclopentadiene) networks." *Chemical Physics Letters*, 637, 103-109. doi: <https://doi.org/10.1016/j.cplett.2015.07.058>.
- 2 *Gao, H. Gillespie, J. Jensen, R. Li, W. Haque, B. Z. and McKnight, S. (2015) "Effect of fiber surface texture on the mechanical properties of glass fiber reinforced epoxy composite." *Composites Part A: Applied Science and Manufacturing*, 74, 10-17. doi: <https://doi.org/10.1016/j.compositesa.2015.03.023>.
- 3 Ghosh, S. (2015) "Foundational aspects of a multi-scale modeling framework for composite materials." *Integrating Materials and Manufacturing Innovation*, 4(9), 1-28. doi: <http://dx.doi.org/10.1186/s40192-015-0036-x>.
- 4 Haque, B. Z. and Gillespie, J. (2015) "A new penetration equation for ballistic limit analysis." *Journal of Thermoplastic Composite Materials*, 28(7), 950-972. doi: <http://dx.doi.org/10.1177/0892705713495430>.
- 5 Haque, B. Z. and Gillespie, J. (2015) "Penetration and Perforation of Composite Structures." *Mechanical Engineering Research Journal*, 9, 37-42. doi: <http://www.cuet.ac.bd/merj/files/MERJ-Vol-9,%20202013,%20page%2037-42.pdf>.
- 6 Hudspeth, M. Claus, B. Parab, N. Lim, B. Sun, T. Fezza, K. and Chen, W. (2015) "In Situ Visual Observation of Fracture Processes in Several High-Performance Fibers." *Journal of Dynamic Behavior of Materials*, 1(1), 55-64. doi: <http://dx.doi.org/10.1007/s40870-015-0009-3>.
- 7 *Jang, C. Holmquist, T. Andzelm, J. and Abrams, C. (2015) "Comparison of Crosslinking Algorithms in Molecular Dynamics Simulation of Thermosetting Polymers." *Macromolecular Theory and Simulations*, 24(3), 260-270. doi: <http://dx.doi.org/10.1002/mats.201400094>.
- 8 Karkkainen, R. (2015) "Dynamic micromechanical modeling of textile composite strength under impact and multi-axial loading." *Composites Part B: Engineering*, 83, 27-35. doi: <https://doi.org/10.1016/j.compositesb.2015.08.009>.
- 9 Knorr, D. Masser, K. Elder, R. Sirk, T. Hindenlang, M. Yu, J. Richardson, A. Boyd, S. Spurgeon, W. and Lenhart, J. (2015) "Overcoming the structural versus energy

- dissipation trade-off in highly crosslinked polymer networks: Ultrahigh strain rate response in polydicyclopentadiene." *Composites Science and Technology*, 114, 17-25. doi: <https://doi.org/10.1016/j.compscitech.2015.03.021>.
- 10 Masser, K. Knorr, D. Hindenlang, M. Yu, J. Richardson, A. Strawhecker, K. Beyer, F. and Lenhart, J. (2015) "Relating structure and chain dynamics to ballistic performance in transparent epoxy networks exhibiting nanometer scale heterogeneity." *Polymer*, 58, 96-106. doi: <https://doi.org/10.1016/j.polymer.2014.12.027>.
 - 11 *Mc Aninch, I. Palmese, G. Lenhart, J. and La Scala, J. (2015) "Epoxy-amine networks with varying epoxy polydispersity." *Journal of Applied Polymer Science*, 132(8), 1097-4628. doi: <http://dx.doi.org/10.1002/app.41503>.
 - 12 Sharifi, M. Jang, C. Abrams, C. and Palmese, G. (2015) "Epoxy Polymer Networks with Improved Thermal and Mechanical Properties via Controlled Dispersion of Reactive Toughening Agents." *Macromolecules*, 48(20), 7495-7502. doi: <http://dx.doi.org/10.1021/acs.macromol.5b00677>.
 - 13 Yeager, M. and Advani, S. (2015) "Numerical model of fiber wetting with finite resin volume." *Integrating Materials and Manufacturing Innovation*, 4(3), 1-16. doi: <http://dx.doi.org/10.1186/s40192-015-0032-1>.

2014

- 1 Dey, M. Deitzel, J. Gillespie, J. and Schweiger, S. (2014) "Influence of sizing formulations on glass/epoxy interphase properties." *Composites Part A: Applied Science and Manufacturing*, 63, 59-67. doi: <http://dx.doi.org/10.1016/j.composites.a.2014.04.006>.
- 2 Jang, C. Sharifi, M. Palmese, G. and Abrams, C. (2014) "Crosslink network rearrangement via reactive encapsulation of solvent in epoxy curing: A combined molecular simulation and experimental study." *Polymer*, 55(16), 3859-3868. doi: <http://dx.doi.org/10.1016/j.polymer.2014.06.022>.
- 3 Kelly, G. Just, M. Advani, S. and Gillespie, J. (2014) "Energy and bond strength development during ultrasonic consolidation." *Journal of Materials Processing Technology*, 214(8), 1665-1672. doi: <http://dx.doi.org/10.1016/j.jmatprotec.2014.03.010>.
- 4 Sharifi, M. Jang, C. Abrams, C. and Palmese, G. (2014) "Toughened epoxy polymers via

- rearrangement of network topology." *J. Mater. Chem. A*, 2, 16071-16082. doi: <http://dx.doi.org/10.1039/C4TA03051F>.
- 5 Sockalingam, S. Gillespie, J. and Keefe, M. (2014) "On the transverse compression response of Kevlar KM2 using fiber-level finite element model." *International Journal of Solids and Structures*, 51(13), 2504-2517. doi: <https://doi.org/10.1016/j.ijsolstr.2014.03.020>. Accepted.
 - 6 Sockalingam, S. Mody, P. Gillespie, J. and Keefe, M. (2014) "Finite element analysis of the microdroplet test method using cohesive zone model of the fiber/matrix interface." *Composites Part A: Applied Science and Manufacturing*, 56, 239-247. doi: <https://doi.org/10.1016/jcomposite.sa.2013.10.021>.

2013

- 1 *Bogetti, T. Staniszewski, J. Burkins, M. Hoppel, C. Gillespie, J. and Tamrakar, S. (2013) "Predicting the nonlinear response and progressive failure of composite laminates under triaxial loading: Correlation with experimental results." *Journal of Composite Materials*, 47, 793-804. doi: <http://dx.doi.org/10.1177/0021998312462616>.
- 2 *McAninch, I. Palmese, G. Lenhart, J. and Lascala, J. (2013) "Characterization of epoxies cured with bimodal blends of polyetheramines." *Journal of Applied Polymer Science*, 130(3), 1621-1631. doi: <http://dx.doi.org/10.1002/app.39322>.

2012

- 1 *Bogetti, T. Staniszewski, J. Burns, B. Hoppel, C. Gillespie, J. and Tierney, J. (2012) "Predicting the nonlinear response and progressive failure of composite laminates under tri-axial loading." *Journal of Composite Materials*, 46(19), 2443-2459. doi: <https://doi.org/10.1177/0021998312449889>.
- 2 Haque, B. Z. and Gillespie, J. (2012) "A combined theoretical-semiempirical penetration model of ballistic penetration of thick section composites." *Journal of Thermoplastic Composite Materials*, 25(5), 631-659. doi: <http://dx.doi.org/10.1177/0892705712450296>.
- 3 Haque, B. Z. Harrington, J. and Gillespie, J. (2012) "Multi-hit ballistic impact on S-2 glass/SC15 thick-section composites: finite

- element analyses." *The Journal of Strain Analysis for Engineering Design*, 47(7), 495-512. doi: <http://dx.doi.org/10.1177/0309324712456823>.
- 4 Karkkainen, R. and McWilliams, B. (2012) "Dynamic micromechanical modeling of textile composites with cohesive interface failure." *Journal of Composite Materials*, 46(18), 2203-2218. doi: <https://doi.org/10.1177/0021998311430544>.
- 5 Karkkainen, R. and Yen, C. (2012) "Dynamic modeling for rate-dependent and mode-dependent cohesive interface failure analysis." *Journal of Composite Materials*, 46(18), 2193-2201. doi: <https://doi.org/10.1177/0021998311430543>.
- 6 Lopatnikov, S. Shevchenko, N. and Gillespie, J. (2012) "Device and Method for Investigation of Mechanical Properties of Fibers under High-Strain Rate Tensile Load." Cornell University Library, 1, 1-6. doi: <https://arxiv.org/pdf/1201.0916.pdf>.

Metals

2018

- 1 Ananthan, V. Krodel, S. and Kochmann, D. (2018) "Microstructural pattern and elastic property evolution during anisotropic spinodal decomposition." *Proceedings of the Royal Society A*, Accepted.
- 2 Ananthan, V. Tutcuoglu, A. and Kochmann, D. (2018) "Deformation patterning in finite-strain crystal plasticity by spectral homogenization with application to magnesium." *Computer Methods in Applied Mechanics and Engineering*, 335, 584-609. doi: <https://doi.org/10.1016/j.cma.2018.03.003>.
- 3 Kannan, V. Hazeli, K. and Ramesh, K. (2018) "The mechanics of dynamic twinning in single crystal magnesium." *Journal of the Mechanics and Physics of Solids*, Volume 120(ISSN 0022-5096), 154-178. doi: <https://doi.org/10.1016/j.jmps.2018.03.010>.
- 4 Nguyen, T. and Wilkerson, J. (2018) "The role of elastic and plastic anisotropy in intergranular spall failure." *Acta Materialia*, Submitted.
- 5 Tutcuoglu, A. Ananthan, V. Bhattacharya, K. and Kochmann, D. (2018) "Stochastic modeling of discontinuous dynamic recrystallization at finite strains in hcp metals." *Journal of the Mechanics*

- and Physics of Solids*, Submitted.
- 6 Zhao, M. Kannan, V. and Ramesh, K. (2018) "The dynamic plasticity and dynamic failure of a magnesium alloy under multiaxial loading." *Acta Materialia*, 154, 124-136. doi: <https://doi.org/10.1016/j.actamat.2018.05.012>.

2017

- 1 Barrett, C. Imandoust, A. Oppedal, A. Inal, K. Tschoff, M. and Kadiri, H. (2017) "Effect of grain boundaries on texture formation during dynamic recrystallization of magnesium alloys." *Acta Materialia*, 128, 270-283. doi: <https://doi.org/10.1016/j.actamat.2017.01.063>.
- 2 *Chang, Y. Lloyd, J. Becker, R. and Kochmann, D. (2017) "Modeling microstructure evolution in magnesium: Comparison of detailed and reduced-order kinematic models." *Mechanics of Materials*, 108, 40-57. doi: <https://doi.org/10.1016/j.mechmat.2017.02.007>.
- 3 Dixit, N. Farbaniec, L. and Ramesh, K. (2017) "Twinning in single crystal Mg under microsecond impact along the < a > axis." *Materials Science and Engineering A-Structural Materials Properties Microstructure and Processing*, 693, 22-25. doi: <http://dx.doi.org/10.1016/j.msea.2017.03.074>.
- 4 Fan, H. Tang, J. Tian, X. Wang, Q. Tian, X. and El-Awady, J. (2017) "Core structures and mobility of dislocations in magnesium." *Scripta Materialia*, 135, 37-40. doi: <https://doi.org/10.1016/j.scriptamat.2017.03.012>.
- 5 Fan, H. Wang, Q. Tian, X. and El-Awady, J. (2017) "Temperature effects on the mobility of pyramidal dislocations in magnesium." *Scripta Materialia*, 127, 68-71. doi: <https://doi.org/10.1016/j.scriptamat.2016.09.002>.
- 6 *Farbaniec, L. Williams, C. Kecske, L. Becker, R. and Ramesh, K. (2017) "Spall response and failure mechanisms associated with a hot-extruded AMX602 Mg alloy." *Materials Science and Engineering: A*, 707, 725-731. doi: <https://doi.org/10.1016/j.msea.2017.09.105>.
- 7 Lloyd, J. and Priddy, M. (2017) "Simulating strain localization in rolled magnesium." *Acta Materialia*, 129, 149-158. doi: <https://doi.org/10.1016/j.actamat.2017.02.043>.
- 8 Nguyen, T. Luscher, D. and Wilkerson, J. (2017) "A dislocation-based crystal plasticity framework for dynamic ductile failure of single crystals." *Journal of the Mechanics and Physics of Solids*, 108, 1-29. doi:

- [https://doi.org/10.1016/j.jmps.2017.07.020.](https://doi.org/10.1016/j.jmps.2017.07.020)
- 9 Paudel, Y. Barrett, C. Tschopp, M. Inal, K. and Kadiri, H. (2017) "Beyond initial twin nucleation in hcp metals: Micromechanical formulation for determining twin spacing during deformation." *Acta Materialia*, 133, 134-146. doi: <https://doi.org/10.1016/j.actamat.2017.05.013>.
 - 10 Sim, G. Kim, G. Lavenstein, S. Hamza, M. Fan, H. and El-Awady, J. (2017) "Anomalous hardening in magnesium driven by a size-dependent transition in deformation modes." *Acta Materialia*, doi: <https://doi.org/10.1016/j.actamat.2017.10.033>. Accepted.
 - 11 Srivastava, K. and El-Awady, J. (2017) "Dislocation Orientation Effects on the on the anisotropy of Pyramidal Slip in Magnesium." *Physical Review Letters*, Submitted.
 - 12 Srivastava, K. and El-Awady, J. (2017) "The dominating role of Jogs in Controlling Plasticity in Magnesium." *Acta Materialia*, Submitted.
 - 13 Srivastava, K. and El-Awady, J. (2017) "Deformation of magnesium during c-axis compression at low temperatures." *Acta Materialia*, 133, 282-292. doi: <https://doi.org/10.1016/j.actamat.2017.05.039>.
 - 14 Wang, P. Gao, W. Wilkerson, J. Liechti, K. and Huang, R. (2017) "Cavitation of water by volume-controlled stretching." *Extreme Mechanics Letters*, 11, 59-67. doi: <https://doi.org/10.1016/j.eml.2016.12.004>.
 - 15 Wang, F. Hazeli, K. Molodov, K. Barrett, C. Al-Samman, T. Molodov, D. Kontsos, A. Ramesh, K. El, K. and Agnew, S. (2017) "Characteristic dislocation substructure in \10(1)over-bar2\ magnesium." *Scripta Materialia*, 143, 8185-8185. doi: <http://dx.doi.org/10.1016/j.scriptamat.2017.09.015>.
 - 16 *Wang, W. Wang, Y. Shang, S. Darling, K. Kim, H. Tang, B. Kou, H. Mathaudhu, S. Hui, X. Li, J. Kecskes, L. and Liu, Z. (2017) "Strengthening Mg by self-dispersed nano-lamellar faults." *Materials Research Letters*, 5(6), 415-425. doi: <http://dx.doi.org/10.1080/21663831.2017.1308973>.
 - 17 Wang, F. Barrett, C. Hazeli, K. Molodov, K. Al-Samman, T. Oppedal, A. Molodov, D. Kontsos, A. Ramesh, K. El, K. and Agnew, S. (2017) "The Effect of \10(1)over-bar2\ Twin Boundary on the Evolution of Defect Substructure." *Magnesium Technology*, 1, 175-180. doi: http://dx.doi.org/10.1007/978-3-319-52392-7_27.
 - 18 Wilkerson, J. (2017) "On the micromechanics of void dynamics at extreme rates." *International Journal of Plasticity*, 95, 21-42. doi: <http://dx.doi.org/10.1016/j.ijplas.2017.03.008>.
- ## 2016
- 1 Aubry, S. Rhee, M. Hommes, G. Bulatov, V. and Arsenlis, A. (2016) "Dislocation dynamics in hexagonal close-packed crystals." *Journal of the Mechanics and Physics of Solids*, 94, 105-126. doi: <http://dx.doi.org/10.1016/j.jmps.2016.04.019>.
 - 2 Becker, R. and Lloyd, J. (2016) "A reduced-order crystal model for HCP metals: Application to Mg." *Mechanics of Materials*, 98, 98-110. doi: <https://doi.org/10.1016/j.mechmat.2016.04.009>.
 - 3 Bleckmann, M. Eichhorst, M. Schuch, M. Kreuzer, W. Hammond, V. Spiller, C. Meyer, L. and Herzig, N. (2016) "The influence of selected ECAP-processing routes on the material properties of Magnesium Elektron 675." *Materials Science and Engineering: A*, 660, 108-117. doi: <https://doi.org/10.1016/j.msea.2016.02.059>.
 - 4 Coleman, S. Tschopp, M. Weinberger, C. and Spearot, D. (2016) "Bridging atomistic simulations and experiments via virtual diffraction: understanding homophase grain boundary and heterophase interface structures." *Journal of Materials Science*, 51(3), 1251-1260. doi: <http://dx.doi.org/10.1007/s10853-015-9087-9>.
 - 5 El-Awady, J. Fan, H. and Hussein, A. (2016) "Advances in Discrete Dislocation Dynamics Modeling of Size-Affected Plasticity." *Multiscale Materials Modeling for Nanomechanics*, 245, 337-371. doi: http://dx.doi.org/10.1007/978-3-319-33480-6_11.
 - 6 Fan, H. Aubry, S. Arsenlis, A. and El-Awady, J. (2016) "Grain size effects on dislocation and twinning mediated plasticity in magnesium." *Scripta Materialia*, 112, 50-53. doi: <http://dx.doi.org/10.1016/j.scriptamat.2015.09.008>.
 - 7 *Farbaniec, L. Williams, C. Kecskes, L. Ramesh, K. and Becker, R. (2016) "Microstructural effects on the spall properties of ECAE-processed AZ31B magnesium alloy." *International Journal of Impact Engineering*, 98, 34-41. doi: <http://dx.doi.org/10.1016/j.ijimpeng.2016.08.001>.
 - 8 Lamberson, L. Eliasson, V. and Weerasooriya, T. (2016) "Quantitative Visualization of Dynamic Material Behavior." *Experimental Mechanics*, 56(1), 1-2. doi:

- http://dx.doi.org/10.1007/s11340-015-0118-x.
- 9 Liu, B. Arsenlis, T. and Aubry, S. (2016) "Computing forces on interface elements exerted by dislocations in an elastically anisotropic crystalline material." *Modelling and Simulation in Materials Science and Engineering*, 24(5), 55013-55013. doi: <http://stacks.iop.org/0965-0393/24/i=5/a=055013>.
 - 10 Lloyd, J. and Becker, R. (2016) "Stress-based crystal analysis of yielding in rolled Mg AZ31B." *Philosophical Magazine*, 96(4), 370-386. doi: <http://dx.doi.org/10.1080/14786435.2015.1132854>.
 - 11 Meredith, C. Lloyd, J. and Sano, T. (2016) "The quasi-static and dynamic response of fine-grained Mg alloy AMX602: An experimental and computational study." *Materials Science and Engineering: A*, 673, 73-82. doi: <https://doi.org/10.1016/j.msea.2016.07.035>.
 - 12 Mo, C. Wisner, B. Cabal, M. Hazeli, K. Ramesh, K. El, K. Al-Samman, T. Molodov, K. Molodov, D. and Kontos, A. (2016) "Acoustic Emission of Deformation Twinning in Magnesium." *Materials*, 9(8), 662-662. doi: <http://dx.doi.org/10.3390/ma9080662>.
 - 13 Ponga, M. Bhattacharya, K. and Ortiz, M. (2016) "A sublinear-scaling approach to density-functional-theory analysis of crystal defects." *Journal of the Mechanics and Physics of Solids*, 95, 530-556. doi: <http://dx.doi.org/10.1016/j.jmps.2016.05.029>.
 - 14 Shen, J. Gärtnerová, V. Kecskes, L. Kondoh, K. Jäger, A. and Wei, Q. (2016) "Residual stress and its effect on the mechanical properties of Y-doped Mg alloy fabricated via back-pressure assisted equal channel angular pressing (ECAP-BP)." *Materials Science and Engineering: A*, 669, 110-117. doi: <https://doi.org/10.1016/j.msea.2016.05.067>.
 - 15 Wilkerson, J. and Ramesh, K. (2016) "A closed-form criterion for dislocation emission in nano-porous materials under arbitrary thermomechanical loading." *Journal of the Mechanics and Physics of Solids*, 86, 94-116. doi: <http://dx.doi.org/10.1016/j.jmps.2015.10.005>.
 - 16 Wilkerson, J. and Ramesh, K. (2016) "Unraveling the Anomalous Grain Size Dependence of Cavitation." *Phys. Rev. Lett.*, 117, 1-5. doi: <http://dx.doi.org/10.1103/PhysRevLett.117.215503>.
 - 17 *Wu, C. Aubry, S. Arsenlis, A. and Chung, P. (2016) "Binary dislocation junction formation and strength in hexagonal close-packed crystals." *International Journal of Plasticity*, 79, 176-195. doi: <https://doi.org/10.1016/j.ijplas.2015.12.003>.
 - 18 Xie, K. Alam, Z. Caffee, A. and Hemker, K. (2016) "Deformation behavior of Mg single crystals compressed along c-axis." *Magnesium Technology*, 16, 209-211. doi: <http://dx.doi.org/10.1002/9781119274803.ch42>.
 - 19 Xie, K. Alam, Z. Caffee, A. and Hemker, K. (2016) "Pyramidal I slip in c-axis compressed Mg single crystals." *Scripta Materialia*, 112, 75-78. doi: <http://dx.doi.org/10.1016/j.scriptamat.2015.09.016>.
 - 20 Yi, P. Cammarata, R. and Falk, M. (2016) "Atomistic simulation of solid solution hardening in Mg/Al alloys: Examination of composition scaling and thermo-mechanical relationships." *Acta Materialia*, 105, 378-389. doi: <https://doi.org/10.1016/j.actamat.2015.12.038>.

2015

- 1 Aitken, Z. Fan, H. El-Awady, J. and Greer, J. (2015) "The effect of size, orientation and alloying on the deformation of AZ31 nanopillars." *Journal of the Mechanics and Physics of Solids*, 76, 208-223. doi: <http://dx.doi.org/10.1016/j.jmps.2014.11.014>.
- 2 Chang, Y. and Kochmann, D. (2015) "A variational constitutive model for slip-twinning interactions in hcp metals: Application to single- and polycrystalline magnesium." *International Journal of Plasticity*, 73, 39-61. doi: <https://doi.org/10.1016/j.ijplas.2015.03.008>.
- 3 Dixit, N. Xie, K. Hemker, K. and Ramesh, K. (2015) "Microstructural evolution of pure magnesium under high strain rate loading." *Acta Materialia*, 87, 56-67. doi: <http://dx.doi.org/10.1016/j.actamat.2014.12.030>.
- 4 Fan, H. and El-Awady, J. (2015) "Molecular Dynamics Simulations of Orientation Effects During Tension, Compression, and Bending Deformations of Magnesium Nanocrystals." *J. Appl. Mech.*, 82(10), 1-11. doi: <http://dx.doi.org/10.1115/1.4030930>.
- 5 Fan, H. Aubry, S. Arsenlis, A. and El-Awady, J. (2015) "Orientation influence on grain size effects in ultrafine-grained magnesium." *Scripta Materialia*, 97, 25-28. doi: <http://dx.doi.org/10.1016/j.scriptamat.2014.10.031>.
- 6 Fan, H. Aubry, S. Arsenlis, T. and El-Awady, J. (2015) "The role of twinning deformation on the hardening response of polycrystalline magnesium from discrete dislocation dynamics simulations." *Acta Materialia*, 92, 126-139. doi: <https://doi.org/10.1016/j.actamat.2015.03.039>.

- 7 Fan, H. and El-Awady, J. (2015) "Towards resolving the anonymity of pyramidal slip in magnesium." *Materials Science and Engineering: A*, 644, 318-324. doi: <https://doi.org/10.1016/j.msea.2015.07.080>.
- 8 Paul, J. and Kimberley, J. (2015) "A Desktop Tensile Kolsky Bar for the Dynamic Testing of Metallic Foils." *Journal of Dynamic Behavior of Materials*, 1(4), 439-446. doi: <http://dx.doi.org/10.1007/s40870-015-0038-y>.
- 9 Ponga, M. Ortiz, M. and Ariza, M. (2015) "Finite-temperature non-equilibrium quasi-continuum analysis of nanovoid growth in copper at low and high strain rates." *Mechanics of Materials*, 90, 253-267. doi: <https://doi.org/10.1016/j.mechmat.2015.02.007>.
- 10 *Wang, W. Shang, S. Wang, Y. Kim, H. Darling, K. Kecskes, L. Mathaudhu, S. Hui, X. and Liu, Z. (2015) "Solid-Solution Hardening in Mg-Gd-TM (TM = Ag, Zn, and Zr) Alloys: An Integrated Density Functional Theory and Electron Work Function Study." *JOM*, 67(10), 2433-2441. doi: <http://dx.doi.org/10.1007/s11837-015-1555-9>.
- 11 Winey, M. Renganathan, P. and Gupta, Y. (2015) "Shock wave compression and release of hexagonal-close-packed metal single crystals: Inelastic deformation of c-axis magnesium." *Journal of Applied Physics*, 117(10), 1-1. doi: <http://dx.doi.org/10.1063/1.4914525>.
- 12 *van Beers, P. Kouznetsova, V. Geers, M. Tschoop, M. and McDowell, D. (2015) "A multiscale model of grain boundary structure and energy: From atomistics to a continuum description." *Acta Materialia*, 82, 513-529. doi: <https://doi.org/10.1016/j.actamat.2014.08.045>.
- 3 Clayton, J. (2014) "Shock Compression of Metal Crystals: A Comparison of Eulerian and Lagrangian Elastic-Plastic Theories." *International Journal of Applied Mechanics*, 6(5), 1450-48. doi: <http://dx.doi.org/10.1142/S1758825114500483>.
- 4 Coleman, S. Sichani, M. and Spearot, D. (2014) "A Computational Algorithm to Produce Virtual X-ray and Electron Diffraction Patterns from Atomistic Simulations." *JOM*, 66(3), 408-416. doi: <http://dx.doi.org/10.1007/s11837-013-0829-3>.
- 5 *Crone, J. Chung, P. Leiter, K. Knap, J. Aubry, S. Hommes, G. and Arsenlis, T. (2014) "A multiply parallel implementation of finite element-based discrete dislocation dynamics for arbitrary geometries." *Modelling and Simulation in Materials Science and Engineering*, 22(3), 35014-35014. doi: <https://doi.org/10.1088/0965-0393/22/3/035014>.
- 6 *Eswar, P. Liu, B. Dixit, N. Shaffer, M. Mathaudhu, S. and Ramesh, K. (2014) "The Dynamic Flow and Failure Behavior of Magnesium and Magnesium Alloys." *JOM*, 66(2), 291-304. doi: <http://dx.doi.org/10.1007/s11837-013-0850-6>.
- 7 *Lambert, P. Hustedt, C. Vecchio, K. Huskins, E. Casem, D. Gruner, S. Tate, M. Philipp, H. Woll, A. Purohit, P. Weiss, J. Kannan, V. Ramesh, K. Kenesei, P. Okasinski, J. Almer, J. Zhao, M. Ananiadis, A. and Hufnagel, T. (2014) "Time-resolved x-ray diffraction techniques for bulk polycrystalline materials under dynamic loading." *Review of Scientific Instruments*, 85(9), 93901-93901. doi: <http://dx.doi.org/10.1063/1.4893881>.
- 8 *Lloyd, J. Clayton, J. Austin, R. and McDowell, D. (2014) "Plane wave simulation of elastic-viscoplastic single crystals." *Journal of the Mechanics and Physics of Solids*, 69, 14-32. doi: <https://doi.org/10.1016/j.jmps.2014.04.009>.
- 9 Prasad, K. and Ramesh, K. (2014) "In-situ observations and quantification of twin boundary mobility in polycrystalline magnesium." *Materials Science and Engineering: A*, 617, 121-126. doi: <https://doi.org/10.1016/j.msea.2014.08.043>.
- 10 Queyreau, S. Marian, J. Wirth, B. and Arsenlis, T. (2014) "Analytical integration of the forces induced by dislocations on a surface element." *Modelling and Simulation in Materials Science and Engineering*, 22(3), 35004-35004. doi: <http://stacks.iop.org/0965-0393/22/i=3/a=035004>.

2014

- 1 Agnew, S. Whittington, W. Oppedal, A. El, K. Shaeffer, M. Ramesh, K. Bhattacharyya, J. Delorme, R. and Davis, B. (2014) "Dynamic Behavior of a Rare-Earth-Containing Mg Alloy, WE43B-T5, Plate with Comparison to Conventional Alloy, AM30-F." *JOM*, 66(2), 277-290. doi: <http://dx.doi.org/10.1007/s11837-013-0830-x>.
- 2 Aubry, S. Fitzgerald, S. and Arsenlis, A. (2014) "Methods to compute dislocation line tension energy and force in anisotropic elasticity." *Modelling and Simulation in Materials Science and Engineering*, 22(1), 15001-15001. doi: <http://stacks.iop.org/0965-0393/22/i=1/a=015001>.
- 3 Clayton, J. (2014) "Shock Compression of Metal Crystals: A Comparison of Eulerian and Lagrangian Elastic-Plastic Theories." *International Journal of Applied Mechanics*, 6(5), 1450-48. doi: <http://dx.doi.org/10.1142/S1758825114500483>.
- 4 Coleman, S. Sichani, M. and Spearot, D. (2014) "A Computational Algorithm to Produce Virtual X-ray and Electron Diffraction Patterns from Atomistic Simulations." *JOM*, 66(3), 408-416. doi: <http://dx.doi.org/10.1007/s11837-013-0829-3>.
- 5 *Crone, J. Chung, P. Leiter, K. Knap, J. Aubry, S. Hommes, G. and Arsenlis, T. (2014) "A multiply parallel implementation of finite element-based discrete dislocation dynamics for arbitrary geometries." *Modelling and Simulation in Materials Science and Engineering*, 22(3), 35014-35014. doi: <https://doi.org/10.1088/0965-0393/22/3/035014>.
- 6 *Eswar, P. Liu, B. Dixit, N. Shaffer, M. Mathaudhu, S. and Ramesh, K. (2014) "The Dynamic Flow and Failure Behavior of Magnesium and Magnesium Alloys." *JOM*, 66(2), 291-304. doi: <http://dx.doi.org/10.1007/s11837-013-0850-6>.
- 7 *Lambert, P. Hustedt, C. Vecchio, K. Huskins, E. Casem, D. Gruner, S. Tate, M. Philipp, H. Woll, A. Purohit, P. Weiss, J. Kannan, V. Ramesh, K. Kenesei, P. Okasinski, J. Almer, J. Zhao, M. Ananiadis, A. and Hufnagel, T. (2014) "Time-resolved x-ray diffraction techniques for bulk polycrystalline materials under dynamic loading." *Review of Scientific Instruments*, 85(9), 93901-93901. doi: <http://dx.doi.org/10.1063/1.4893881>.
- 8 *Lloyd, J. Clayton, J. Austin, R. and McDowell, D. (2014) "Plane wave simulation of elastic-viscoplastic single crystals." *Journal of the Mechanics and Physics of Solids*, 69, 14-32. doi: <https://doi.org/10.1016/j.jmps.2014.04.009>.
- 9 Prasad, K. and Ramesh, K. (2014) "In-situ observations and quantification of twin boundary mobility in polycrystalline magnesium." *Materials Science and Engineering: A*, 617, 121-126. doi: <https://doi.org/10.1016/j.msea.2014.08.043>.
- 10 Queyreau, S. Marian, J. Wirth, B. and Arsenlis, T. (2014) "Analytical integration of the forces induced by dislocations on a surface element." *Modelling and Simulation in Materials Science and Engineering*, 22(3), 35004-35004. doi: <http://stacks.iop.org/0965-0393/22/i=3/a=035004>.

- 11 Tang, Y. and El-Awady, J. (2014) "Formation and slip of pyramidal dislocations in hexagonal close-packed magnesium single crystals." *Acta Materialia*, 71, 319-332. doi: <https://doi.org/10.1016/j.actamat.2014.03.022>.
- 12 Tang, Y. and El-Awady, J. (2014) "Highly anisotropic slip-behavior of pyramidal I dislocations in hexagonal close-packed magnesium." *Materials Science and Engineering: A*, 618, 424-432. doi: <https://doi.org/10.1016/j.msea.2014.09.032>.
- 13 Venturini, G. Wang, K. Romero, I. Ariza, M. and Ortiz, M. (2014) "Atomistic long-term simulation of heat and mass transport." *Journal of the Mechanics and Physics of Solids*, 73, 242-268. doi: <http://dx.doi.org/10.1016/j.jmps.2014.09.008>.
- 14 *Wang, W. Shang, S. Wang, Y. Mei, Z. Darling, K. Kecske, L. Mathaudhu, S. Hui, X. and Liu, Z. (2014) "Effects of Alloying Elements on Stacking Fault Energies and Electronic Structures of Binary Mg Alloys: A First-Principles Study." *Materials Research Letters*, 2(1), 29-36. doi: <http://dx.doi.org/10.1080/21663831.2013.858085>.
- 15 *Wang, W. Shang, S. Wang, Y. Darling, K. Kecske, L. Mathaudhu, S. Hui, X. and Liu, Z. (2014) "Electronic structures of long periodic stacking order structures in Mg: A first-principles study." *Journal of Alloys and Compounds*, 586, 656-662. doi: <https://doi.org/10.1016/j.jallcom.2013.10.068>.
- 16 Wilkerson, J. and Ramesh, K. (2014) "A dynamic void growth model governed by dislocation kinetics." *Journal of the Mechanics and Physics of Solids*, 70, 262-280. doi: <http://dx.doi.org/10.1016/j.jmps.2014.05.018>.
- 17 *Williams, C. Chen, C. Ramesh, K. and Dandekar, D. (2014) "On the shock stress, substructure evolution, and spall response of commercially pure 1100-O aluminum." *Materials Science and Engineering: A*, 618, 596-604. doi: <https://doi.org/10.1016/j.msea.2014.09.030>.
- 18 Winey, M. and Gupta, Y. (2014) "Shock wave compression of hexagonal-close-packed metal single crystals: Time-dependent, anisotropic elastic-plastic response of beryllium." *Journal of Applied Physics*, 116(3), 33505-33505. doi: <http://dx.doi.org/10.1063/1.4889886>.
- 19 Wright, T. Daphalapurkar, N. and Ramesh, K. (2014) "Stability of ideal fcc twin boundaries." *Journal of the Mechanics and Physics of Solids*, 73, 228-241. doi: <http://dx.doi.org/10.1016/j.jmps.2014.09.007>.
- 20 Zhang, J. Ramesh, K. and Joshi, S. (2014) "Stochastic size-dependent slip-twinning competition in hexagonal close packed single crystals." *Modelling and Simulation in Materials Science and Engineering*, 22(7), 75003-75003. doi: <http://stacks.iop.org/0965-0393/22/i=7/a=075003>.

2013

- 1 Aubry, S. and Arsenlis, A. (2013) "Use of spherical harmonics for dislocation dynamics in anisotropic elastic media." *Modelling and Simulation in Materials Science and Engineering*, 21(6), 65013-65013. doi: <http://stacks.iop.org/0965-0393/21/i=6/a=065013>.
- 2 Bhatia, M. Solanki, K. Moitra, A. and Tschoop, M. (2013) "Investigating Damage Evolution at the Nanoscale: Molecular Dynamics Simulations of Nanovoid Growth in Single-Crystal Aluminum." *Metallurgical and Materials Transactions A*, 44(2), 617-626. doi: <http://dx.doi.org/10.1007/s11661-012-1082-z>.
- 3 Byer, C. and Ramesh, K. (2013) "Effects of the initial dislocation density on size effects in single-crystal magnesium." *Acta Materialia*, 61(10), 3808-3818. doi: <http://dx.doi.org/10.1016/j.actamat.2013.03.019>.
- 4 Casem, D. and Zellner, M. (2013) "Kolsky Bar Wave Separation Using a Photon Doppler Velocimeter." *Experimental Mechanics*, 53(8), 1467-1473. doi: <http://dx.doi.org/10.1007/s11340-013-9735-4>.
- 5 Clayton, J. and Knap, J. (2013) "Phase-field analysis of fracture-induced twinning in single crystals." *Acta Materialia*, 61(14), 5341-5353. doi: <https://doi.org/10.1016/j.actamat.2013.05.023>.
- 6 *Guo, Y. Behm, N. Ligda, J. Li, Y. Pan, Z. Horita, Z. and Wei, Q. (2013) "Critical issues related to instrumented indentation on non-uniform materials: Application to niobium subjected to high pressure torsion." *Materials Science and Engineering: A*, 586, 149-159. doi: <https://doi.org/10.1016/j.msea.2013.08.015>.
- 7 Kadiri, H. Barrett, C. and Tschoop, M. (2013) "The candidacy of shuffle and shear during compound twinning in hexagonal close-packed structures." *Acta Materialia*, 61(20), 7646-7659. doi: <https://doi.org/10.1016/j.actamat.2013.09.002>.
- 8 Kim, C. Sohn, I. Nezafati, M. Ferguson, J. Schultz, B. Bajestani-Gohari, Z. Rohatgi, P. and

- Cho, K. (2013) "Prediction models for the yield strength of particle-reinforced unimodal pure magnesium (Mg) metal matrix nanocomposites (MMNCs)." *Journal of Materials Science*, 48(12), 4191-4204. doi: <http://dx.doi.org/10.1007/s10853-013-7232-x>.
- 9 *Vignes, R. Becker, R. Stölken, J. and Kumar, M. (2013) "An assessment of diamond anvil cell measurements on material strength." *Journal of Applied Physics*, 113(21), 213-503. doi: <http://dx.doi.org/10.1063/1.4807786>.
- 10 *Williams, C. Chen, C. Ramesh, K. and Dandekar, D. (2013) "The effects of cold rolling on the microstructural and spall response of 1100 aluminum." *Journal of Applied Physics*, 114(9), 93502-93502. doi: <http://dx.doi.org/10.1063/1.4817844>.
- 11 *Wu, C. Chung, P. Aubry, S. Munday, L. and Arsenlis, A. (2013) "The strength of binary junctions in hexagonal close-packed crystals." *Acta Materialia*, 61(9), 3422-3431. doi: <https://doi.org/10.1016/j.actamat.2013.02.033>.

2012

- 1 Casem, D. Grunschel, S. and Schuster, B. (2012) "Normal and Transverse Displacement Interferometers Applied to Small Diameter Kolsky Bars." *Experimental Mechanics*, 52(2), 173-184. doi: <http://dx.doi.org/10.1007/s11340-011-9524-x>.
- 2 Daphalapurkar, N. and Ramesh, K. (2012) "Orientation dependence of the nucleation and growth of partial dislocations and possible twinning mechanisms in aluminum." *Journal of the Mechanics and Physics of Solids*, 60(2), 277-294. doi: <http://dx.doi.org/10.1016/j.jmps.2011.10.009>.
- 3 Grujicic, M. Pandurangan, B. Cheeseman, B. and Yen, C. (2012) "Spall-Fracture Physics and Spallation-Resistance-Based Material Selection." *Journal of Materials Engineering and Performance*, 21(9), 1813-1823. doi: <http://dx.doi.org/10.1007/s11665-011-0068-0>.
- 4 Panigrahi, S. Kumar, K. Kumar, N. Yuan, W. Mishra, R. DeLorme, R. Davis, B. Howell, R. and Cho, K. (2012) "Transition of deformation behavior in an ultrafine grained magnesium alloy." *Materials Science and Engineering: A*, 549, 123-127. doi: <https://doi.org/10.1016/j.msea.2012.04.017>.
- 5 *Razavi, S. Foley, D. Karaman, I. Hartwig, K. Duygulu, O. Kecskes, L. Mathaudhu, S. and Hammond, V. (2012) "Effect of grain size on prismatic slip in Mg-3Al-1Zn alloy." *Scripta Materialia*, 67(5), 439-442. doi: <https://doi.org/10.1016/j.scriptamat.2012.05.017>.
- 6 *Williams, C. Ramesh, K. and Dandekar, D. (2012) "Spall response of 1100-O aluminum." *Journal of Applied Physics*, 111(12), 123-528. doi: <http://dx.doi.org/10.1063/1.4729305>.

Polymers

2018

- 1 Dong, H. Wang, Z. O'Connor, T. Azoug, A. Robbins, M. O. and Nguyen, V. (2018) "Micromechanical models for the stiffness and strength of UHMWPE macro fibrils." *JMPS*, 116, 70-98. doi: <https://doi.org/10.1016/j.jmps.2018.03.015>.
- 2 Galvani Cunha, M. and Robbins, M. O. (2018) "Determination of pressure-viscosity relation of 2,2,4-trimethylhexane by all-atom molecular dynamics simulations." *Fluid Phase Equilib.*, Submitted.
- 3 *McDaniel, P. Deitzel, J. Gillespie, J. and Strawhecker, K. (2018) "Nanoscale Interfibrillar Adhesion in UHMWPE Fibers." *Journal of Polymer Science Part B: Polymer Physics*, 56(5), 391-401. doi: <https://doi.org/10.1002/polb.24552>.
- 4 O'Connor, T. Elder, R. Sliozberg, Y. Sirk, T. Andzelm, J. and Robbins, M. O. (2018) "Molecular origins of anisotropic shock propagation in crystalline and amorphous polyethylene." *Phys. Rev. Materials*, 2(3), doi: <https://doi.org/10.1103/PhysRevMaterials.2.035601>.
- 5 O'Connor, T. Alvarez, N. and Robbins, M. O. (2018) "Relating Chain Conformations to Extensional Stress in Entangled Polymer Melts." *Phys. Rev. Lett.*, 121(4), doi: <http://doi.org/10.1103/PhysRevLett.121.047801>.
- 6 Polakovic, T. Gregory, D. McDaniel, P. Deitzel, J. and Gillespie, J. (2018) "A Single Fiber Peel Test to Assess Ultra High Molecular Weight Polyethylene Fiber Mesostructured Interactions." *Journal of Applied Polymer Science*, 1135(16), 46-156. doi: <https://doi.org/10.1002/app.46156>.
- 7 *Staniszewski, J. Sockalingam, S. Bogetti, T. and Gillespie, J. (2018) "Modeling the Fibrillation of Kevlar KM2 Single Fibers Subjected to Transverse Compression." *Fibers and Polymers*, 19(7), 1479-1489. doi:

<https://doi.org/10.1007/s12221-018-8127-x>.
Submitted.

2017

- 1 Bogetti, T. Walter, M. Staniszewski, J. and Cline, J. (2017) "Interlaminar shear characterization of ultra-high molecular weight polyethylene (UHMWPE) composite laminates." *Composites Part A: Applied Science and Manufacturing*, 98, 105-115. doi: <https://doi.org/10.1016/j.compositesa.2017.03.018>.
- 2 Brayton, A. Yeh, I. Andzelm, J. and Rutledge, G. (2017) "Vibrational Analysis of Semicrystalline Polyethylene Using Molecular Dynamics Simulation." *Macromolecules*, 50(17), 6690-6701. doi: <https://dx.doi.org/10.1021/acs.acromol.7b00995>.
- 3 Chowdhury, S. Sockalingam, S. and Gillespie, J. (2017) "Molecular Dynamics Modeling of the Effect of Axial and Transverse Compression on the Residual Tensile Properties of Ballistic Fiber." *Fibers*, 5(7), 1-16. doi: <http://www.mdpi.com/2079-6439/5/1/7.htm>.
- 4 Deitzel, J. McDaniel, P. and Gillespie, J. (2017) "Chapter 10: High Performance Polyethylene Fibers." *Structure and Properties of High-Performance Fibers*, 1(1), 167-185. doi: <https://doi.org/10.1016/B978-0-08-100550-7.00007-3>. Accepted.
- 5 *Elder, R. O'Connor, T. Chantawansri, T. Sliozberg, Y. Sirk, T. Yeh, I. Robbins, M. O. and Andzelm, J. (2017) "Shock-wave propagation and reflection in semicrystalline polyethylene: A molecular-level investigation." *Phys. Rev. Materials*, 1, 43606-43606. doi: <http://dx.doi.org/10.1103/PhysRevMaterials.1.043606>.
- 6 Haque, B. Z. Ali, M. and Gillespie, J. (2017) "Modeling Transverse Impact on UHMWPE Soft Ballistic Sub-Laminate." *Journal of Thermoplastic Composite Materials*, 30(11), 1441-1483. doi: <https://doi.org/10.1177/0892705716637114>.
- 7 Jadhao, V. and Robbins, M. O. (2017) "Correction for Jadhao and Robbins, Probing large viscosities in glass-formers with nonequilibrium simulations." *Proceedings of the National Academy of Sciences*, 114(39), 8317-8317. doi: <https://doi.org/10.1073/pnas.1715376114>.
- 8 Jadhao, V. and Robbins, M. O. (2017) "Probing large viscosities in glass-formers with nonequilibrium simulations." *Proceedings of the National Academy of Sciences*, 114(30), 7952-7957. doi: <http://dx.doi.org/10.1073/pnas.1705978114>.
- 9 Jadhao, V. and Robbins, M. O. (2017) "Reply to Bair: Crossover to Arrhenius behavior at high viscosities in squalane." *Proceedings of the National Academy of Sciences*, 114(42), 8807-8808. doi: <http://dx.doi.org/10.1073/pnas.1715298114>.
- 10 *McDaniel, P. Sockalingam, S. Deitzel, J. Gillespie, J. Keefe, M. Bogetti, T. Casem, D. and Weerasooriya, T. (2017) "The effect of fiber meso/nanostructure on the transverse compression response of ballistic fibers." *Composites Part A: Applied Science and Manufacturing*, 94, 133-145. doi: <https://doi.org/10.1016/j.compositesa.2016.12.003>.
- 11 *McDaniel, P. Deitzel, J. Gillespie, J. and Strawhecker, K. (2017) "Influence of sub-filament structure on failure mechanisms for mode I and II loading conditions in UHMWPE filaments." Submitted.
- 12 *McDaniel, P. Deitzel, J. Gillespie, J. and Strawhecker, K. (2017) "Measurement of Microfibril Adhesion in UHMW PE fibers through Nanomechanical testing." Submitted.
- 13 *O'Connor, T. Elder, R. Sliozberg, Y. Sirk, T. Andzelm, J. and Robbins, M. O. (2017) "Molecular Origins of Anisotropic Shock Propagation in Crystalline and Amorphous Polyethylene." *Physical Review Materials*, Submitted.
- 14 *Sockalingam, S. Casem, D. Weerasooriya, T. McDaniel, P. and Gillespie, J. (2017) "Experimental Investigation of the High Strain Rate Transverse Compression Behavior of Ballistic Single Fibers." *Journal of Dynamic Behavior of Materials*, 3(3), 474-484. doi: <http://dx.doi.org/10.1007/s40870-017-0126-2>.
- 15 Sockalingam, S. Gillespie, J. and Keefe, M. (2017) "Role of Inelastic Transverse Compressive Behavior and Multiaxial Loading on the Transverse Impact of Kevlar KM2 Single Fiber." *Fibers*, 5(1), 1-9. doi: <http://dx.doi.org/10.3390/fib5010009>.
- 16 *Sockalingam, S. Casem, D. Gillespie, J. and Weerasooriya, T. (2017) "High strain rate transverse compression behavior of Kevlar KM2 and Dyneema SK76 ballistic single fibers." *Polymer Testing*, Submitted.
- 17 Sockalingam, S. Gillespie, J. and Keefe, M. (2017) "Influence of inelastic transverse compressive behavior on the transverse impact of Kevlar KM2 single fiber." *Textile Research*

- Journal, Submitted.
- 18 Sockalingam, S. Gillespie, J. and Keefe, M. (2017) "Modeling the Fiber Length-Scale Response of Kevlar KM2 Yarn During Transverse Impact." *Textile Research Journal*, 87(8), 2242-2254. doi: <https://doi.org/10.1177/0040517516669074>.
 - 19 Sockalingam, S. Chowdhury, S. Gillespie, J. and Keefe, M. (2017) "Recent Advances in Modeling and Experiments of Kevlar Ballistic Fibrils, Fibers, Yarns and Flexible Textile Fabrics – A Review." *Textile Research Journal*, 87(8), 984-1010. doi: <https://doi.org/10.1177/0040517516646039>.
 - 20 Yeh, I. Lenhart, J. Rutledge, G. and Andzelm, J. (2017) "Molecular Dynamics Simulation of the Effects of Layer Thickness and Chain Tilt on Tensile Deformation Mechanisms of Semicrystalline Polyethylene." *Macromolecules*, 50(4), 1700-1712. doi: <http://dx.doi.org/10.1021/acs.macromol.6b01748>.

2016

- 1 Elder, R. Knorr, D. Andzelm, J. Lenhart, J. and Sirk, T. (2016) "Nanovoid formation and mechanics: a comparison of poly(dicyclopentadiene) and epoxy networks from molecular dynamics simulations." *Soft Matter*, 12, 4418-4434. doi: <http://dx.doi.org/10.1039/C6SM00691D>.
- 2 Hsieh, A. Chantawansri, T. Hu, W. Cain, J. and Yu, J. (2016) "New insight into the influence of molecular dynamics of matrix elastomers on ballistic impact deformation in UHMWPE composites." *Polymer*, 95, 52-61. doi: <https://doi.org/10.1016/j.polymer.2016.04.048>.
- 3 O'Connor, T. and Robbins, M. O. (2016) "Chain Ends and the Ultimate Strength of Polyethylene Fibers." *ACS Macro Letters*, 5(3), 263-267. doi: <http://dx.doi.org/10.1021/acsmacrolett.5b00838>.
- 4 Sliozberg, Y. Kröger, M. and Chantawansri, T. (2016) "Fast equilibration protocol for million atom systems of highly entangled linear polyethylene chains." *The Journal of Chemical Physics*, 144(15), 154-901. doi: <http://dx.doi.org/10.1063/1.4946802>.
- 5 Sockalingam, S. Gillespie, J. and Keefe, M. (2016) "Influence of multiaxial loading on the failure of Kevlar KM2 single fiber." *Textile Research Journal*, 88(5), 483-498. doi: <http://dx.doi.org/10.1177/0040517516681961>.

- 6 Sockalingam, S. Gillespie, J. and Keefe, M. (2016) "Modeling the fiber length-scale response of Kevlar KM2 yarn during transverse impact." *Textile Research Journal*, 1(0), 2242-2254. doi: <http://dx.doi.org/10.1177/0040517516669074>.
- 7 Sockalingam, S. Bremble, R. Gillespie, J. and Keefe, M. (2016) "Transverse compression behavior of Kevlar KM2 single fiber." *Composites Part A: Applied Science and Manufacturing*, 81, 271-281. doi: <https://doi.org/10.1016/j.compositesa.2015.11.032>.
- 8 Veysset, D. Hsieh, A. Kooi, S. Maznev, A. Masser, K. and Nelson, K. (2016) "Dynamics of supersonic microparticle impact on elastomers revealed by real-time multi-frame imaging." *Scientific Reports*, 6, 25577-25577. doi: <http://doi.org/10.1038/srep25577>.
- 9 Wang, Y. Miao, Y. Huang, L. Swenson, D. Yen, C. Yu, J. and Zheng, J. (2016) "Effect of the inter-fiber friction on fiber damage propagation and ballistic limit of 2-D woven fabrics under a fully confined boundary condition." *International Journal of Impact Engineering*, 97, 66-78. doi: <https://doi.org/10.1016/j.ijimpeng.2016.06.007>.

2015

- 1 Chantawansri, T. Yeh, I. and Hsieh, A. (2015) "Investigating the glass transition temperature at the atom-level in select model polyamides: A molecular dynamics study." *Polymer*, 81, 50-61. doi: <https://doi.org/10.1016/j.polymer.2015.09.069>.
- 2 McDaniel, P. Deitzel, J. and Gillespie, J. (2015) "Structural Hierarchy and Surface Morphology of Highly Drawn Ultra High Molecular Weight Polyethylene Fibers Studied by Atomic Force Microscopy and Wide Angle X-Ray Diffraction." *Journal of Polymer Research*, 69, 148-158. doi: <https://doi.org/10.1016/j.polymer.2015.05.010>.
- 3 *O'Connor, T. Andzelm, J. and Robbins, M. O. (2015) "AIREBO-M: A reactive model for hydrocarbons at extreme pressures." *The Journal of Chemical Physics*, 142(2), 24903-24903. doi: <http://dx.doi.org/10.1063/1.4905549>.
- 4 Rahman, R. and Foster, J. (2015) "A molecular dynamics based investigation of thermally vibrating graphene under different boundary conditions." *Physica E: Low-dimensional Systems and Nanostructures*, 72, 25-47. doi: <https://doi.org/10.1016/j.physe.2015.04.007>.

- 5 Rahman, R. and Foster, J. (2015) "A molecular dynamics based investigation of thermally vibrating graphene under different boundary conditions." *Physica E: Low-dimensional Systems and Nanostructures*, 72, 25-47. doi: <http://dx.doi.org/10.1016/j.physe.2015.04.007>.
- 6 Rahman, R. and Foster, J. (2015) "Peridynamic theory of solids from the perspective of classical statistical mechanics." *Physica A: Statistical Mechanics and its Applications*, 437, 162-183. doi: <http://dx.doi.org/10.1016/j.physa.2015.05.099>.
- 7 Sockalingam, S. Gillespie, J. and Keefe, M. (2015) "Dynamic modeling of Kevlar KM2 single fiber subjected to transverse impact." *International Journal of Solids and Structures*, 67, 297-310. doi: <https://doi.org/10.1016/j.ijsolstr.2015.04.031>.
- 8 Yeh, I. Andzelm, J. and Rutledge, G. (2015) "Mechanical and Structural Characterization of Semicrystalline Polyethylene under Tensile Deformation by Molecular Dynamics Simulations." *Macromolecules*, 48(12), 4228-4239. doi: <http://dx.doi.org/10.1021/acs.macromol.5b00697>.

2014

- 1 Chantawansri, T. and Sliozberg, Y. (2014) "Computational study of the morphology and mechanical properties of dilute ABC triblock copolymers." *Korea-Australia Rheology Journal*, 26(1), 49-61. doi: <http://dx.doi.org/10.1007/s13367-014-0006-4>.
- 2 Cole, D. and Strawhecker, K. (2014) "An improved instrumented indentation technique for single microfibers." *Journal of Materials Research*, 29(9), 1104-1112. doi: <http://dx.doi.org/10.1557/jmr.2014.83>.
- 3 Lopatnikov, S. and Gillespie, J. (2014) "Simple analytical model for fiber tensile failure due to droplet impact." *Journal of Applied Physics*, 115(6), 63511-63511. doi: <http://dx.doi.org/10.1063/1.4863207>.
- 4 McAllister, Q. Gillespie, J. and VanLandingham, M. (2014) "The energy dissipative mechanisms of particle-fiber interactions in a textile composite." *Journal of Composite Materials*, 48(28), 3553-3567. doi: <http://dx.doi.org/10.1177/0021998313511651>.
- 5 *Nilakantan, G. Merrill, R. Keefe, M. Gillespie, J. and Wetzel, E. (2014) "Experimental investigation of the role of frictional yarn pull-out and windowing on the probabilistic impact response of kevlar fabrics." *Composites Part B: Engineering*, 68, 215-229. doi: <https://doi.org/10.1016/j.compositesb.2014.08.033>.

- 6 Rahman, R. Haque, A. and Foster, J. (2014) "A Multiscale Modeling Scheme Based on Peridynamic Theory." *International Journal for Multiscale Computational Engineering*, 12(3), 223-248. doi: <http://doi.org/10.1615/IntJMultCompEng.2014007954>.
- 7 Rahman, R. and Foster, J. (2014) "Bridging the length scales through nonlocal hierarchical multiscale modeling scheme." *Computational Materials Science*, 92, 401-415. doi: <http://dx.doi.org/10.1016/j.commatsci.2014.05.052>.
- 8 Rahman, R. and Foster, J. (2014) "Deformation mechanism of graphene in amorphous polyethylene: A molecular dynamics based study." *Computational Materials Science*, 87, 232-240. doi: <https://doi.org/10.1016/j.commatsci.2014.02.023>.
- 9 *Sanborn, B. and Weerasooriya, T. (2014) "Quantifying damage at multiple loading rates to Kevlar KM2 fibers due to weaving, finishing, and pre-twist." *International Journal of Impact Engineering*, 71, 50-59. doi: <https://doi.org/10.1016/j.ijimpeng.2014.04.005>.

- 10 Sockalingam, S. Gillespie, J. and Keefe, M. (2014) "On the transverse compression response of Kevlar KM2 using fiber-level finite element model." *International Journal of Solids and Structures*, 51(13), 2504-2517. doi: <http://dx.doi.org/10.1016/j.ijsolstr.2014.03.020>.
- 11 Strawhecker, K. and Cole, D. (2014) "Morphological and local mechanical surface characterization of ballistic fibers via AFM." *Journal of Applied Polymer Science*, 131(19), 1-1. doi: <http://dx.doi.org/10.1002/app.40880>.

2013

- 1 Grujicic, M. Pandurangan, B. Snipes, J. Yen, C. and Cheeseman, B. (2013) "Multi-Length Scale-Enriched Continuum-Level Material Model for Kevlar®-Fiber-Reinforced Polymer-Matrix Composites." *Journal of Materials Engineering and Performance*, 22(3), 681-695. doi: <http://dx.doi.org/10.1007/s11665-012-0329-6>.
- 2 McAllister, Q. Gillespie, J. and VanLandingham, M. (2013) "The influence of surface microstructure on the scratch characteristics of Kevlar fibers." *Journal of Materials Science*, 48(3), 1292-1302. doi:

- http://dx.doi.org/10.1007/s10853-012-6872-6.
- 3 McAllister, Q. Gillespie, J. and VanLandingham, M. (2013) "The sub-micron scale energy dissipative deformation mechanisms of Kevlar fibrils." *Journal of Materials Science*, 48(18), 6245-6261. doi: http://dx.doi.org/10.1007/s10853-013-7422-6.
 - 4 *Nilakantan, G. Wetzel, E. Bogetti, T. and Gillespie, J. (2013) "A deterministic finite element analysis of the effects of projectile characteristics on the impact response of fully clamped flexible woven fabrics." *Composite Structures*, 95, 191-201. doi: https://doi.org/10.1016/j.compstruc.t.2012.07.023.
 - 5 Nilakantan, G. and Gillespie, J. (2013) "Yarn pull-out behavior of plain woven Kevlar fabrics: Effect of yarn sizing, pullout rate, and fabric pre-tension." *Composite Structures*, 101, 215-224. doi: https://doi.org/10.1016/j.compstruc.t.2013.02.018.
 - 6 Rahman, R. Foster, J. and Haque, A. (2013) "Molecular dynamics simulation and characterization of graphene-cellulose nanocomposites." *The Journal of Physical Chemistry A*, 117(25), 5344-5353. doi: https://doi.org/10.1021/jp402814t.
 - 7 Sirk, T. Khare, K. Karim, M. Lenhart, J. Andzelm, J. McKenna, G. and Khare, R. (2013) "High strain rate mechanical properties of a cross-linked epoxy across the glass transition." *Polymer*, 54(26), 7048-7057. doi: https://doi.org/10.1016/j.polymer.2013.10.051.
 - 8 Sliozberg, Y. and Chantawansri, T. (2013) "Computational study of imperfect networks using a coarse-grained model." *The Journal of Chemical Physics*, 139(19), 194-904. doi: http://dx.doi.org/10.1063/1.4832140.

2012

- 1 Chantawansri, T. Sliozberg, Y. Andzelm, J. and Hsieh, A. (2012) "Coarse-grained modeling of model poly(urethane urea)s: Microstructure and interface aspects." *Polymer*, 53(20), 4512-4524. doi: https://doi.org/10.1016/j.polymer.2012.07.056.
- 2 Grujicic, M. Hariharan, A. Pandurangan, B. Yen, C. Cheeseman, B. Wang, Y. Miao, Y. and Zheng, J. (2012) "Fiber-Level Modeling of Dynamic Strength of Kevlar® KM2 Ballistic Fabric." *Journal of Materials Engineering and Performance*, 21(7), 1107-1119. doi: http://dx.doi.org/10.1007/s11665-011-0006-1.

- 3 McAllister, Q. Gillespie, J. and VanLandingham, M. (2012) "Evaluation of the three-dimensional properties of Kevlar across length scales." *Journal of Materials Research*, 27(14), 1824-1837. doi: https://doi.org/10.1557/jmr.2012.80.
- 4 McAllister, Q. Gillespie, J. and VanLandingham, M. (2012) "Nonlinear indentation of fibers." *Journal of Materials Research*, 27(1), 197-213. doi: https://doi.org/10.1557/jmr.2011.336.
- 5 Nilakantan, G. and Gillespie, J. (2012) "Ballistic impact modeling of woven fabrics considering yarn strength, friction, projectile impact location, and fabric boundary condition effects." *Composite Structures*, 94(12), 3624-3634. doi: https://doi.org/10.1016/j.compstruct.2012.05.030.
- 6 *Nilakantan, G. Keefe, M. Wetzel, E. Bogetti, T. and Gillespie, J. (2012) "Effect of statistical yarn tensile strength on the probabilistic impact response of woven fabrics." *Composites Science and Technology*, 72(2), 320-329. doi: https://doi.org/10.1016/j.compscitech.2011.11.021.
- 7 *Nilakantan, G. Wetzel, E. Bogetti, T. and Gillespie, J. (2012) "Finite element analysis of projectile size and shape effects on the probabilistic penetration response of high strength fabrics." *Composite Structures*, 94(5), 1846-1854. doi: https://doi.org/10.1016/j.compstruct.2011.12.028.
- 8 Sirk, T. Sliozberg, Y. Brennan, J. Lisal, M. and Andzelm, J. (2012) "An enhanced entangled polymer model for dissipative particle dynamics." *The Journal of Chemical Physics*, 136(13), 134-903. doi: https://doi.org/10.1063/1.3698476.
- 9 Sliozberg, Y. Sirk, T. Brennan, J. and Andzelm, J. (2012) "Bead-spring models of entangled polymer melts: Comparison of hard-core and soft-core potentials." *Journal of Polymer Science Part B: Polymer Physics*, 50(24), 1694-1698. doi: http://dx.doi.org/10.1002/polb.23175.
- 10 Sliozberg, Y. and Andzelm, J. (2012) "Fast protocol for equilibration of entangled and branched polymer chains." *Chemical Physics Letters*, 523, 139-143. doi: https://doi.org/10.1016/j.cplett.2011.12.040.

Integrative

2017

- 1 Barnes, B. Leiter, K. Becker, R. Knap, J. and Brennan, J. (2017) "LAMMPS integrated

- materials engine (LIME) for efficient automation of particle-based simulations: application to equation of state generation." *Modelling and Simulation in Materials Science and Engineering*, 25(5), 55006-55006. doi: <https://doi.org/10.1088/1361-651X/aa6e36>.
- 2 *Voisin, T. Grapes, M. Zhang, Y. Lorenzo, N. Ligda, J. Schuster, B. and Weihs, T. (2017) "TEM sample preparation by femtosecond laser machining and ion milling for high-rate TEM straining experiments." *Ultramicroscopy*, 175, 1-8. doi: <https://doi.org/10.1016/j.ultramic.2016.12.001>.
 - 3 Wildman, R. O'Grady, J. and Gazonas, G. (2017) "A hybrid multiscale finite element/peridynamics method." *International Journal of Fracture*, 207(1), 41-53. doi: <http://dx.doi.org/10.1007/s10704-017-0218-y>.

2016

- 1 Carey, N. Budavari, T. Daphalapurkar, N. and Ramesh, K. (2016) "Data integration for materials research." *Integrating Materials and Manufacturing Innovation*, 5(1), 7-7. doi: <https://doi.org/10.1186/s40192-016-0049-0>.
- 2 Clayton, J. and Knap, J. (2016) "Phase field modeling and simulation of coupled fracture and twinning in single crystals and polycrystals." *Computer Methods in Applied Mechanics and Engineering*, 312, 447-467. doi: <https://doi.org/10.1016/j.cma.2016.01.023>.
- 3 Knap, J. Spear, C. Leiter, K. Becker, R. and Powell, D. (2016) "A computational framework for scale-bridging in multi-scale simulations." *International Journal for Numerical Methods in Engineering*, 108(13), 1649-1666. doi: <http://dx.doi.org/10.1002/nme.5270>.

2015

- 1 Clayton, J. and Knap, J. (2015) "Nonlinear phase field theory for fracture and twinning with analysis of simple shear." *Philosophical Magazine*, 95(24), 2661-2696. doi: <http://dx.doi.org/10.1080/14786435.2015.1076176>.
- 2 Clayton, J. and Knap, J. (2015) "Phase field modeling of directional fracture in anisotropic polycrystals." *Computational Materials Science*, 98, 158-169. doi: <https://doi.org/10.1016/j.commatsci.2014.11.009>.
- 3 *Strack, O. Leavy, B. and Brannon, R. (2015) "Aleatory uncertainty and scale effects in

computational damage models for failure and fragmentation." *International Journal for Numerical Methods in Engineering*, 102, 468-495. doi: <http://dx.doi.org/10.1002/nme.4699>.

- 4 Zhang, L. Jasa, J. Gazonas, G. Jérusalem, A. and Negahban, M. (2015) "Extracting continuum-like deformation and stress from molecular dynamics simulations." *Computer Methods in Applied Mechanics and Engineering*, 283, 1010-1031. doi: <https://doi.org/10.1016/j.cma.2014.10.018>.

2014

- 1 Brennan, J. Lisal, M. Moore, J. Izvekov, S. Schweigert, I. and Larentzos, J. (2014) "Coarse-Grain Model Simulations of Nonequilibrium Dynamics in Heterogeneous Materials." *The Journal of Physical Chemistry Letters*, 5(12), 2144-2149. doi: <https://doi.org/10.1021/jz500756s>.
- 2 Clayton, J. (2014) "Article Navigation An alternative three-term decomposition for single crystal deformation motivated by non-linear elastic dislocation solutions." *The Quarterly Journal of Mechanics and Applied Mathematics*, 67(1), 127-158. doi: <https://doi.org/10.1093/qjmam/hbt026>.
- 3 Izvekov, S. and Rice, B. (2014) "Multi-scale coarse-graining of non-conservative interactions in molecular liquids." *The Journal of Chemical Physics*, 140(10), 104-104. doi: <http://dx.doi.org/10.1063/1.4866142>.
- 4 Weile, D. Hopkins, D. Gazonas, G. and Powers, B. (2014) "On the proper formulation of Maxwellian electrodynamics for continuum mechanics." *Continuum Mechanics and Thermodynamics*, 26(3), 387-401. doi: <http://dx.doi.org/10.1007/s00161-013-0308-7>.
- 5 Wildman, R. and Gazonas, G. (2014) "A finite difference-augmented peridynamics method for reducing wave dispersion." *International Journal of Fracture*, 190(1), 39-52. doi: <http://dx.doi.org/10.1007/s10704-014-9973-1>.
- 6 Zimmerman, J. Sabau, A. Zaeem, M. Tschopp, M. and Spearot, D. (2014) "Algorithm Development in Computational Materials Science." *JOM*, 66(3), 397-398. doi: <http://dx.doi.org/10.1007/s11837-013-0846-2>.

2013

- 1 Beaudet, T. Mattson, W. and Rice, B. (2013) "New form of polymeric nitrogen from dynamic shock simulation." *The Journal of Chemical Physics*, 138(5), 54503-54503. doi: <http://dx.doi.org/10.1063/1.4789307>.
- 2 Grinfeld (a.k.a. Greenfield), M. (2013) "Thermodynamic models of phase transformations and failure waves." *Wave Motion*, 50(7), 1118-1126. doi: <https://doi.org/10.1016/j.wavemoti.2013.04.010>.
- 3 Satapathy, S. and Hsieh, K. (2013) "Jump conditions for Maxwell equations and their consequences." *AIP Advances*, 3(1), 12120-12120. doi: <http://dx.doi.org/10.1063/1.4789794>.
- 4 Taylor, D. (2013) "Intermolecular Forces and Molecular Dynamics Simulation of 1,3,5-Triamino-2,4,6-trinitrobenzene (TATB) Using Symmetry Adapted Perturbation Theory." *The Journal of Physical Chemistry A*, 117(16), 3507-3520. doi: <http://dx.doi.org/10.1021/jp4005289>.

2012

- 1 Gazonas, G. and Velo, A. (2012) "Analytical solutions for the resonance response of Gouillaud-type elastic media using z-transform methods." *Wave Motion*, 49(1), 135-151. doi: <https://doi.org/10.1016/j.wavemoti.2011.08.002>.
- 2 McWilliams, R. Kadry, Y. Mahmood, M. Goncharov, A. and Ciezak-Jenkins, J. (2012) "Structural and chemical properties of the nitrogen-rich energetic material triaminoguanidinium 1-methyl-5-nitriminotetrazolate under pressure." *The Journal of Chemical Physics*, 137(5), 54501-54501. doi: <http://dx.doi.org/10.1063/1.4732097>.

Uncategorized

2018

- 1 Lloyd, J. Matejunas, A. Becker, R. Walter, T. Priddy, M. and Kimberley, J. (2018) "Dynamic tensile failure of rolled magnesium: Simulations and experiments quantifying the role of texture and second-phase particles." *International Journal of Plasticity*, Accepted.

Summary

submitted, published, or accepted

	2012	2013	2014	2015	2016	2017	2018	2019	Total
Ceramics	7	4	6	21	23	17	6	0	84
Composites	6	2	6	13	17	9	18	0	71
Metals	6	11	20	12	20	18	6	0	93
Polymers	10	8	11	8	9	20	7	0	73
Integrative	2	4	6	4	3	3	0	0	22
Uncategorized	0	0	0	0	0	0	1	0	1
Total	31	29	49	58	72	67	38	0	344
Joint	8	8	10	9	13	15	8	0	71