RÉMI DINGREVILLE, PH.D.

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Center for Integrated NanoTechnologies ⋄ Sandia National Laboratories

CINT Scientist ⋄ Principal Member of the Technical Staff

SUMMARY

My research expertise is at the intersection of computational material science, experimental materials science and emerging fields in integrated computational mechanics. I employ and combine various theoretical and computational techniques (molecular dynamics, cluster dynamics, phase field, mean field, data mining) to understand and characterize materials aging and performance in solid matter. My research emphasizes designing materials with enhanced functionality through understanding and control of interface and defect phenomena. My research strategy is built on "reduced order mesoscale models", which enable insights into how computational materials science and engineering can be exploited as discovery tools for applications into technologies such as nanostructures or advanced alloys.

EDUCATION

Georgia Institute of Technology *2007*
Ph.D. in Mechanical Engineering

Université de Rennes (France) *2001*
M.S. in Materials Science

École Nationale Supérieure des Techniques Avancées (France) *2001*
B.S. in Mechanical Engineering

RESEARCH AND PROFESSIONAL EXPERIENCE

Sandia National Laboratories *03/2018 – Present*
CINT Scientist — Nanostructure Physics Dept.

Sandia National Laboratories *08/2011 – 03/2018*
Principal Member of the Technical Staff — Dept. of Structural & Thermal Analysis

New York University *09/2009 – 08/2011*
Assistant Professor — Dept. of Mechanical & Aerospace Eng.

Sandia National Laboratories *07/2007 – 09/2009*
Postdoctoral Appointee — Dept. of Computational Materials Science

RESEARCH INTERESTS

- Mechanical behavior and aging of materials under extreme environments (e.g., irradiation or high strain rate), with an emphasis on characterizing the impact of coupled effects (e.g., stress and irradiation) on properties and microstructure evolution.
- Materials design through interface engineering to enhance performance under extreme environments.
- Atomic-scale defect mechanisms and collective response of interfaces under extreme environments.
- Integration of computational materials science simulations with experimental capabilities (simulated experimental measurements).

HONOR AND AWARDS

2017	International visiting scholar fellowship at CNRS, Labex DAMAS.
2017	Sandia National Laboratories SPOT Award for exceptional accomplishments.
2015	Division 6000 (Energy Division) 2015 Up & coming innovator award.
2015	International visiting scholar fellowship at CNRS, Labex DAMAS.
2015	ASME recognition award for tutorial on "Probabilistic Fracture Mechanics" at PVP.
2013	TMS fellowship for the emerging leaders alliance capstone program.
2013	TMS Materials Processing and Manufacturing Division (MPMD) young leader professional development award.
2010	NSF fellowship summer institute of nano mechanics and materials.
2010	R. Dingreville et al., JMPS, 2005, vol. 53(8), p. 1827–1854, #1 most cited journal article for 2005-2010 in the Journal of Mechanics and Physics of Solids.
2009	Sandia National Laboratories SPOT Award for technical accomplishments.
2001	M.S. degree with Honors of the Jury, Université de Rennes, France, 2001.

CURRENT AND PENDING SUPPORT (PRINCIPAL INVESTIGATOR)

Current:

2018–current	*Center for Integrated Nanotechnology.* Source of Funding: Department of Energy – Office of Science (DOE-BES); Amount: 0.5fte/yr.
2017–2019	*Probabilistic Fracture Mechanics.* Source of Funding: U.S. Nuclear Regulatory Commission (USNRC); Amount: \$1.1M.
2017–2019	*Developing Microstructure-Property Correlation of Radiation-Tolerant Nanoporous and Nanostructured Materials for High Irradiation Environments.* Source of Funding: Sandia Nat'l Labs – LDRD; Amount: \$1.85M.
2016–2018	*Fundamentals of Pellet-Clad Debonding.* Source of Funding: Sandia Nat'l Labs – LDRD; Amount: \$1.72M.
2015	*Feasibility of Observing and Characterizing Single Ion Strikes in Microelectronic Components.* Sandia Nat'l Labs – LDRD; Amount: \$100k.
2013–2015	*Predictive Characterization of Aging and Degradation of Reactor Materials in Extreme Environments.* Source of Funding: Department of Energy – Nuclear Energy (DOE-NE) – NEET-3; Amount: \$ 1M.
2012–2018	*Environmental Stress Corrosion Cracking of Welded Canisters.* Source of Funding: Department of Energy – Nuclear Energy (DOE-NE) Amount: \$1.2M
2012–2018	*extremely low probability of rupture (xLPR).* Source of Funding: U.S. Nuclear Regulatory Commission (USNRC); Amount: \$3.1M.

Pending:

2018–2022	*Energy Frontier Research Center: MAterials Discovery for Combined Extremes.* Source of Funding: Department of Energy-Office of Science (DOE-BES); Amount: \$15.5M
2018–2021	*Multi-Resolution Characterization of the Coupling Effects of Molten Salts, High Temperature and Irradiation on Intergranular Fracture.* Source of Funding: Sandia Nat'l Labs – LDRD; Amount: \$ 1.4M.

SYNERGETIC ACTIVITIES

Invited lectures:

2018	International Conference on Plasticity, Damage & Fracture (keynote)	San Juan, PR.
2018	German and European Physical Societies (DPG & EPS), Spring Meeting 2018	Berlin, Germany.
2017	SIAM Annual Meeting	Pittsburgh, PA.
2017	DAMAS Technical Seminar Series	Labex DAMAS, Metz, France.
2017	ME Technical Seminar	UNM, Albuquerque, NM.
2016	ME Technical Seminar	C.U. Boulder, Boulder, CO.
2016	NE/ME Technical Seminar	Georgia Tech, Atlanta, GA.
2016	ME Technical Seminar	LEM3, Metz, France.
2015	DAMAS Technical Seminar Series	Labex DAMAS, Metz, France.
2014	ME Technical Seminar Series	Northwestern, Evanston, IL.
2012	Technical Seminar	Los Alamos National Laboratory, Los Alamos, NM.
2011	ME Technical Seminar	Lehigh University, Bethlehem, PA.
2010	NE Technical Seminar	RMC, Kingston, Canada.
2010	ME Technical Seminar	ETS, Montréal, Canada.
2010	Special Seminar	AECL Chalk River Laboratories, Chalk River, Canada.
2009	ME Technical Seminar	Columbia University, New York, NY.

Chair of organizational committees:

2018–2021	TMS Public & Governmental Affairs Committee.
2017	Lead organizer (co-organizer P.-A. Juan, Sandia Nat'l Labs), "Characterization of fracture and fragmentation phenomena across multiple length scales: from atomistic to macroscopic approaches", MS&T Fall meeting, Pittsburgh, PA.
2014	Lead organizer (co-organizer R.A. Karnesky, Sandia Nat'l Labs; G. Puel, Centrale/Supélec, Université Paris-Saclay; J.-H. Schmitt, Centrale/Supélec, Université Paris-Saclay), "Symposium on Synergies between Computational Modeling and Experimental Characterization", 7^{th} MMM (Multiscale Materials Modeling) Conference, Berkeley, CA.
2013	Lead organizer (co-organizer K. Janssens, PSI, Switzerland), "Integrated computational modeling of materials for nuclear energy", TMS Annual meeting, San Antonio, TX.
2012–2016	TMS Programming Committee, Materials Processing & Manufacturing Division (MPMD).
2010–2012	Chair of TMS Computational Materials Science & Engineering committee, MPMD.
2010	Lead organizer (co-organizer K. Janssens, PSI, Switzerland), "Computational Plasticity", TMS Annual Meeting, Seattle, WA.
2010	Co-organizer (Lead organizer: T.J. Bartel, Sandia National Laboratories), "Material Point and other Particle Methods: Advances and Applications", WCCM, Sydney, Australia.

Guest editorial activities:

2015	Guest editor Journal of Materials Science (Volume 51 Issue 2), 2015.

Evaluation panels:

2010	NSF review panelist for Condensed Matter and Materials Theory (CMMT) (Diana Farkas, Program Director.
2008	NSF review panelist for Infrastructural Materials SBIR/STTR Phase I (Ben Schrag, Program Director).

Reviewer of journal articles:

Journal of the Mechanics and Physics of Solids, International Journal of Solids and Structures, Acta Materialia, Scripta Materialia, International Journal of Plasticity, Computational Materials Science, Philosophical Magazine, International Journal of Mechanical Sciences, Applied Surface Science, Computational Mechanics, International Journal for Numerical Methods in Engineering, Mechanics of Materials, Mechanics Research Communications, Thin Solid Films.

Reviewer of Research Proposals and Activities:

USA: National Science Foundation (NSF), Army Research Office (ARO), Laboratory Directed Research and Development (LDRD) program; **Switzerland**: Swiss National Science Foundation (SNF); **Canada**: Natural Sciences and Engineering Research Council of Canada (CRSNG).

GRADUATE AND POSTDOCTORAL ADVISEES

Postdoctoral associates:	P.-A. Juan, J. Stewart, C.J. O'Brien.
Graduate student associates (serving as advisor/co-advisor):	D. Aksoy (Ph.D. student, U. Florida), M. Andriamisandratra (M.S. student, ETS, Canada), W. Barrows (M.S. student, U. Arkansas), E. Chen (Ph.D. student, Georgia Tech), A.Y. Dunn (Ph.D. student, Georgia Tech), C. Nellis (Virginia Tech), P. Zarnas (Ph.D. student, Northwestern).

RECENT COLLABORATORS

O. Anderoglu (UNM), T.J. Balk (U. Kentucky), T. Bartel (SNL), J. Bignell (SNL), S. Berbenni (LEM3-CNRS, France), L. Capolungo (LANL), A. Chartier (CEA, France), C. Deo (GeorgiaTech), P. Edmonson (ORNL), S. Foiles (SNL), K. Hattar (SNL), R. Karnesky (SNL), H. Lim (SNL), E. Martínez (LANL), B. Muntifering (SNL), J. Qu (Tufts U.), A. Schleife (UIUC), D.E. Spearot (Florida U.), R.A. Regueiro (C.U. Boulder), J. Robbins (SNL), T. Richeton (LEM3-CNRS, France), V. Tomar (Purdue U.), L. Van Brutzel (CEA, France), T. Voth (SNL), P. Weck (SNL), X.W. Zhou (SNL).

PEER REVIEWED PUBLICATIONS (1045 CITATIONS/ H-INDEX 11)

1. **Dingreville, R.**, J. Qu, and M. Cherkaoui, "Surface free energy and its effect on the elastic behavior of nano-size particles, wires and films". *Journal of the Mechanics and Physics of Solids*, 53(8), 1827–1854, 2005.
2. **Dingreville, R.**, and J. Qu, "A semi-analytical method to compute surface elastic properties". *Acta Materialia*, 55(1), 141–147, 2007.
3. **Dingreville, R.**, A.J. Kulkarni, M. Zhou, and J. Qu, "A semi-analytical method for quantifying the size-dependent elasticity of nanostructures". *Modelling and Simulation in Materials Science and Engineering*, 16(2), 025002, 2008.
4. **Dingreville, R.**, and J. Qu, "Interfacial excess energy, excess stress and excess strain in elastic solids: planar interfaces". *Journal of the Mechanics and Physics of Solids*, 56(5), 1944–1954, 2008.
5. **Dingreville, R.**, and J. Qu, 'A semi-analytical method to estimate interface elastic properties". *Computational Materials Science*, 46(1), 83–91, 2009.

6. **Dingreville, R.**, C.C. Battaile, L.N. Brewer, E.A. Holm, and B.L. Boyce, "The effect of microstructural representation on simulations of microplastic ratcheting". *International Journal of Plasticity*, 26(5), 617–633, 2010.

7. Zhang, L., **R. Dingreville**, T.J. Bartel, and M.T. Lusk, "Hybrid Monte Carlo simulation of stress-induced texture evolution with inelastic effects". *Metallurgical and Materials Transactions A*, 43(3), 575–581, 2011.

8. Zhang, L., **R. Dingreville**, T.J. Bartel, and M.T. Lusk, "A stochastic approach to capture crystal plasticity". *International Journal of Plasticity*, 27(9), 1432–1444, 2011.

9. **Dingreville, R.**, J. Robbins, and T. E. Voth, "Multiresolution modeling of the dynamic loading of metal matrix composites". *JOM*, 65(2), 203–214, 2013.

10. **Dingreville, R.**, J. Robbins, and T. E. Voth, "Wave propagation and dispersion in elasto-plastic microstructured materials". *International Journal of Solids and Structures*, 51(11), 203–214, 2014.

11. **Dingreville, R.**, A. Hallil, and S. Berbenni, "From coherent to incoherent mismatched interfaces: A generalized continuum formulation of surface stresses". *Journal of the Mechanics and Physics of Solids*, 72, 40–60, 2014.

12. **Dingreville, R.**, A. Eckert-Gallup, and C. Sallaberry, "Uncertainty analysis for the net-section-collapse failure criterion of circumferentially cracked cylinders for multiple arbitrary-shaped circumferential cracks". *International Journal of Pressure Vessels and Piping*, 123, 30–45, 2014.

13. Muntifering, B., **R. Dingreville**, K. Hattar, and J. Qu, "Electron Beam Effects during In-Situ Annealing of Self-Ion Irradiated Nanocrystalline Nickel". *Materials Research Letters*, 4(2), 96–103, 2016.

14. Rudland, D., C. Harrington, and **R. Dingreville, R.**, "Development of the extremely low probability of rupture (xLPR) Version 2.0 code". *Proceedings of the 2015 ASME Pressure Vessels and Piping Conference*, PVP2015-45134, 2015.

15. Dunn, A., **R. Dingreville**, and L. Capolungo, "Multi-scale simulation of radiation damage accumulation and subsequent hardening in neutron-irradiated α-Fe". *Modelling and Simulation in Materials Science and Engineering*, 24(1), 015005, 2015.

16. **Dingreville, R.**, R.A. Karnesky, G. Puel, and J.-H. Schmitt, "Review of the synergies between computational modeling and experimental characterization of materials across length scales". *Journal of Materials Science*, 51(3), 1178–1203, 2016.

17. Muntifering, B., S.J. Blair, C. Gong, A. Dunn, **R. Dingreville**, J. Qu, K. Hattar, "Cavity evolution at grain boundaries as a function of radiation damage and thermal conditions in nanocrystalline nickel". *MRS Proceedings, 1809, 13–18, 2015.*

18. Lim, H., **R. Dingreville**, L.A. Deibler, T.E. Buchheit, C.C. Battaile, "Investigation of grain-scale microstructural variability in tantalum using crystal plasticity-finite element simulations". *Computational Materials Science*, 117, 437–444, 2016.

19. Dunn, A., **R. Dingreville**, and L. Capolungo, "Identification of dominant damage accumulation processes at grain boundaries during irradiation in nanocrystalline α-Fe: A statistical study". *Acta Materialia*, 110, 306–323, 2016.

20. Dunn, A., **R. Dingreville**, E. Martínez and L. Capolungo, "Synchronous parallel spatially resolved stochastic cluster dynamics". *Computational Materials Science*, 120, 43–52, 2016.

21. **Dingreville, R.**, and S. Berbenni, "On the interaction of solutes with grain boundaries". *Acta Materialia*, 104(104), 237–249, 2015.

22. Barrows, W., **R. Dingreville**, and D.E. Spearot, "Traction-separation relationships for hydrogen induced grain boundary embrittlement in nickel via molecular dynamics simulations". *Materials Science and Engineering: A*, 560(5), 354–364, 2016.

23. Muntifering, B., Y. Fang, A.C. Leff, A. Dunn, J. Qu, M.L. Taheri, **R. Dingreville**, and K. Hattar, "*In situ* Transmission Electron Microscopy He^+ implantation and thermal aging of nanocrystalline iron". *Journal of Nuclear Materials*, 482, 139–146, 2016.

24. Dunn, A., B. Muntifering, **R. Dingreville**, K. Hattar, and L. Capolungo, "Displacement rate and temperature equivalence in stochastic cluster dynamics simulations of irradiated pure α-Fe". *Journal of Nuclear Materials*, 480, 129–137, 2016.

25. Weck, P.F, P.-A. Juan, **R. Dingreville**, E. Kim, "Density functional analysis of fluorite-structured (Ce, Zr)O_2/CeO_2 interfaces". *The Journal of Physical Chemistry C*, 121(27), 14678–14687, 2017.

26. Juan, P.-A., and **R. Dingreville**, "Mechanics of finite cracks in dissimilar anisotropic elastic media considering interfacial elasticity". *Journal of the Mechanics and Physics of Solids*, 99, 1–18, 2017.

27. **Dingreville, R.**, D. Aksoy, and D.E. Spearot, "A primer on selecting grain boundary sets for comparison of interfacial fracture properties in molecular dynamics simulations". *Scientific Reports*, 7(1), 8332, 2017.

28. C.J. O'Brien, P.-A. Juan, J. Bignell, and **R. Dingreville**, "Fragmentation prediction for a brittle ceramic: An integrated two-scale model approach". *Transactions of the American Nuclear Society*, 116, 2017.

29. Schleife, A., C.W. Lee, K. Hattar, **R. Dingreville**, S. Foiles, "Multiscale modeling of electron-ion dynamics in silicon under particle radiation". *Bulletin of the American Physical Society*, 62, 2017.

30. Zarnas, P., **R. Dingreville** and J. Qu, "Mechanics of radiation-induced defects segregation to dislocations and grain boundaries: a chemomechanical framework". *Computational Materials Science*, 144, 99–112, 2018.

31. Stewart, J., A. Kohnert, L. Capolungo and **R. Dingreville** and J. Qu, "Design and Analysis of Cluster Dynamics Simulations for Predicting Radiation Damage Parameter Spaces". *Computational Materials Science*, XXX, 2018 (special issue; invited).

32. Zhou, X.W., **R. Dingreville** and R.A. Karnesky, "Molecular dynamics studies of irradiation effects on hydrogen isotope diffusion through nickel crystals and grain boundaries". *Physical Chemistry Chemical Physics*, 20, 520–534, 2018.

33. Stewart, J., G. Brookman, P. Price, M. Franco, W. Ji, K. Hattar, and **R. Dingreville** R.A. Karnesky, "Characterizing single isolated radiation-damage events from molecular dynamics via virtual diffraction methods". *Journal of Applied Physics*, 123(16), 165902, 2018.

34. Juan, P.-A., and **R. Dingreville**, "Elastic Green's function in anisotropic bimaterials considering interfacial elasticity". *Journal of Elasticity*, 131(2), 277–296, 2018.

BOOK CHAPTERS

1. Van Brutzel, L., **R. Dingreville**, and T.J. Bartel, "Nuclear fuel deformation phenomena". *State-of-the-Art Report on Multi-scale Modelling of Nuclear Fuels. OECD/NEA Working Party on Multi-scale Modelling of Fuels and Structural Materials for Nuclear Systems*, 59, 2015.

2. Spearot, D.E. **R. Dingreville**, C.J. O'Brien, "Atomistic Simulation Techniques to Model Hydrogen Segregation and Hydrogen Embrittlement in Metallic Materials". *Springer Nature Singapore Pte Ltd., C.-H. Hsueh et al. (eds.), Handbook of Mechanics of Materials*, 2018.

INTERNAL (SANDIA NAT'L LABS) REFERENCES

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EXTERNAL REFERENCES

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