

Jaime Marian

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University of California, Los Angeles
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Personal

United States Citizen

Marital Status: married.

Education

M.Sc. Power Engineering, [Universidad Politécnica de Madrid](#), 1997.

Ph.D. Nuclear Engineering, [University of California at Berkeley](#), 2002.

Postdoctoral Scholar, [California Institute of Technology](#), 2002-2004.

Employment

Flexible Term Employee, [Lawrence Livermore National Laboratory](#), 2005-2009.

Staff Scientist, [Lawrence Livermore National Laboratory](#), 2009-2014.

Associate Professor, [Department of Materials Science and Engineering, University of California Los Angeles](#), since June 2014.

Joint appointment in the [Mechanical and Aerospace Engineering Department](#), since December 2016

Honors

Featured speaker at the 2016 Modeling Experimentation Validation (MeV) Summer School, Oak Ridge National Laboratory, July 18-29, 2016.

Paper highlighted in [Advances in Engineering](#).

Winner of DOE's Early Career Research Award (April 2012).

Finalist of the Nicholas Metropolis Award to the best thesis in computational physics, 2003.

Winner of a "Ramón y Cajal" Fellowship from the Spanish Ministry of Education and Science, May 2003 (declined).

Current Active Projects

Title: **Early Career Research Award: Computational Modeling and Design of Radiation Tolerant Materials in Fusion Environments.**

PI: Jaime Marian.

Sponsor: DOE-Office of Fusion Energy Sciences, Sponsor Award Number: DE-SC0012774:0001.

Effort on Project: 2 months per year of summer salary support. 12 months per year of postdoctoral researcher support.

Total Award Amount: \$450,000.

Period of Performance: 11/01/14-11/01/17.

Title: **A Physically-Based Model for the Degradation of Zirconium Cladding in LWR Environments.**

PI: Jaime Marian.

Sponsor: Consortium for Advanced Simulation of Light Water Reactors (CASL/DOE-ORNL), Project Subcontract 4000139957.

Effort on Project: 1 month per year of summer salary, 12 months per year of postdoctoral researcher support.

Total Award Amount: \$120,000.

Period of Performance: 10/01/16-09/30/17

Title: **Understanding the Fundamental Mechanisms of Serrated Flow in BCC Alloys and their Impact on Mechanical Response: A Validated Mesoscopic Computational Study.**

PI: Jaime Marian. *Co-PI:* Marta Pozuelo.

Sponsor: National Science Foundation, DMR - 1611342.

Effort on Project: 0.5 summer month per year. 18 months effort per year of graduate student support.

Total Award Amount: \$444,654.

Period of Performance: 9/01/16-08/31/19.

Title: **Resilient Self-Healing Materials for the Extreme Environment of Space Electric Propulsion & Power**

PI: Nasr Ghoniem. *Co-PI:* Jaime Marian.

Sponsor: Air Force Office of Scientific Research, AFOSR - 16RT0799.

Effort on Project: 1.0 summer month per year. 9 months effort per year of graduate student support.

Total Award Amount: \$1,800,000.

Period of Performance: 10/01/16-09/30/19.

Academic activities

Teaching

MS 143A: "Mechanical behavior of Materials" (Upper division undergraduate class, WQ 2015, 2016, 2017)

MS 298SEM: "Numerical Methods to Study Materials Behavior across Multiple Length and Time Scales" (graduate class, spring quarter 2015)

MS 243C: "Dislocations and Strengthening Mechanisms in Solids" (graduate class, FQ 2015, 2016)

MS 132: "Structure and Properties of Metallic Alloys" (Upper division undergraduate class, SQ 2016)

Service in qualifying oral examinations

Owen Liang/MSE and Zhanlue Yang/MSE (December 2016)

Junsoo Park/MSE, Yu-Sheng Kuo/MSE (September 2016)

Roxanne Radpour/MSE (July 2016)

Sheng-Yung Chang/MSE and Brian Ramirez/MAE (March 2016)
Dustin Chen/MSE (February 2016)
Yue Huang/MSE, Jiatong Chen/MSE, and Xinke Yu/MSE (December 2015)
Bandar Al-Mangour/MSE (November 2015)
Yun-Chiao Huang/MSE (September 2015)
Hongxiang Zhao/MSE (August 2015)
Jon Van Lew/MAE (June 2015)
Chezheng Cao /MSE (May 2015)
Christopher Matthes/MAE (April 2015)
Andrew Sheng/MAE (April 2015)
Edward Gao/MAE (April 2015)
Cheng-Hsi Huang/MSE (March 2015)
Po-Yuan Wang/MSE (February 2015)
Yao-Tsung Hsieh/MSE (December 2014)
Hongjie Zhang/MAE (December 2014)
Zhongbo Yan/MSE (August 2014)

PhD defense committee participation

Dustin Chen/MSE (December 2016)
Bandar Al-Mangour/MSE (November 2016)
Yi Xia/MSE (July 2016)
Jon Van Lew/MAE (June 2016)
Christopher Matthes/MAE (May 2016)

Advised Students

PhD graduates

David Cereceda, UPM (co-advised)
Celia Reina, Caltech (co-advised)
Gabriela Venturini, Caltech (co-advised)
Enrique Martinez, UPM (co-advised)

Current students

Nicholas Julian (PhD)
Hsing-Yin Chang (PhD)
Cheng-Hsi Huang (PhD)
Yue Zhao (PhD)
Michael Reyes (PhD/MAE)

Qianran Yu (MSc)

Feng Cao (BSc)
Kevin Chu (BSc)

Other students

Xiaoxi Huang, Cross-disciplinary Scholars in Science and Technology (CSST), summer 2016.
Ricardo Garcia and Preston Rozwood, HSSEAS High School Summer Research Program (HSSRP), summer 2016.

Patents

J. Marian, P. DeMange, M. Caro, A. Caro and J. C. Farmer.
"Beryllium Pebble Designs for Neutron Multiplication in (Inertial Confinement) Fusion/Fission Hybrids"
Attorney Docket No: 027512-001501US
Client Reference No: IL-12128-I

E. Moses, M. Serrano de Caro, J. Marian, P. Demange, A. Arsenlis, J. H. Satcher, J. F. Latkowski, R. P. Abbott, T. Diaz de la Rubia and J. C. Farmer.
"TRISO Fuel for High Burn-up Nuclear Engine"
Attorney Docket No:
Client Reference No: IL-12021

Peer-reviewed Publications

Journal Articles

1. Jaime Marian, Charlotte Becquart, Christophe Domain, Sergei Dudarev, Mark Gilbert, Richard Kurtz, Daniel Mason, Kai Nordlund, Andrea Sand, Lance Snead, Tomoaki Suzudo, and Brian Wirth, "Recent advances in computational materials modeling of tungsten as plasma-facing material for fusion energy applications", accepted in *Nuclear Fusion* (2016).
2. Nikhil Admal Chandra, Jaime Marian, Giacomo Po, "The atomistic representation of first strain-gradient elastic tensors", *Journal of the Mechanics and Physics of Solids* **99** (2017) 93-115.
3. M. Pozuelo, Y. W. Chang, J. Marian, J.-M. Yang, "Serrated flow in Nanostructured Binary Mg-Al alloys", *Scripta Materialia* **127** (2017) 178-181.
--- 2016 -----
4. Asghar Aryanfar, John Thomas, Anton Van der Ven, Donghua Xu, Mostafa Youssef, Jing Yang, Bilge Yildiz, and Jaime Marian, "Integrated Computational Modeling of Waterside Corrosion in Zirconium Metal Clad under Nominal LWR Operating Conditions", *JOM* **68** (2016) 2900-2911.
5. Giacomo Po, Yinan Cui, David Rivera, David Cereceda, Tom D. Swinburne, Jaime Marian, and Nasr Ghoniem, "A phenomenological dislocation mobility law for bcc metals", *Acta Materialia* **119** (2016) 123-135.
6. Chen-Hsi Huang and Jaime Marian, "A Generalized Ising Model for studying Alloy Evolution under Irradiation and its use in Kinetic Monte Carlo Simulations", *Journal of Physics: Condensed Matter* **28** (2016) 425201.
7. Leili Gharaee, Jaime Marian, and Paul Erhart, "Role of interstitial binding in radiation-induced segregation in W-Re alloys", *Journal of Applied Physics* **120** (2016) 025901.

8. Luigi E. Perotti, Sanjay Dharmavaram, William S. Klug, [Jaime Marian](#), Joseph Rudnick, Robijn Bruinsma, "Useful Scars: Physics of the Capsids of Archaeal Viruses", *Physical Review E* **94** (2016) 012404.
9. David Cereceda, Martin Diehl, Franz Roters, Dierk Raabe, J. Manuel Perlado, [Jaime Marian](#), "Unraveling the temperature dependence of the yield strength in single-crystal tungsten using atomistically-informed crystal plasticity calculations", *International Journal of Plasticity* **78** (2016) 242-265.
--- 2015 -----
10. Luis A. Sandoval, Celia Reina, and [Jaime Marian](#), "Formation of Nanotwin Networks during High-Temperature Crystallization of Amorphous Germanium", *Scientific Reports* **5** (2015) 17251.
11. M. R. Gilbert, [J. Marian](#), J.-Ch. Sublet, "Energy spectra of primary knock-on atoms under neutron irradiation", *Journal of Nuclear Materials* **467** (2015) 121-134.
12. David Cereceda, Martin Diehl, Franz Roters, Pratheek Shanthraj, Dierk Raabe, José Manuel Perlado, and [Jaime Marian](#), "Linking atomistic, kinetic Monte Carlo and crystal plasticity simulations of single-crystal tungsten strength", *GAMM-Mitteilungen* **38** (2015) 213-227.
13. Tuan Hoang, [Jaime Marian](#), Vasily V. Bulatov and Peter Hosemann, "Computationally-efficient stochastic cluster dynamics method for modeling damage accumulation in irradiated materials", *Journal of Computational Physics* **300** (2015) 254-268.
14. [Jaime Marian](#), Tuan Hoang, Michael Fluss and Luke Hsiung, "A Review of Helium-Hydrogen Synergistic Effects in Radiation Damage Observed in Fusion Energy Steels and an Interaction Model to Guide Future Understanding", *Journal of Nuclear Materials* **462** (2015) 409-421.
15. Alexander Stukowski, David Cereceda, Thomas D. Swinburne, [Jaime Marian](#), "Thermally-activated Non-Schmid Glide of Screw Dislocations in W using Atomistically-informed Kinetic Monte Carlo Simulations", *International Journal of Plasticity* **65** (2015) 108-130.
--- 2014 -----
16. M. Z. Hossain and [J. Marian](#), "Stress-dependent solute energetics in W-Re alloys from first-principles calculations", *Acta Materialia* **80** (2014) 107.
17. Jerome Nilmeier and [Jaime Marian](#), "A rigorous sequential update strategy for parallel kinetic Monte Carlo simulation", *Computer Physics Communications* **185** (2014) 2467.
18. C. Reina, L. Sandoval, and [J. Marian](#), "Mesoscale computational study of the nanocrystallization of amorphous Ge via a self-consistent atomistic phase-field model", *Acta Materialia* **77** (2014) 335.
19. C. Reina and [J. Marian](#), "Slip-induced conservation laws for dislocation structures in the finite kinematic framework", *Journal of Mechanics and Physics of Solids* **69** (2014) 123.
20. Meijie Tang and [Jaime Marian](#), "Temperature and high strain rate dependence of tensile deformation behavior in single crystal iron from dislocation dynamics simulations", *Acta Materialia* **70** (2014) 123.
21. Sylvain Queyreau, [Jaime Marian](#), Brian D. Wirth, A. Arsenlis, "Analytical integration of the forces induced by dislocations on a surface element", *Modelling and Simulation in Materials Science and Engineering* **22** (2014) 035004.
22. Luis Sandoval, Geoffrey H. Campbell, and [Jaime Marian](#), "Thermodynamic interpretation of reactive processes in Ni-Al nanolayers from atomistic simulations", *Modelling and Simulation in Materials Science and Engineering* **22** (2014) 025022.
--- 2013 -----

23. M.-C. Marinica, Lisa Ventelon, M. R. Gilbert, L. Proville, S. L. Dudarev, J. Marian, G. Bencteux, F. Willaime, "Interatomic potentials for modelling radiation defects and dislocations in tungsten", *Journal of Physics: Condensed Matter* **25** (2013) 395502.
24. M. R. Gilbert, P. Schuck, B. Sadigh, and J. Marian, "Free energy generalization of the Peierls potential in iron", *Physical Review Letters* **111** (2013) 095502.
25. P. Erhart, J. Marian, and B. Sadigh, "Thermodynamic and mechanical properties of copper precipitates in α -iron from atomistic simulations", *Physical Review B* **88** (2013) 024116.
26. Y. Morris Wang, Frederic Sansoz, Thomas LaGrange, Ryan T. Ott, Jaime Marian, Troy W. Barbee Jr and Alex V. Hamza, "Defective twin boundaries in nanotwinned metals", *Nature Materials* **12** (2013) 697.
27. D. Cereceda, A. Stukowski, M. R. Gilbert, S. Queyreau, L. Ventelon, M.-C. Marinica, J. M. Perlado and J. Marian, "Assessment of interatomic potentials for atomistic analysis of static and dynamic properties of screw dislocations in W", *Journal of Physics: Condensed Matter* **25** (2013) 085702.
28. N. Barton, A. Arsenlis, and J. Marian, "A Polycrystal Plasticity Model of Strain Localization in Irradiated Iron", *Journal of the Mechanics and Physics of Solids* **61** (2013) 341-351.
29. I. R. Vatne, A. Stukowski, C. Thaulow, E. Østby and Jaime Marian, "Three-dimensional crack initiation mechanisms in bcc-Fe under loading modes I, II and III", *Materials Science and Engineering A* **560** (2013) 306-314.
--- 2012 -----
30. J. Marian, T. Hoang, "Modeling fast neutron irradiation damage accumulation in tungsten", *Journal of Nuclear Materials* **429** (2012) 293-297.
31. D. Cereceda, J. M. Perlado, and J. Marian, "Techniques to accelerate convergence of stress-controlled molecular dynamics simulations of dislocation motion", *Computational Materials Science* **62** (2012) 272-275.
32. A. Arsenlis, M. Rhee, G. Hommes, R. Cook and J. Marian, "A dislocation dynamics study of the transition from homogeneous to heterogeneous deformation in irradiated body-centered cubic iron", *Acta Materialia* **60** (2012) 3748-3757.
33. G. Venturini, J. Marian, J. Knap, G. Campbell, M. Ortiz, "Thermal Expansion Behavior of Al and Ta using a Finite-Temperature Extension of the Quasicontinuum Method", *International Journal for Multiscale Computational Engineering* **10** (2012) 1-11.
--- 2011 -----
34. M. R. Gilbert, S. Queyreau, and J. Marian, "Stress and temperature dependence of screw dislocation mobility in α -Fe by molecular dynamics", *Physical Review B* **84** (2011) 174103.
35. C. Reina, J. Marian, and M. Ortiz, "Nanovoid nucleation by vacancy aggregation and vacancy-cluster coarsening in high-purity metallic single crystals", *Physical Review B* **84** (2011) 104117.
36. S. Queyreau, J. Marian, M. R. Gilbert, and B. D. Wirth, "Edge dislocation mobilities in bcc Fe obtained by molecular dynamics", *Physical Review B* **84** (2011) 064106.
37. J. Marian and V. V. Bulatov, "Stochastic cluster dynamics method for simulations of multispecies irradiation damage accumulation", *Journal of Nuclear Materials* **415** (2011) 84-95.
38. Paul Erhart and Jaime Marian, "Calculation of the substitutional fraction of ion-implanted He in an α -Fe target", *Journal of Nuclear Materials* **414** (2011) 426-430.

39. N. Barton, J. V. Bernier, R. Becker, A. Arsenlis, R. Cavallo, J. Marian, M. Rhee, H.-S. Park, B. A Remington, R. T. Olson, "A multi-scale strength model for extreme loading conditions", *Journal of Applied Physics* **109** (2011) 073501.
40. A. Higginbotham, E. M. Bringa, J. Marian, N. Park, M. Suggit, and J. S. Wark, "Simulations of copper single crystals subjected to rapid shear", *Journal of Applied Physics* **109** (2011) 063530.
41. J. Marian, "Generation of an amorphous graphite substrate by cumulative deuterium bombardment using molecular dynamics with full non-bonded interactions", *Journal of Applied Physics* **109** (2011) 063501.
42. E. Martinez, P. R. Monasterio and J. Marian, "Billion-atom Synchronous Parallel Kinetic Monte Carlo Simulations of Critical 3D Ising Systems", *Journal of Computational Physics* **230** (2011) 1359-1369.
--- 2010 -----
43. P. S. DeMange, J. Marian, M. Caro and A. Caro, "TRISO-fuel element thermo-mechanical performance modeling for the hybrid LIFE engine with Pu fuel blanket", *Journal of Nuclear Materials* **405** (2010) 144-155.
44. J. Marian, G. Venturini, B. L. Hansen, J. Knap, M. Ortiz and G. H. Campbell, "Finite-Temperature Extension of the Quasicontinuum Method using Langevin Dynamics: Entropy Losses and Analysis of Errors", *Modelling and Simulation in Materials Science and Engineering* **18** (2010) 01500317.
--- 2009 -----
45. J. Marian, E. Martinez, H-J. Lee and B. D. Wirth, "Micro/Mesoscale Study of Dislocation-Stacking Fault Tetrahedra in Irradiated Copper", *Journal of Materials Research* **24** (2009) 3628-3635.
46. P. C. Schuck, J. Marian, J. B. Adams and B. Sadigh, "Vibrational properties of straight dislocations in bcc and fcc metals within the harmonic approximation", *Philosophical Magazine* **89** (2009) 2861-2882.
47. P. DeMange, J. Marian, M. Caro and A. Caro, "Thermo-mechanical and neutron lifetime modeling and design of Be pebbles in the neutron multiplier for the LIFE engine", *Nuclear Fusion* **49** (2009) 115013.
--- 2008 -----
48. J. Marian, J. Knap and G. H. Campbell, "A Quasicontinuum Study of Nanovoid Collapse under Uniaxial Loading in Ta", *Acta Materialia* **56** (2008) 2839
49. E. Martinez, J. Marian and J. M. Perlado, "A Dislocation Dynamics Study of the Strength of Stacking Fault Tetrahedra. Part II: Interactions with Mixed and Edge Dislocations", *Philosophical Magazine* **88** (2008) 841
50. E. Martinez, J. Marian, A. Arsenlis, M. Victoria and J. M. Perlado, "A Dislocation Dynamics Study of the Strength of Stacking Fault Tetrahedra. Part I: Interactions with Screw Dislocations", *Philosophical Magazine* **88** (2008) 809
51. E. Martinez, J. Marian, M.H. Kalos and J.M. Perlado, "Synchronous parallel kinetic Monte Carlo for continuum diffusion-reaction systems", *Journal of Computational Physics* **227** (2008) 3804-3823.
52. E. Martinez, J. Marian, A. Arsenlis, M. Victoria, J. M. Perlado, "Atomistically-informed dislocation dynamics in fcc crystals", *Journal of the Mechanics and Physics of Solids* **56** (2008) 869-895.
--- 2007 -----
53. J. Marian and J. Knap, "Breakdown of self-similar hardening behavior in Au nanopillar microplasticity", *International Journal for Multiscale Computational Engineering* **5** (3&4) (2007) 287-294.

54. J. Marian, L. A. Zepeda-Ruiz, N. Couto, E. M. Bringa, G. H. Gilmer, P. C. Stangeby and T. D. Rognlien, "Characterization of sputtering products during graphite exposure to deuterium ions by molecular dynamics", *Journal of Applied Physics* **101** (2007) 044506
 --- 2006 -----
55. J. Marian and A. Caro, "Moving dislocations in disordered alloys: Connecting continuum and discrete models with atomistic simulations", *Physical Review B* **74** (2006) 024113/1-12.
56. J. Marian, L. A. Zepeda-Ruiz, G. H. Gilmer, E. M. Bringa, T. Rognlien, "Simulations of carbon sputtering in fusion reactor divertor plates", *Physica Scripta T124* (2006) 65-69.
 --- 2005 -----
57. J. Marian, J. Knap and M. Ortiz, "Nanovoid deformation in Al under simple shear", *Acta Materialia* **53** (2005) 2893-2900.
58. L. A. Zepeda-Ruiz, J. Marian and B. D. Wirth, "On the character of self-interstitial dislocation loops in vanadium", *Philosophical Magazine* **85** (2005) 697-702.
 --- 2004 -----
59. J. Marian, J. Knap and M. Ortiz, "Nanovoid Cavitation by Dislocation Emission in Aluminum", *Physical Review Letters* **93** (2004) p. 165503/1-4.
60. J. Marian, B. D. Wirth, G. R. Odette and J. M. Perlado, "Cu Diffusion in α -Fe: Determination of Solute Diffusivities using Atomic-Scale Simulations", *Computational Materials Science* **31** (2004) 347-367
61. B.D. Wirth, G.R. Odette, J. Marian, L. Ventelon, J.A. Young-Vandersall, L.A. Zepeda-Ruiz, "Multiscale modeling of radiation damage in Fe-based alloys in the fusion environment", *Journal of Nuclear Materials* **329-333** (2004) 103-111.
62. J. Marian, W. Cai and V. V. Bulatov, "Dynamic transitions from smooth to rough to twinning in dislocation motion", *Nature Materials* **3** (2004) 158-163.
 --- 2003 -----
63. J. Marian, B. D. Wirth, R. Schäublin, G. R. Odette and J. M. Perlado, "MD modeling of defects in Fe and their interactions", *Journal of Nuclear Materials* **323** (2003) 181-191.
64. J. M. Perlado, D. Lodi, J. Marian, A. Gonzalez Plata, M. Salvador, L. Colombo, M. J. Caturla, T. Diaz de la Rubia, "Time-Dependent Neutronics in Structural Materials of Inertial Fusion Reactors and Simulation of Defect Accumulation in Pulsed Fe and SiC", *Fusion Science and Technology* **43** (2003) 384-392.
 --- 2002 -----
65. J. Marian, B. D. Wirth and J. M. Perlado, "Mechanism of Formation and Growth of $\langle 100 \rangle$ Interstitial Loops in Ferritic Materials", *Physical Review Letters* **88** (2002) 255507/1-4.
66. J. Marian, B. D. Wirth, A. Caro, B. Sadigh, G. R. Odette, J. M. Perlado and T. Diaz de la Rubia, "Dynamics of self-interstitial cluster migration in pure α -Fe and Fe-Cu alloys", *Physical Review B* **65** (2002) p. 094303/1-5
67. J. Marian, B. D. Wirth, R. Schäublin, J. M. Perlado and T. Diaz de la Rubia, " $\langle 100 \rangle$ -Loop characterization in α -Fe: comparison between experiments and modeling", *Journal of Nuclear Materials* **307-311** (2002) 871-875
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68. J. Marian, B. D. Wirth, J. M. Perlado, G. R. Odette and T. Diaz de la Rubia, "Dynamics of self-interstitial migration in Fe-Cu alloys", *Physical Review B* **64** (2001) p. 144102/1-11
69. J. M. Perlado, E. Dominguez, D. Lodi, L. Malerba, J. Marian, J. Prieto, M. Salvador, T. Diaz de la Rubia, E. Alonso, M. J. Caturla and L. Colombo, "Multiscale modeling of radiation damage of metals and SiC in inertial fusion reactors", *Fusion Technology* **39** (2001) 579-584
70. G. Velarde, J. M. Perlado, E. Alonso, M. Alonso, E. Dominguez, J. G. Rubiano, J. M. Gil, J. Gomez del Rio, D. Lodi, L. Malerba, J. Marian, P. Martel, J. M. Martinez-Val, E. Minguez, M. Piera, F. Ogando, S. Reyes, M. Salvador, J. Sanz, P. Sauvan, M. Velarde and P. Velarde, "Advances in implosion physics, alternative target designs, and neutron effects on heavy ion fusion reactors", *Nuclear Instruments & Methods in Physics Research, Section A* **464** (2001) 61-71
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71. J. M. Perlado, J. Marian and J. G. Sanz, "Neutron fluence, dosimetry and damage response determination in in-core/ex-core components of the VENUS CEN/SCK LWR using 3-D Monte Carlo simulations: NEA's VENUS-3 benchmark", *Nuclear Technology* **129** (2000) 285-296
72. E. Alonso, M. J. Caturla, T. Diaz de la Rubia, N. Soneda, J. Marian, J. M. Perlado and R. E. Stoller, "Comparative study of damage accumulation in iron under magnetic and inertial fusion conditions", *Journal of Nuclear Materials* **283-287** (2000) 768-772.

Book Chapters

Michael J. Fluss, Peter Hosemann, Jaime Marian, "Charged-Particle Irradiation for Neutron Radiation Damage Studies", in *Characterization of Materials*, 10/2012, ISBN: 0471266965.

Conference and Symposium Proceedings

R. E. Rudd, A. Arsenlis, N. R. Barton, R. M. Cavallo, A. J. Comley, B. R. Maddox, J. Marian, H.-S. Park, S. T. Prsbrey, C. E. Wehrenberg, L. Zepeda-Ruiz and B. A. Remington, "Multiscale strength (MS) models: their foundation, their successes, and their challenges", 18th APS-SCCM and 24th AIRAPT, *Journal of Physics: Conference Series* **500** (2014) 112055.

Nathan Barton, Athanasios Arsenlis, Moono Rhee, Jaime Marian, Joel V. Bernier, Meijie Tang, and Lin Yang. "A multi-scale strength model with phase transformation", AIP Conference Proceedings **1426** (2012) 1513.

J. M. Perlado, D. Lodi, J. Marian, A. Gonzalez Plata, M. Salvador, L. Colombo, M. J. Caturla, T. Diaz de la Rubia, "Time-Dependent Neutronics in Structural Materials of Inertial Fusion Reactors y Simulation of Defect Accumulation in Pulsed Fe y SiC", *Fusion Science y Technology* **43** (2003) p. 384-392.

J. Marian, B. D. Wirth, R. Schäublin and J. M. Perlado, " $\langle 100 \rangle$ Dislocation Loop Formation and Characterization in Ferritic Materials: Comparison between Experiments and Modeling", in *Modeling and Numerical Simulation of Materials Behavior and Evolution*, editado por V. Tikare, E. A. Olevsky, A. Zavaliangos y R. G. Elliman (Mater. Res. Soc. Proc. **731**, Warrendale, PA, 2002) W1.4

G. Velarde, J. M. Perlado, E. Alonso, M. Alonso, E. Dominguez, J. G. Rubiano, J. M. Gil, J. Gomez del Rio, D. Lodi, L. Malerba, J. Marian, P. Martel, J. M. Martinez-Val, E. Minguez, M. Piera, F. Ogando, S. Reyes, M. Salvador, J. Sanz, P. Sauvan, M. Velarde and P. Velarde, "Advances in implosion physics, alternative target designs, and neutron effects on heavy ion fusion reactors", *Nuclear Instruments & Methods in Physics Research, Section A* **464** (2001) 61-71.

J. M. Perlado, E. Dominguez, D. Lodi, L. Malerba, J. Marian, J. Prieto, M. Salvador, T. Diaz de la Rubia, E. Alonso, M. J. Caturla and L. Colombo, "Multiscale modeling of radiation damage of metals and SiC in inertial fusion reactors", *Fusion Technology* **39** (2001) 579-584.

J. Marian, B. D. Wirth, J. M. Perlado, T. Diaz de la Rubia, R. Schäublin, D. Lodi, M. Hernandez, G. de Diego, D. Gomez-Briceño and R. E. Stoller, "Direct comparison between modeling and experiment: an α -Fe implantation study", in *Microstructural Processes in Irradiated Materials*, edited by G. E. Lucas, L. L. Snead, M. A. Kirk y R. G. Elliman (Mater. Res. Soc. Proc. **650**, Warrendale, PA, 2001) R3.2.

J. Marian, B. D. Wirth, J. M. Perlado, G. R. Odette and T. Diaz de la Rubia, "Atomistic simulation of vacancy and self-interstitial diffusion in Fe-Cu alloys", in *Microstructural Processes in Irradiated Materials*, editado por G. E. Lucas, L. L. Snead, M. A. Kirk y R. G. Elliman (Mater. Res. Soc. Proc. **650**, Warrendale, PA, 2001) R6.9.

E. Alonso, M. Caturla, T. Diaz de la Rubia, J. Marian, J. M. Perlado and R. Stoller, "Flux Effects on Defect Production and Damage Accumulation in Cu and Fe to Exposed IFE-like Conditions", proceedings of *The First International Conference on Inertial Fusion Sciences and Applications*, Bordeaux, France, September 12-17, 1999.

J. Sanz, J. Marian and J. F. Latkowski, "Activation Analysis of Target Debris in the National Ignition Facility", proceedings of *The First International Conference on Inertial Fusion Sciences and Applications*, Bordeaux, France, September 12-17, 1999

J. M. Perlado, L. Malerba, J. Marian, D. Lodi, T. Diaz de la Rubia and E. Alonso, "Neutron Dynamics y Materials Damage in Inertial Fusion Reactors", proceedings of *The First International Conference on Inertial Fusion Sciences and Applications*, Bordeaux, France, September 12-17, 1999.

J. M. Perlado, J. Marian, D. Lodi and T. Diaz de la Rubia, "Computer simulation of the effect of copper on defect production and damage evolution in ferritic steels", in *Multiscale Phenomena in Materials-Experiments and Modeling*, eds.: B. Devincere, D. H. Lassila, R. Phillips and I. M. Robertson (Mater. Res. Soc. Proc. **578**, Warrendale, PA, 1999) p. 243-248.

J. M. Perlado, J. Marian, D. Lodi, T. Diaz de la Rubia, E. Alonso and M. J. Caturla, "Computer Simulation of Neutron Irradiation Damage in Metallic Systems", in *Proceedings of the IAEA Specialists Meeting on Irradiation Embrittlement and Mitigation*, Madrid, Spain, 26-29 April 1999.

Invited Talks

"Predicting the Temperature Dependence of the Yield Strength in BCC Metals using Atomistically-Informed Crystal Plasticity Calculations", Dislocations-2016, September 19-23, Purdue University.

"Predicting the Temperature Dependence of the Yield Strength in BCC Metals using Atomistically-Informed Crystal Plasticity Calculations", Workshop on Recent Advances in Computational Methods for Nanoscale Phenomena, August 29-31, Ann Arbor, MI.

"Modeling and Simulation Techniques for Structural Materials", invited lecturer at the [MeV Summer School](#), Oak Ridge National Laboratory, 19 July 2016.

"Mesoscale Modeling of Laser-Induced Crystallization of Amorphous Ge", in *Multiscale Behavior of Materials in Extreme Environments*, Symposium MD8, Materials Research Society Spring Meeting, March 28-April 1, 2016, Phoenix, AZ.

"Recent Research Highlights in BCC Alloys: Fundamental Modeling and Microstructure", International Conference on Fusion Reactor Materials, ICFRM-17, October 10-17, 2015, Aachen, Germany. (invited plenary)

"Calculating the release fraction of W tendrils into the plasma using polymeric reptation theory", 2014 Joint ICTP-IAEA Conference on Models and Data for Plasma-Material Interaction in Fusion Devices, November 3-7, 2014, ICTP-Miramare, Trieste, Italy.

"Atomistically-informed Kinetic Monte Carlo Simulations of Screw Dislocation Motion in Tungsten", IUTAM Symposium on Innovative Numerical Approaches for Materials and Structures in Multi-field and Multi-scale Problems, September 1-4, 2014, Burg Schnellenberg, Germany.

"Modeling Fast Neutron Irradiation Damage in Tungsten for Fusion Applications", in Symposium FJ: *Materials Challenges for Future Nuclear Fission and Fusion Technologies*, 6th Forum on New Materials, CIMTEC 2014, June 15-19, 2014, Montecatini Terme, Italy.

"Stochastic Cluster Dynamics Simulations of Irradiation Damage Accumulation in Fusion Materials", 12th Conference on Computer Simulation of Radiation Effects in Solids (COSIRES 2014), June 8-13, 2014, Alicante, Spain.

"Modeling Plastic Flow Localization in Iron: A Multiscale Study connecting Atomistics with Polycrystals", IUTAM Symposium on Micromechanics of Defects in Solids, June 9-13, 2014, Sevilla, Spain.

"Plastic localization in irradiated fusion steels: New insights from modeling and simulation", in *Radiation Hardened Materials for Accelerators, Reactors and Spacecraft*, 247th ACS National Meeting and Exposition, March 16-20, 2014, Dallas, TX.

"Parallelization of Kinetic Monte Carlo Using Synchronous Algorithms: Applications and Differences in Continuum and Discrete Systems", in symposium *Parallel Kinetic Monte Carlo and Discrete-Event Simulation*, SIAM Conference on Parallel Processing for Scientific Computing, February 18-21, 2014, Portland, OR.

"Modelling Irradiation Damage in Tungsten", Workshop on Tungsten for Nuclear Applications, 23-25 September, 2013, Oxford, UK.

"Plastic Localization in Irradiated Ferritic Systems: New Insights from Modeling and Simulation", in Minisymposium TS5: *Predictive Modeling of the Co-Evolution of Microstructure and Properties*, 12th US National Congress on Computational Mechanics, July 22-25, 2013, Raleigh, North Carolina.

"Plastic Localization in Irradiated Ferritic Systems: New Insights from Modeling and Simulation" in *Advances in Materials for Nuclear Energy*, Symposium HH, Materials Research Society Fall Meeting, November 25-30, 2012, Boston, MA.

"Applications of the dislocation dynamics method to irradiation hardening in metals", Conference on Computational Physics CCP11, October 30-November 3, 2011, Gatlinburg, TN.

"Some Accelerated Stochastic Techniques for Irradiation Damage Kinetics", CECAM (Centre European de Calcul Atomique et Moléculaire) Conference Series: Materials Modelling in Nuclear Energy Environments: State of the Art and Beyond, April 26-29, 2010, ETHZ, Zurich, Switzerland.

"Dislocations Dynamics Simulations of Dislocation-Obstacle Interactions in FCC Materials", International Conference on Particle-based Methods (Particles-2009), November 25-27, 2009, Barcelona, Spain.

"Accelerated kinetic Monte Carlo techniques for defect diffusion and agglomeration", *The First International Workshop on Measuring, Modeling and Managing Helium-DPA Effects*, June 15-17, 2009, Paul Scherrer Institut, Switzerland.

"Dislocation Dynamics in fcc Metals" in *Structural and Refractory Materials for Fusion and Fission Technologies*, Symposium JJ, Materials Research Society Fall Meeting, November 27- December 1, 2006, Boston, MA

“Characterization of Sputtering Species in amorphous C:D Thin Films by Molecular Dynamics”, given at the *Plasma Facing Components Meeting*, February 28-March 2, 2006, UCSD, San Diego, CA.

“Simulations of Carbon Sputtering and Sheath Chemistry in Fusion Reactor Divertor Plates”, given at the *US-Japan Fusion Workshop on Low-energy ion sputtering*, University of Wisconsin, Madison, WI, May 19-20, 2005

“Mixed Atomistic/Continuum Modeling of Nanovoid Cavitation and Growth in Al”, in *Multiscale and Stochastic Modeling Methods*, Fourth SIAM Conference on Mathematical Aspects of Materials Science, May 22-26, 2004, Los Angeles, CA.

“MD Modeling of Defects in Fe and their Interaction”, Second IEA Fusion Materials Agreement Workshop on Modeling and Experimental Validation, September 30-October 4, 2002, Les Diablerets, Switzerland.

Conferences Organized

“*Modeling dislocation and hardening processes from atomistic scale to microstructure*” Multiscale Modeling of Materials Conference.
Dijon, France, October 2016.

“*Radiation Damage in Materials--A Grand Multiscale Challenge*”
Symposium EE12--Spring 2016 MRS Meeting.
Phoenix, AZ, March 28-April 1, 2016.

“*Quasicontinuum and other Atomistic-to-Continuum Coupling Techniques*”.
Mini-symposium at the 13th US Congress on Computational Mechanics (USCCM-13).
San Diego, CA, July 26-30, 2015.

“*Predictive Modeling of Irradiation Effects in Structural and Functional Materials?*” 7th International Conference on Multiscale Materials Modeling (MMM-2014), Berkeley, CA, October 6-10, 2014.

“*Recent Advances in Quasicontinuum and Other Atomistic/Continuum Methods*” and
“*Validated Materials Modeling with Quantified Uncertainties Across Scales and Physics*”
Mini-symposia at the 11th World Congress on Computational Mechanics.
Barcelona, Spain, July 20-25, 2014.

International Energy Agency Fusion Modeling Workshop
Lawrence Livermore National Laboratory, April 20-22, 2011
Attendance: 40 registered participants.

“*Quasicontinuum Method & Other Atomistic/Continuum Coupling Techniques & Studies of Microstructural Deformation in Materials*”
Mini-symposium at the 11th US Congress on Computational Mechanics (USNCCM-11)
Minneapolis, MN, July 24-29, 2011.

Synergistic Activities

Member of the *Materials Research Society (MRS)*, *The Minerals, Metals and Materials Society (TMS)*, and *The United States Society for Computational Mechanics (USACM)*.

Invited panelist in the 2015 Mechanical Engineering Graduate Student Association (MEGSA) Research Symposium at UC Riverside: “The Transition from Graduate School into the Professional World”, Thursday, May 14th, 2015.

Referee for technical papers submitted to:

Nature Materials, Nature Communications, Physical Review Letters, International Journal of Plasticity, Physical Review B, Acta Materialia, Journal of Computational Physics, Philosophical Magazine, Journal of Nuclear Materials, Nanotechnology Reviews, Journal of Physics D (Applied Physics), Journal of Materials Research, Nano Letters, Materials Research Letters, Materials Science and Engineering A, Modelling and Simulation in Materials Science and Engineering, Computer Physics Communications, Physics Letters A, International Journal of Solids and Structures, Scripta Materialia, Current Opinion in Solid State & Materials Science, Materials Letters, Advanced Engineering Materials.

Reviewer of technical proposals for: BES, FES, NSF.

Reviewer for DOE's Lawrence Award for Energy Science and Innovation.

Reviewer for the *Deutsche Forschungsgemeinschaft* (German Research Foundation).

Reviewer for EUROfusion Enabling Research projects.

Reviewer for Hong Kong's University Grants Committee Secretariat.

Reviewer for the UC MEXUS-CONACYT postdoctoral and collaborative grant program.

References

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Last updated: December 18, 2016

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