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Department of Materials Science and Engineering
Department of Mechanical Engineering (Joint Appointment)

Arróyave, Raymundo

Education

2004 • **PhD in Materials Science**
Massachusetts Institute of Technology (Cambridge, MA)
Title of Dissertation:*Thermodynamics and Kinetics of Ceramic/Metal Interfacial Interactions*
Minor: Systems Design, Strategy and Policy.
Advisor: Thomas W. Eagar

2000 • **MS in Materials Science and Engineering**
Massachusetts Institute of Technology (Cambridge, MA)
Advisor: Thomas W. Eagar

1996 • **BS in Mechanical and Electrical Engineering**
Instituto Tecnológico y de Estudios Superiores de Monterrey (Monterrey, México)

Positions

2013-present • **Associate Professor. Department of Materials Science and Engineering; Department of Mechanical Engineering (Joint Appointment)**
Texas A & M University, (College Station, TX)

2012-2013 • **Associate Professor. Department of Mechanical Engineering; Interdisciplinary Graduate Program in Materials Science and Engineering**
Texas A & M University, (College Station, TX)

2006-2012 • **Assistant Professor. Department of Mechanical Engineering; Interdisciplinary Graduate Program in Materials Science and Engineering**
Texas A & M University, (College Station, TX)

2004-2006 • **Postdoctoral Scholar**
Pennsylvania State University, (University Park, PA)
Prof. Zi-Kui Liu's Group

1998-2003 • **Research Assistant**
Massachusetts Institute of Technology, (Cambridge, MA)

1997-1998 • **Researcher**
HYLSAMEX, S.A. de C.V., (Monterrey, México)

Interests

Research • Computational materials science; integration of first-principles methods and phenomenological (i.e CALPHAD method) thermodynamic descriptions; alloy theory; development of phase-field methods to describe microstructural evolution; interfacial and surface effects on materials; materials for energy applications; high-temperature materials; multi-functional materials; computational materials design.

Interests (continued)

Teaching

- Thermodynamics; Kinetics; Computational Methods in Materials Science; Phase Transformations; Materials Design; Numerical Analysis; Design of Experiments.

Teaching Experience

2006-present

- Principal Investigator: CCLI: Scaling Up: Classroom-wide Student-led Undergraduate Research Experience for the Introductory Materials Science Course. Funding Agency: National Science Foundation. 08/2010-08/2015.

- **Instructor**
  Texas A&M University, (College Station, TX)
  Average Student Evaluation of 4.0/5.0 in both Graduate and Undergraduate Courses.
  Courses taught:

  ◦ Introduction to Materials Science and Engineering (MEEN 222), Sophomore Level Course. Times taught: 5.

  ◦ Numerical Analysis for Mechanical Engineers (MEEN 357), Junior Level Course. Times taught: 4.

  ◦ Engineering Laboratory (Design of Experiments) (MEEN 404), Senior Level Course. Times taught: 5.

  ◦ Fundamentals of Materials Science and Engineering (MSEN 601), Graduate Level Course. Times taught: 2.

  ◦ Thermodynamics in Materials Science (MSEN 640), Graduate Level Course. Times taught: 7. Note: This course was designed and implemented by R. Arróyave. The course is currently part of the Core Curriculum of the MSEN PhD at Texas A&M University.

  ◦ Kinetics of Materials (MSEN 620), Graduate Level Course. Times taught: 4. Note: This course was designed and implemented by R. Arróyave. The course is currently part of the Core Curriculum of the MSEN PhD at Texas A&M University.

Spring 2005

- **Teaching Assistant, Computational Thermodynamics (MatSE597C)**
  Pennsylvania State University, (University Park, PA)
  Instructor: Prof. Zi-Kui Liu

Fall 2003

- **Teaching Assistant, Materials at Equilibrium (3.20)**
  Massachusetts Institute of Technology, (Cambridge, MA)
  Instructor: Prof. Gerbrand Ceder.

Fall 2001

- **Teaching Assistant, Thermodynamics of Materials (3.00)**
  Massachusetts Institute of Technology, (Cambridge, MA)
  Instructor: Prof. W. Craig Carter.

Honors and Awards

2016

- Engineering Genesis Award. Awarded by the Texas Engineering Experiment Station at Texas A&M University
- TEES Faculty Fellow Award. Awarded by the Texas Engineering Experiment Station at Texas A&M University

Honors and Awards (continued)

2015
- William O. and Montine P. Head Faculty Fellow Award. Awarded by Texas A&M's Dwight Look College of Engineering.

2014
- FMD Journal of Electronic Materials Best Paper Award: Park, M. S.; Gibbons, S. L..; **Arróyave, R.**. *Confinement Effects on Evolution of Intermetallic Compounds during Metallurgical Joint Formation.* Journal of Electronic Materials, (2014), 43, pp. 2510-2520.
- TMS-EMPMD Distinguished Service Award.

2013-2018
- Member Level II—highest ranking is Level III—of the Sistema Nacional de Investigadores (National System of Investigators) of CONACyT, México.

2012
- TEES Select Young Faculty Fellow. Texas Engineering Experiment Station, Texas A&M University.
- Early Career Faculty Fellow Award-Honorable Mention, TMS.

2010
- NSF CAREER Award: "Ab Initio Calculations for Design of High Temperature Materials". Sponsored by NSF-CMMI-MSE Program under Dr. Clark V. Cooper.

2006-2007
- Young Leaders Professional Development Award, EPMD Division. (Formerly known as the Young Leaders Internship Award). The Minerals, Metals and Materials Society (TMS).

2002-2003
- Graduate Research Fellowship. American Welding Society (AWS).

1996
- Academic Excellence Award. Instituto Tecnológico y de Estudios Superiores de Monterrey (Monterrey, México).
- Second Place Statewide, Mechanical Engineer. Awarded by the state of Nuevo León, México and the state professional societies.

Publications

- 101 publications in refereed journals. 21 conference papers published in archived proceedings. One book/report. Students are underlined. 2020 citations. 304 citations in 2015. h-index:24. i-10 index: 50. Source: *Google Scholar Citations*, (Click to Access Google Scholar Profile).

Books, Book Sections and Reports

- Fowler, D.; **Arróyave, R.**, Ross, J. H.; Malak, R.; Banerjee, S. *Looking Outwards from the "Central Science": An Interdisciplinary Perspective on Graduate Education in Materials Chemistry.* In: Educational and Outreach Projects from the Cottrell Scholars Collaborative. Waterman, R.; Feig, A. (Eds.); ACS Symposium Series. (2017)
- Agren J.; **Arróyave, R.**; Asta, M.; Battaile, C. C.; Campbell, C. E.; Guest, J. K.; Krajewski, P. E.; Lewis, A. C.; Liu, W. K.; McDowell, D. L.; Rollet, R.; Trinkle, D. R.; Voorhees, P. W.; *Modelling Across Scales: A Roadmapping Study for Connecting Materials Models and Simulations Across Length and Time Scales.* The Minerals, Metals and Materials Society. Warrendale, PA. (2015)

Refereed Journals

- **101.** Hudak, B. M.; Depner, S. W.; Waetzig, G.; Talapatra, A.; **Arróyave, R.**; Banerjee, S.; Guiton, B. S. *Real-Time Atomistic Observations of Structural Phase Transformations in Individual Hafnia Rods* Nature Communications (2017), Accepted
- **100.** Tapia, G.; Johnson, L.; Franco, B.; Karayagiz, K.; Ma, J.; **Arróyave, R.**; Karaman, I,; Elwany, A. *Bayesian Calibration and Uncertainty Quantification for a Physics-based Precipitation Model of Nickel-Titanium Shape-Memory Alloys.* Journal of Manufacturing Science and Engineering (2017), Accepted

Publications (continued)

- **99.** Honarmandi, P.; **Arróyave, R.** *Using a Bayesian Framework to Calibrate a Physically Based Model Describing Strain-Stress Behavior of TRIP Steels.* Computational Materials Science (2017), 129, pp. 66-81
- **98.** Junkaew, A.; Maitarad, P.; **Arróyave, R.**; Kungwan, N.; Zhang, D.; Shi, L.; Namuangruk, S. *Complete Reaction Mechanism of H2S Desulfurization on Anatase TiO2(001) Surface: A Density Functional Theory Investigation.* Catalysis Science & Technology (2017), 7, pp. 356-365
- **97.** Galvan, E.; Malak, R. J.; Gibbons, S. L.;**Arróyave, R.** *A Constraint Satisfaction Algorithm for Inverse Phase Stability Problems.* Journal of Mechanical Design (2017), 139(1), pp. 011401
- **96.** Entel, P.; Talapatra, A.; **Arróyave, R.**; Singh, N.; Gruner, M.; Dronskowski, R.; Bogdanovski, D.; Hucht, A. *First-principles and Monte Carlo Studies of Magnetocaloric Effects.* Advances in Science and Technology (2017), 97, pp. 124-133
- **95.** **Arróyave, R.**; Talapatra, A.; Duong, T.; Son, W.; Gao, H.; Radovic, M. *Does Aluminum Play Well with Others? Intrinsic Al-A Alloying Behavior in 211/312 MAX Phases.* Materials Research Letters (2016), Accepted.
- **94.** Duong, T. C.; Hackenberg, R. E.; Landa, A.; Honarmandi, P.; Talapatra, A.; Volz, H. M.; Llobet, A.; Smith, A. I.; King, G.; Bajaj, S.; Rubam A.; Vitos, L.; Turchi, P. E. A.; **Arróyave, R.** *Revisiting the Thermodynamics and Kinetic Diffusivities of Uranium-Niobium with Bayesian Uncertainty Analysis.* CALPHAD (2016), 55, pp. 219-230.
- **93.** Talapatra, A.; Duong, T.; Son, W.; Gao, H.; Radovic, M.; **Arróyave, R.** *A High Throughput Combinatorial Study of the effect of M site Alloying on the Solid Solution behavior of M_2AlC MAX Phases.* Physical Review B (2016), 94, p. 104016.
- **92.** Son, W.; Duong, T.; Talapatra, A.; Gao, H.; **Arróyave, R.**; Radovic, M. *Ab-initio Investigation of the Finite-Temperature Structural, Elastic and Thermodynamic Properties of Ti_3AlC_2 and Ti_3SiC_2.* Computational Materials Science (2016), 124, pp. 420-427.
- **91.** Cáceres-Dıaz, L. A.; Alvarado-Orozco, J. M.; Ruiz-Luna, H.; García-Herrera, J. E.; Mora-García, A. G.; Trápaga-Martínez; **Arróyave, R.**; Muñoz-Saldañ a, J. *Study of the Isothermal Oxidation Process and Phase Transformations in B2-(Ni, Pt)Al/RENE-N5 System.* Metals (2016), 6(9), p. 208.
- **90.** Gao, H.; Benitez, R.; Son, W.;**Arróyave, R.**; Radovic, M. *Structural, Physical and Mechanical Properties of $Ti_3(Al_{1-x}Si_x)C_2$ Solid Solution with x=0-1.* Materials Science and Engineering A (2016), 676 pp. 197-208.
- **89.** Attari, V.; **Arróyave, R.** *Phase Field Modeling of Joint Formation During Isothermal Solidification in 3DIC Micro Packaging.* Journal of Phase Equilibria & Diffusion (2016), 37(4), pp.469-480.
- **88.** Johnson, L.; **Arróyave, R.** *An Inverse Design Framework for Prescribing Precipitation Heat Treatments from a Target Microstructure.* Materials & Design (2016), 107(5), pp. 7-17.
- **87.** **Arróyave, R.**; Gibbons, S. L.; Galvan, E.; Malak, R. J. *The Inverse Phase Stability Problem as a Constraint Satisfaction Problem: Application to Materials Design.* JOM (2016), 68(5), pp. 1385-1395.
- **86.** Monroe, J. A.; Karaman, I.; **Arróyave, R.**; Brown, D. W.; Clausen, B. *Tailored Thermal Expansion Alloys.* Acta Materialia (2016), 102 (33), pp. 333-341 .
- **85.** Singh, N.; Talapatra, A.; Gibbons, S.; Duong, T.; Thawabi, H.; Li, S.; **Arróyave, R.** *Effect of Ternary Additions to Structural Properties of NiTi Alloys.* Computational Materials Science (2016), 112, pp. 347-355.
- **84.** Talapatra, A.; **Arróyave, R.**; *Investigation of the Energetics of Structural Transformations in Co-based Shape Memory Alloys.* Journal of Alloys and Compounds (2016), 663(5), pp. 693-700.

Publications (continued)

- **83.** Stonaha, P. J.; Manley, M. E.; Bruno, N. M.; Karaman, I.; **Arróyave, R.**; Singh, N.; Abernathy, D. L.; Chi, S. *Lattice Vibrations Boost Demagnetization Entropy in a Shape Memory Alloy.* Physical Review B: Rapid Communications (2015), 92 (14), p. 140406.
- **82.** **Arróyave, R.**; Talapatra, A.; Johnson, L.; Singh, N.; Ma, J.; Karaman, I. *Computational Thermodynamics and Kinetics-Based ICME Framework for High-Temperature Shape Memory Alloys.* Shape Memory and Superelasticity (2015), 4(1), pp. 429-449.
- **81.** Monroe, J. A.; Raymond, J. E.; Karaman, I.; **Arróyave, R.**; Xu, X.; Kainuma, R.; Chumlyakov, Y. I. *Multiple Ferroic Glasses via Ordering.* Acta Materialia (2015), 101, pp. 107-115.
- **80.** Zhou, Y.; Eunju, J.; **Arróyave, R.**; Radovic, M.; Shamberger, P. *Incorporating Research Experiences into an Introductory Materials Science Course.* International Journal of Engineering Education (2015), 31(6), pp. 1491-1503.
- **79.** Talapatra, A.; **Arróyave, R.**; Entel, P.; Valencia-Jaime, I.; Romero, Aldo H. *Stability analysis of the martensitic phase transformation in Co_2NiGa Heusler Alloy.* Physical Review B (2015), 92 (5) p. 054107.
- **78.** Junkaew, A.; C. Rungnim; M. Kunaseth; J. Meeprasert; **Arróyave, R.**; S. Namuangruk *Metal cluster-deposited Graphene as Adsorptive Materials for m-Xylene.* New Journal of Chemistry (2015), 39 (12), pp. 9650-9658.
- **77.** Junkaew, A.; Ham, B.; Zhang, X.; **Arróyave, R.** *Investigation of Interfaces in Multi-layer Mg/Nb Thin Films.* Computational Materials Science (2015), 108A, pp. 212-225.
- **76.** Li, S.; Honarmandi, P.; **Arróyave, R.**; Rivera-Diaz-del-Castillo, P. E. J. *Describing the Deformation Behavior of TRIP and Dual Phase Steels Employing an Irreversible Thermodynamics Formulation.* Materials Science and Technology (2015), 31 (15), pp. 1658-1663.
- **75.** Bajaj, S.; Haverty, M. G.; **Arróyave, R.**; Goddard III, W. A.; Shankar, S. *Phase Stability in Nanoscale Materials Systems: Extension from Bulk Phase Diagrams.* Nanoscale (2015), 7, pp.9868-9877.
- **74.** Entel, P.; **Arróyave, R.**; Fähler, S.; Kainuma, R.; Planes, A.; Ren, X.; Saxena, A. *Ferroic Glasses: Magnetic, Polar and Strain Glass.* Physica Status Solidi B (2014), 10.
- **73.** Comtesse, D.; Gruner, M. E.; Ogura, M.; Sokolovskiy, V. V.; Buchelnikov, V. D.; Grünebohm; **Arróyave, R.**; Singh, N.; Gottschall, T.; Gutfleisch, O.; Chernenko, V.; Albertini, F.; Fähler, S.; Entel, P. *First-principles Calculation of the Instability Leading to Giant Inverse Magnetocaloric Effects.* Physical Review B (2014), pp. 184403.
- **72.** Lis, A.; Park, M. S.; **Arróyave, R.**; Leinenbach, C. *Early Stage Growth Characteristics of Ag_3Sn Intermetallic Compounds during Solid-Solid and Solid-Liquid Reactions in the Ag-Sn Interlayer System: Experiments and Simulations.* Journal of Alloys and Compounds, (2014), 617, pp. 763-773.
- **71.** Junkaew, A.; Ham, B.; Zhang, X.; **Arróyave, R.** *Ab Initio Calculations of the Elastic and Finite-temperature Thermodynamic Properties of Niobium and Magnesium Hydrides.* International Journal of Hydrogen Energy, (2014), 39 (28), pp. 15530-15539.
- **70.** Park, M. S.; Gibbons, S. L.; **Arróyave, R.** *Confinement Effects on Evolution of Intermetallic Compounds during Metallurgical Joint Formation.* Journal of Electronic Materials, (2014), 43, pp. 2510-2520.
- **69.** Park, M. S.; Gibbons, S. L.; **Arróyave, R.** *Prediction of Processing Maps for Transient Liquid Phase Diffusion Bonding of Cu/Sn/Cu Joints in Microelectronics Packaging.* Microelectronics Reliability,(2014), 54, pp. 1401-1411.

Publications (continued)

- **68.** Ham, B.; Junkaew, A.; **Arróyave, R.**; Foley, D.; Rios, S.; Wang, H.; Zhang, X. *Size and Stress Dependent Hydrogen Desorption in Metastable Mg Hydride Films.* International Journal of Hydrogen Energy, (2014), 39, pp. 2597-2607.
- **67.** Chari, A.; Dogan, E.; Talapatra, A.; Chivukula, A.; Garay, A.; Karaman, I.; **Arróyave, R.** *Computational Thermodynamics of the CoNiGa High Temperature Shape Memory Alloy System.* CALPHAD, (2014), 45, pp. 167-177.
- **66.** Junkaew, A.; Ham, B.; Zhang, X.; **Arróyave, R.** *Tailoring the Formation of Metastable Mg through Interfacial Engineering: a Phase Stability Analysis.* CALPHAD, (2014), 45, pp. 145-150.
- **65.** Ham, B.; Junkaew, A.; Wang, H.; **Arróyave, R.**; Zhang, X. *Fabrication of Porous and Pillar-shaped Mg by Magnetron Sputtering.* Thin Solid Films, (2014), 550, pp. 220-226.
- **64.** Thawabi, H. S.; Duong, T.; **Arróyave, R.** *Thermodynamic and Mechanical Stabilities of α-Ta_4AlC_3 via First-Principles Investigations.* Journal of Applied Physics, (2013), 114(21), pp. 213517.
- **63.** Park, M. S.; Gibbons, S. L.; **Arróyave, R.** *Phase-field Simulations of Intermetallic Compound Evolution in Cu/Sn Solder Joints under Electromigration.* Acta Materialia (2013), 61(19), pp. 7142-7154.
- **62.** Sanchez-Martinez, A.; Ceballos-Sanchez, O; Vazques-Lepe, M. O.; Duong, T.; **Arróyave, R.**; Espinoza-Magana, F.; Herrera-Gomez, A. *Diffusion of In and Ga in TiN/HfO_2/InGaAs Nanofilms.* Journal of Applied Physics (2013), 114, pp. 143504.
- **61.** Santamarta, R.; **Arróyave, R.**; Pons, J.; Evirgen, A.; Karaman, I.; Karaca, H. E.; Noebe, R. D. *TEM Study of Structural and Microstructural Characteristics of a Precipitate Phase in Ni-rich Ni-Ti-Hf and Ni-Ti-Zr Shape Memory Alloys.* Acta Materialia (2013), 61(16), pp.6191-6206.
- **60.** Duong, T.; **Arróyave, R.** *First-Principles Calculations of Finite-Temperature Elastic Properties of Ti_2AlX (X = C or N).* Computational Materials Science (2013), 79, pp. 296-302.
- **59.** Ham, B.; Junkaew, A.; **Arróyave, R.**; Chen, J.; Wang, H.; Wang, P.; Majewski, J.; Park, J.; Zhou, H.-C.; Arvapally, R.; Kaipa, U.; Omary, M. A.; Zhang, X.; Ren, Y.; Zhang, X. *Hydrogen Sorption in Orthorhombic Mg Hydride at Ultralow Temperature.* International Journal of Hydrogen Energy, (2013), 38(20), pp. 8328-8341.
- **58.** Junkaew, A.; Ham, B.; Zhang, X.; Talapatra, A., **Arróyave, R.** *REPORT: Stabilization of bcc Mg in Thin Films at Ambient Pressure: Experimental Evidence and Ab Initio Calculation.* Materials Research Letters (2013), 1(3), pp. 161-167.
- **57.** Singh, N.; **Arróyave, R.** *Magnetocaloric effects in Ni-Mn-Ga-Fe alloys using Monte Carlo Simulations.* Journal of Applied Physics (2013), 113(18), pp. 183904/1-11.
- **56.** Gruenebohm, A., Entel, P.; Gruener, M. E.; Hucth, A.; Comtesse, D.; **Arróyave, R.** *Complex Magnetic Ordering and Spin Glass Behavior as a Driving Mechanism of Multifunctional Properties of Heusler Alloys from First Principles.* Bulletin of the American Physical Society (2013), 58(1).
- **55.** Park, M. S.; Gibbons, S. L.; **Arróyave, R.** *Computational Investigation of Intermetallic Compounds Evolution Affected by Microvoids during Solid-state Aging Process in the Cu-Sn System.* Journal of Electronic Materials (2013), 42(6), pp. 999-1009.
- **54.** Zhu, R.; Li, S.; Song, M.; Karaman, I.; **Arróyave, R.** *Phase Constitution Effect on the Ductility of Low Alloy Multiphase Transformation.* Materials Science and Engineering A (2013), 569(1), pp. 137-143.
- **53.** Li, S.; Zhu, R.; Karaman, I.; **Arróyave, R.** *Development of a Kinetic Model to Predict the Volume Fraction of Retained Austenite after the Two-stage Heat Treatment in TRIP Steels.* Acta Materialia (2013), 61(8), pp. 2884-2894.

Publications (continued)

- **52.** Entel, P.; Siewert, M.; Gruner, M. E.; Herper, H. C.; Comtesse, D.; **Arróyave, R.**; Singh, N.; Talapatra, A.; Sokolowskiy, V. V.; Buchelnikov, V. D.; Albertini, F.; Righi, L.; Chernenko, V. A. *Complex Magnetic Ordering as a Driving Mechanism of Multifunctional Properties of Heusler Alloys from First Principles.* European Physical Journal B, Special Issue on New Trends in Magnetism and Magnetic Materials (2013), 86(2), pp. 1-11 .
- **51.** Ceballos-Sanchez, O.; Sanchez-Martinez, A.; Vazquez-Lepe, M. O.; Duong, T.; **Arróyave, R.**; Espinosa-Magana, F.; Herrera-Gomez, A. *Mass Transport and Thermal Stability of TiN/Al2O3/InGaAs Nanofilms.* Journal of Applied Physics (2012), 112(5), pp. 053527.
- **50.** Li, S.; Zhu, R.; Karaman, I.; **Arróyave, R.** *Thermodynamic Analysis of Two-Stage Heat Treatment of TRIP Steels.* Acta Materialia (2012), 60(17), pp.6120-6130.
- **49.** Park, M.-S.; Gibbons, S.; **Arróyave, R.** *Phase-field Simulations of Intermetallic Compound Growth in the Cu/Sn/Cu Sandwich Structure during the Transient Liquid Phase Bonding.* Acta Materialia (2012), 60(18), pp.6278-6287.
- **48.** Mantina, M; Wang, Y.;**Arróyave, R.**; Shang, S.; Chen, L. Q.; Liu, Z.-K. *First-principles Approach to Transition States of Diffusion.* Journal of Physics: Condensed Matter (2012), 24(30), pp.305402.
- **47.** Stephenson, M. K.; Park, M.-S.; Shannon, C.; Cáceres-Dıaz, L. A.; Hudspeth, K. A.; Gibbons, S. L.; Munoz-Saldana, J.; **Arróyave, R.** *Experimental and Computational Study of the Morphological Evolution of Intermetallic Compound (Cu_6Sn_5) layers at the Cu/Sn Interface under Isothermal Soldering Conditions.* Acta Materialia (2012), 60(13-14), pp.5125-5134.
- **46.** Siewert, M.; Gruner, M. E.; Hucht, A.; Herper, H. C.; Dannenberg, A.; Chakrabarti, A.; Singh, N.; **Arróyave, R.**; Entel, P. *A First-Principles Investigation of the Compositional Dependent Properties of Magnetic Shape Memory Heusler Alloys.* Advanced Engineering Materials (2012), 14(8), pp. 530-546.
- **45.** Dogan, E.; Singh, N.;Chivukula, A.; Thawabi, H. S.; Karaman, I.; **Arróyave, R.** *The Effect of Valence Electron Concentration and Magnetic Properties on the Martensitic Transformation of CoNiGa Shape Memory Alloys.* Acta Materialia (2012), 60 (8), pp.3545-3558.
- **44.** Bajaj, S.; Sevik, C.; Cagin, T.; Garay, A.; Turchi, P. E. A.; **Arróyave, R.** *On the limitations of the DFT+U Approach to Energetics of Actinides.* Computational Materials Science (2012), 59, pp. 48-56.
- **43.** Zhu, R.; Li, S.-Y.; Karaman, I.; **Arró**yave, R.; Niendorf, T.; Maier, H. *Multi-phase Microstructure Design of a Low-Alloy-TRIP-Assisted Steel Through A combined Computational and Experimental Methodology.* Acta Materialia (2012), 60(6-7), pp. 3022-3033.
- **42.** Olivos, E.; Miranda, A. L.; **Arró**yave, R.; Singh, N.; Romero, A. H. *Spin Excitations in Co_2NiGa under Pressure from a Theoretical Approach.* Annalen der Physik (2012), 524 (3-4), pp. 212-226.
- **41.** Park, M.-S.; **Arróyave, R.** *Concurrent Nucleation, Formation and Growth of two Intermetallic Compounds (Cu_6Sn_5 and Cu_3Sn) during Early Stages of Pb-free Soldering.* Acta Materialia (2012), 60(3), pp. 923-934.
- **40.** **Arróyave, R.**; Radovic, M. *Ab-Initio Investigation of $Ti_2Al(C,N)$ Solid Solutions.* Physical Review B (2011), 84, pp. 134112/1-11.
- **39.** Duong, T.; Gibbons, S.; Kinra, R.; **Arróyave, R.** *Ab-Initio Approach to the Electronic, Structural, Elastic and Finite-Temperature Thermodynamic Properties of Ti_2AX (A=Al or Ga and X=C or N).* Journal of Applied Physics (2011), 110, pp. 093504/1-15.
- **38.** Bajaj, S.; Landa, A.; Söderlind, P.; Turchi, P.; **Arróyave, R.** *The U-Ti System: Strengths and Weaknesses of the CALPHAD Method.* Journal of Nuclear Materials (2011), 419, pp. 177-185.

Publications (continued)

- **37.** Singh, N.; Dogan, E.; Karaman, I.; **Arróyave, R.** *The Effect of Configurational Order on the Magnetic Characteristics of Co-Ni-Ga Ferromagnetic Shape Memory Alloys.* Physical Review B (2011), 84, pp. 184201/1-11.
- **36.** Garay-Tapia, A. M.; Romero, A. H.; Trapaga, G.; **Arróyave, R.** *First-principles Investigation of the Al-Si-Sr Ternary System: Ground State Determination and Mechanical Properties.* Intermetallics (2012), 21, pp. 31-44.
- **35.** Pham, H.; Williams, M. E.; Mahaffey, P.; Radovic, M.; **Arróyave, R.**; Cagin, T. *Finite Temperature Elasticity of fcc Al: Atomistic Simulations and Ultrasonic Measurements.* Physical Review B (2011), 84, pp. 064101.
- **34.** Garay-Tapia, A.; Trapaga, G.; Romero, A. H.; **Arróyave, R.** *An ab-initio Study of the Electronic, Mechanical and Vibrational Properties of different Al_2Si_2Sr crystalline phases.* Physical Review B (2011), 83, pp.214111.
- **33.** Dezellus, O.; **Arróyave, R.**; Fries, S. G. *Thermodynamic Modelling of the Ag-Cu-Ti Ternary System.* International Journal of Materials Research (2011), 102(3), pp.286-294.
- **32.** Park, M.-S.; **Arróyave, R.** *Computational Investigation of Intermetallic Compounds (Cu_6Sn_5 and Cu_3Sn) Growth during Solid-state Aging Process.* Computational Materials Science (2011), 50(5), pp.1692-1700.
- **31.** Bajaj, S.; Garay, A.; Landa, A.; Söderlind, P.; Turchi, P.; **Arróyave, R.** *Thermodynamic Study of the Neptunium-Zirconium System.* Journal of Nuclear Materials (2011), 409(1) pp.1-8.
- **30.** **Arróyave, R.**; Junkaew, A.; Chivukula, A.; Bajaj, S.; Yao, C.-Y.; Garay, A. *Investigation of the Structural Stability of Co_2NiGa Shape Memory Alloys via* Ab *Initio Methods.* Acta Materialia (2010), 58(16) pp. 5220-5231.
- **29.** Park, M.-S.; **Arróyave, R.** *Formation and Growth of Intermetallic Compound Cu_6Sn_5 at Early Stages in Lead-free Soldering.* Journal of Electronic Materials (2010), 39(12) pp.2574-2582.
- **28.** Park, M.-S.; **Arróyave, R.** *Early Stages of Intermetallic Compound Formation and Growth during Lead-free Soldering.* Acta Materialia (2010), 58(14) pp.4900-4910.
- **27.** Chari, A.; Garay, A.;**Arróyave,R.***Thermodynamic remodeling of the Co-Ga system.* CALPHAD (2010), 34(2), pp.189-195.
- **26.** Garay, A.; Trápaga, G.; Liu, Z.-K.;**Arróyave, R.** *Thermodynamic Modelling of the Si-Sr System.* CALPHAD (2009), 33(3), pp. 550-556.
- **25.** Garay, A.; Williams, M. E.; Trápaga, G.; **Arróyave, R.** *Thermodynamics, Lattice Stability and Defect Structure of Strontium Silicides via First-Principles Calculations.* Journal of Alloys and Compounds (2009), 484(1-2), pp. 822-831.
- **24.** Park, M.-S.; **Arróyave, R.** *Multi-phase Field Simulation of Intermetallic Compound Growth during Lead Free Soldering.* Journal of Electronic Materials (2009), 38(12), pp. 2525-2533.
- **23.** Mantina, M.; Wang, Y.; **Arróyave, R.**; Wolverton, C.; Chen, L. Q.; Liu, Z.-K. *First principles Calculations of Self-Diffusion Coefficients.* Physical Review Letters (2008), 100, p. 215901.
- **22.** Powell IV, A. C.; **Arróyave, R.** *Open Source Tools for Materials and Process Modeling.* JOM (2008), 60(5), pp.32-37.
- **21.** Kozlov, A.; Ohno, M.; **Arróyave, R.**; Liu, Z.-K.; Schmid-Fetzer, R. *Phase Equilibria and Thermodynamics of the Mg-Ca-Sn System Part 1. Thermodynamic Modeling of Ternary Mg-Sn-Ca Phase Equilibria.* Intermetallics (2008), 16(2), pp.299-315.
- **20.** Ge, L.; Hui, X.; Wang, E. R.; Chen, G. L.; **Arróyave, R.**; Liu, Z.-K. *Prediction of the Glass Forming ability in Cu-Zr binary and Cu-Zr-Ti Ternary Alloys.* Intermetallics (2008), 16(1), pp. 27-33.

Publications (continued)

- **19.** Prins, S; **Arróyave, R.**; Liu, Z.-K. *Defect Structures and Ternary Lattice Site Preference of the B2 Phase in the Al-Ni-Ru System.* Acta Materialia (2007), 55(14), pp. 4781-4787.
- **18.** Shang, S.; Wang, Y.; **Arróyave, R.**; Liu, Z.-K. *Phase Stability in Alpha- and Beta-rhombohedral Boron.* Physical Review B (2007), 75(9), pp. 092101-1/4.
- **17.** Shin, D.; **Arróyave, R.**; Liu, Z.-K. *Thermodynamic Modeling of the Hf-Si-O System.* CALPHAD (2006), 30(4), pp.375-386.
- **16.** **Arróyave, R.**; Liu, Z.-K. *Intermetallics in the Mg-Ca-Sn Ternary System: Structural, Vibrational and Thermodynamic Properties from First Principles.* Physical Review B (2006), 74(3), pp. 174118/1-15.
- **15.** Ohno, M.; Kozlov A.; **Arróyave R.**; Liu, Z.-K.; Schmid-Fetzer, R. *Thermodynamic Modeling of the Ca-Sn System based on Finite Temperature Quantities from First-Principles and Experiment.* Acta Materialia (2006), 54(18), pp. 4939-4951.
- **14.** Shin, D.; **Arróyave, R.**; Liu, Z.-K. *Thermodynamic Properties of Binary HCP Solution Phases from Special Quasirandom Structures.* Physical Review B (2006), 74(2), pp. 024204/1-13.
- **13.** **Arróyave, R.**; Liu, Z.-K. *Thermodynamic Modelling of the Zn-Zr System.* CALPHAD, (2006), 30(1), pp. 1-13.
- **12.** Golumbfskie, W. J.; **Arróyave, R.**; Shin, D.; Liu, Z.-K. *Finite-Temperature Thermodynamic and Vibrational Properties of Al-Ni-Y Compounds via First-Principles Calculations.* Acta Materialia (2006), 54(8), pp. 2291-2304.
- **11.** Venimadhave, A.; Soukiasian, A.; Tenne, D. A.; Li, Q.; Xi, X. X.; Schlom, D. G.; **Arróyave, R.**; Liu, Z. K.; Sun, H. P.; Pan, X.; Lee, M.; Ong, P. *Structural and Transport Properties of Epitaxial Na_xCoO_2 Thin Films.* Applied Physics Letters (2005), 87(17), pp. 172104 1-3.
- **10.** **Arróyave, R.**; Liu, Z.-K; van der Walle, A. *First Principles Calculations of the Zn-Zr System.* Acta Materialia (2005), 54(2), pp. 473-482.
- **9.** **Arróyave, R.**; Shin D.; Liu, Z.-K. *Modification of the Thermodynamic Model for the Mg-Zr System.* CALPHAD (2005), 29(3), pp. 230-238.
- **8.** Zhou, S.; **Arróyave, R.**; Randall, C. A.; Liu, Z. K. *Thermodynamic Modeling of the Binary Barium-Oxygen System.* Journal of the American Ceramic Society (2005), 88(7) pp. 1943-1948.
- **7.** **Arróyave, R.**; Shin, D.; Liu, Z. K. *Ab Initio Thermodynamic Properties of Stoichiometric Phases in the Ni-Al System.* Acta Materialia, (2005) , 53(6), pp. 1809-1819.
- **6.** **Arróyave, R.**; Eagar, T.W. *Thermodynamic Assessment of the Ag-Cu-Ti System.* TMS Letters (2004), 1(5), pp. 87-88.
- **5.** Wang, Y.; Curtarolo, S.; Jiang, C.; **Arróyave, R.**; Wang, T.; Ceder, G.; Chen, L. Q.; Liu, Z. K. *Ab Initio Lattice Stability in Comparison with CALPHAD Lattice Stability.* CALPHAD (2004), 28(1), pp. 79-90. *20^{th} most downloaded paper in CALPHAD journal in 2011.*
- **4.** **Arróyave, R.**; Eagar, T. W. *Metal Substrate Effects on the Thermochemistry of Active Braze Interfaces.* Acta Materialia, (2003) 51(16), pp. 4871-4880.
- **3.** **Arróyave, R.**; Eagar, T. W., Kaufman, L. *Thermodynamic Assessment of the System Cu-Ti-Zr.* Journal of Alloys and Compounds, (2003), 351(1-2), pp. 158-170.
- **2.** **Arróyave, R.**; Kaufman, L.; Eagar, T. W. *Thermodynamic Modeling of the Zr-O system.* CALPHAD(2002), 26(1), pp. 95-118.
- **1.** Flores-Verdugo, M. A.; Perez, A.; Martinez, D.; **Arróyave, R.**; Velasco, A.; Viramontes, R. *Wear of the Pneumatic Transport Elements.* Tribologia (2000), 31(1), pp. 23-37.

Publications (continued)

Conference Proceedings

- **22.** Chang, C.-N.; Semma, B.; Pardo, M.; Fowler, P.; Shamberger, P. J.; **Arróyave, R.** *Data-Enabled Discovery and Design of Energy Materials (D^3EM): Structure of an Interdisciplinary Materials Design Graduate Program.* Proceedings of the 2016 MRS Annual Fall Meeting. Boston, MA, Nov. 28^{th}-Dec. 2^{nd}, 2016
- **21.** Honarmandi, P.; **Arróyave, R.** *Bayesian Calibration of a Physical Model for Plastic Flow Behavior of TRIP Steels.* Proceedings of the 2016 TMS Annual Meeting. Nashville, TN, Feb 2016.
- **20.** Duong, T.; Hackenberg, R. E.; Volz, H. M.; Llobet, A.; Smith, A. I.; King, G.; Landa, A.; Gibbons, S.; Bajaj, S.; Ruban, A.; Vitos, L.; Turchi, P. E. A.; **Arróyave, R.**; *A Hierarchical Computational Thermodynamic and Kinetic Approach to Discontinuous Precipitation in the U-Nb System.* Proceedings of the International Conference on Solid-Solid Phase Transformations in Inorganic Materials (PTM 2015), Whistler, British Columbia, Canada, June 2015. **This paper has been selected as part of the Los Alamos National Laboratory Science Highlights**.
- **19.** **Arróyave, R.**; Li, S.; Zhu, R.; Karaman, I. *Alloy Design Strategies through Computational Thermodynamics and Kinetic Approaches.* Proceedings of the TMS Middle East Mediterranean Materials Congress on Energy and Infrastructure Materials Systems. Doha, Qatar, Jan 2015.
- **18.** Entel, P.; **Arróyave, R.**; Singh, N.; Sokolovskiy, V. V.; Buchelnikov, V. D. *Calculation of Electronic Structure and Field Induced Magnetic Collapse in Ferroic Materials.* Proceedings of the TMS Middle East Mediterranean Materials Congress on Energy and Infrastructure Materials Systems. Doha, Qatar, Jan 2015.
- **17.** Duong, T.; **Arróyave, R.** *Multiscale Modeling of Discontinuous Precipitation in U-Nb.* Proceedings of the TMS Middle East Mediterranean Materials Congress on Energy and Infrastructure Materials Systems. Doha, Qatar, Jan 2015.
- **16.** Galvan, E.; Malak, R.; Gibbons, S. L.; **Arróyave, R.** *Constraint Satisfaction Approach to the Design of Multi-Component Multi-phase Alloys*. Proceedings of the ASME International Design Engineering Technical Conference & Computers and Information in Engineering Conference (IDETC), Buffalo, NY, August, 2014.
- **15.** Zhou, Y. Y.; Radovic, M.; **Arróyave, R.** *Effect of Student-Led Undergraduate Research Experience on Learning and Attitudes –A Practice in An Introductory Materials Science Course*. Proceedings of the MRS Fall Meeting, Boston, MA, December 2013.
- **14.** **Arróyave, R.**; Radovic, M.; Froyd, J. E. *Effects of Student-led Undergraduate Research Experience on Learning and Attitude toward Engineering in an Introductory Materials Science Course*. ASEE Annual Meeting, San Antonio, TX, June 2012.
- **13.** Singh, N.; **Arróyave, R.** *Effect of Atomic Ordering on the Magnetic Behavior of Co_2NiGa Alloys*. Symposium on Shape Memory Alloys. Materials Science and Technology Conference 2011. Columbus, OH, Oct. 16-20^{th}, 2011.
- **12.** Fernandes-Eleno, L. T.; Chivukula, A.; **Arróyave, R.**; Sch´on, C. G. *Metastable BCC Phase Diagram in the Co-Ni-Ga System*. Proceedings of the Discussion Meeting on Thermodynamics of Alloys (2010). Porto, Portugal, Sept. 12th-16th, 2010.
- **11.** Park, M. S.; **Arróyave, R.** *Computational Investigations of Intermetallic Compound Formation and Growth in Cu/Sn Soldering*. Proceedings of the Discussion Meeting on Thermodynamics of Alloys (2010), Porto, Portugal, Sept. 12th-16th, 2010.
- **10.** Bajaj, S.; Garay, A.; **Arróyave, R.**; Sevik, C.; Cagin, T.; Turchi, P. *Thermodynamic Study of the Neptunium-Zirconium System*. The Vasek Vitek Honorary Symposium on Crystal Defects. Proceedings of the TMS Annual Meeting (2010). Seattle, WA, Feb. 14-18th, 2010.

Publications (continued)

- **9.** **Arróyave, R.**; Junkaew, A.; Garay, A.; Chari, A.; Yao, C.-W. *Thermodynamic, Structural Properties and Transformation Behavior in CoNiGa Alloys from First Principles*. Symposium on Computational Thermodynamics and Kinetics. Proceedings of the TMS Annual Meeting (2010). Seattle, Washington, Feb. 14th-18th, 2010.
- **8.** Radovic, M.; **Arróyave, R.**; Froyd, J. E. *Classroom-wide Student-led Undergraduate Research Experience for the Introductory Materials Science Course.* ASEE Gulf-Southwest Conference, Baylor University, Waco, TX, March 2009.
- **7.** Venimadhav, A.; Ma, Z.; Li, Qi; Soukiassian, A.; Xi, X. X.; Schlom, D. G.; **Arróyave, R.**; Liu, Z. K.; Lee, Minhyea; Ong, N. P. *Thermoelectric Properties of Epitaxial and Topotaxial Na_XCoO_2 Thin Films.* Materials Research Society Symposium Proceedings (2006), 886 (Materials and Technologies for Direct Thermal-to-Electric Energy Conversion), pp. 64-74.
- **6.** **Arróyave, R.**; Ohno, M.; Liu, Z. K.; Schmid-Fetzer, R. *Finite-Temperature Thermodynamic Properties of Intermetallics in the Mg-Ca-Sn System via First-Principles Methods.* Magnesium Technology 2006, Proceedings of the Symposium on Magnesium Technology, TMS 2006 Annual Meeting, (2006), pp. 429-434.
- **5.** Prins, S.; **Arróyave, R.**; Jiang, C.; Liu, Z.-K. *B2 Phases and their Defect Structures: Part I. Ab initio Enthalpy of Formation and Enthalpy of Mixing in the Al-Ni-Pt-Ru System.* Materials Research Society Symposium Proceedings (2005), Volume Date 2004 842 (Integrative and Interdisciplinary Aspects of Intermetallics), pp. 529-534.
- **4.** **Arróyave, R.**; Prins, S.; Liu, Z.-K. *B2 Phases and their Defect Structures: Part II. Ab initio Vibrational and Electronic Free Energy in the Al-Ni-Pt-Ru System.* Materials Research Society Symposium Proceedings (2005), Volume Date 2004 842 (Integrative and Interdisciplinary Aspects of Intermetallics), pp. 523-528.
- **3.** **Arróyave, R.**; Liu, Z.-K. *Thermodynamic Model of the Mg-Zn-Zr System and its Application to the Grain Refinement of Mg-Zn-Zr Alloys.* Magnesium Technology 2005, Proceedings of the Symposium on Magnesium Technology, TMS 2005 Annual Meeting, (2005), pp. 203-208.
- **2.** **Arróyave, R.**; Eagar, T.W.; Larson, H. *Joining $LaMO_3$ Perovskite Ceramics to Nickel-based Super Alloys using Liquid Brazing/TLPB Techniques.* Fuel Chemistry Division Preprints, (2003), 48(1), pp. 247-250.
- **1.** Perez-Unzueta, Alberto; Martinez, Dora; Flores, Marco A.; **Arróyave, R.**; Velasco, A.; Viramontes, R. *Erosion and Corrosion Mechanisms in Pneumatic conveying of Direct Reduced Iron Pellets.* ASTM Special Technical Publication (1998), STP 1362 (Wear Processes in Manufacturing), pp. 137-149.

Funding

External Grants

- **24**. Title:*Workshop Support: Interdisciplinary Frontiers of Designing Engineering Material Systems*. Sponsor: NSF. PI: D. Allaire. co-PI(s): **R. Arróyave**; R. Malak; D. Fowler 0 graduate student. Dates: 07/01/16-01/01/17. Amount: $50,000. **Share: N/A**.
- **23**. Title:*High-Throughput Experimentally and Computationally Guided Discovery of Next Generation High-Temperature Shape Memory Alloys*. Sponsor: AFOSR. PI: J. Vlassak. co-PI: **R. Arróyave**. 1 graduate student. Dates: 07/15/16-07/16/19. Amount: $400,000. **Share: $170,000**.
- **22**. Title:*Multi-Material Bulk Deposition and Characterization System for Accelerated Materials Discovery and Design*. Sponsor: AFOSR-DURIP. PI: I. Karaman Co-PI(s):**R. Arróyave**, A. Elwany, D. Lagoudas, M. Radovic, P. Shamberger 1 graduate student. Dates: 07/15/16-07/16/19. Amount: $550,000. **Share: $91,000**.

Funding (continued)

- **21**. Title:*Development of ES-1 Ultra High Strength Alloy*. Sponsor: AFRL. PI: **R. Arróyave** Co-PIs: I. Karaman 1 graduate student. Dates: 03/01/15-12/31/15. **Amount: $70,000**.
- **20**. Title: *Hysteresis Engineering of Adaptive Materials for Electronic and Optoelectronic Devices*. Sponsor: Missile Defense Agency. PI: P. Shamberger Co-PI(s):**R. Arróyave**, S. Banerjee. 1 graduate student. Dates: 11/1/1510/31/18. Amount: $584,878. **Share:$150,000**.
- **19**. Title:*NRT-DESE: Data-Enabled Discovery and Design of Energy Materials (D^3EM)*. Sponsor: NSF-DGE. PI: **R. Arróyave**. Co-PI(s): E. Dougherty, D. Fowler, R. Malak, J. Ross. Dates: 09/01/201508/31/2020. Amount:$2,977,000. **Share: $2,000,000**.
- **18**.Title: *Glassy Ferromagnetic Shape Memory Alloys: Interplay Between Disorder, Phase Transitions, and Multi-Physics Coupling*. Sponsor: NSFDMR. PI: I. Karaman. Co-PI(s):**R. Arróyave**. Dates: 09/01/15- 08/31/18. Amount: $450,622. **Share: $220,000.**
- **17**. Title: *DMREF: Accelerating the Development of Phase-Transforming Heterogeneous Materials: Application to High Temperature Shape Memory Alloys*. Sponsor: NSFCMMI. PI: **R. Arróyave**. Co-PI(s): A. Benzerga, E. Dougherty, I. Karaman, D.C. Lagoudas, T. Baxevanis 3 graduate students. Dates: 09/01/15-08/31/18. Amount: $1,467,133. **Share: $420,000**.
- **16**. Title: *Collaborative Research: Computational Study of Low Volume Solder Interconnects for 3D Integrated Circuit Packaging*. Sponsor: NSF-CMMI-MPE. PI: **R. Arróyave**. Co-PI(s): Y. M. Jin. 1 graduate student. Dates: 02/01/2015-02/01/2018. Amount: $300,000. **Share: $170,000**.
- **15**. Title: *Control of Variability in the Performance of Selective Laser Melting (SLM) Parts through Microstructure Control and Design*. Sponsor: NASA. PI: A. Elwany. Co-PI(s): I. Karaman, **R. Arróyave**. 1 graduate student. Dates: 06/01/2014-06/01/2017. Amount: $500,000. **Share: $150,000**.
- **14**. Title: *Enabling Advanced Design of Novel High-Temperature Nano-laminated Ternary Carbides and Nitrides through Synergetic Experimental and Computational Research*. Sponsor: NSF-DMR. PI: **R. Arróyave**. Co-PI(s): M. Radovic. 1 graduate student. Dates: 06/01/2014-06/01/2017. Amount: $440,104. **Share: $220,000**.
- **13**. Title: *EAGER: Collaborative Research: Simultaneously Controlling Multi-Scale Material Structures Based on Fluid Layering With Self-Assembly and Eutectic Growth*. Sponsor: NSF-DMREF. PI: C. Yu. Co-PI(s): **R. Arróyave**, M. Stremler. 0 graduate student. Dates: 09/01/2013-09/01/2014. Amount:$100,000. **Share:$33,000**.
- **12**. Title: *Tailored Thermal Expansion Alloys*. Sponsor: NSF-I-CORPS. PI: **R. Arróyave**. Co-PI(s): N/A. 0 graduate student. Dates: 10/01/2013-05/01/2015. **Amount: $50,000**.
- **11**. Title: *Synergistic Computational and Microstructural Design of Next-Generation High-Temperature Austenitic Stainless Steels with Thermally Stable Nanotwins*. Sponsor: ARL. PI: **R. Arróyave**, Co-PI: I. Karaman. 1 graduate student supported. Dates: 09/2012-09/2013. Amount: $50,000 (No-IDC). **Share: $25,000**.
- **10**. Title: *Synergistic Computational and Microstructural Design of Next-Generation High-Temperature Austenitic Stainless Steels (TOPIC AREA B)*. Sponsor: DOE-NETL. PI: I. Karaman, Co-PI: **R. Arróyave**. 1 graduate student supported. Dates: 08/2012-08/2015. Amount: $300,000. **Share: $150,000**.
- **9**. Title: *Support of Stockpile Stewardship Program-Phase 2*. Sponsor: Lawrence Livermore National Laboratory. PI: Jim Morel. Co-PI(s): **R. Arróyave**, B. Popov, M. Adams, J.-L Guermond, B. Mallick, N. Amato, L. Rauchwerger, T. Cagin, A. Benzerga. Sponsor: LLNL. 1 graduate student supported. Dates: 10/2011-09/2014. Amount: $2,000,000. **Share: $210,000**.

Funding (continued)

- **8**. Title: *CCLI: Scaling Up Undergraduate Research Experience through Student-led Class-wide Projects in an Introductory Materials Science.: Scaling Up Undergraduate Research Experience through Student-led Class-wide Projects in an Introductory Materials Science Course*. Sponsor: NSF-DUE. PI: **R. Arróyave**. Co-PI(s): M. Radovic, J. Froyd. 0.5 graduate students supported. Dates: 08/2010-08/2013. Amount: $158,000. **Share: $52,000**.
- **7**. Title: *International Institute on Multifunctional Materials for Energy (IIMEC)*. Sponsor: NSF. PI: D. C. Lagoudas. Co-PIs: I. Karaman, Z. Ounaies, **R. Arróyave**, T. Cagin, G. T. Almes, A. A. Benzerga. 1 graduate student supported. Dates: 09/01/2009 02/28/14. Amount: $4,030,000. **Share: $200,000**.
- **6**. Title: *CAREER: Ab Initio Calculations for Design of High Temperature Materials*. Sponsor: NSF-CMMI. PI: **R. Arróyave**. 2 graduate students, 1 postdoc supported. Dates: 03/2010-03/2015. **Amount: $458,000**.
- **5**. Title: *Hydrogen Sorption Mechanisms in Magnesium-based Nanolayers*. Sponsor: NSF-CBET. PI: X. Zhang. Co-PI(s): **R. Arróyave**. 1 graduate student supported. Dates: 08/1/2009-08/1/2012. Amount: $300,000. **Share: $150,000**.
- **4**. Title: *Advanced High Strength Multiphase Steels through a Combined Alloy Microstructural Design*. Sponsor. NSF-CMMI. PI: I. Karaman. Co-PI(s): **R. Arróyave**. 1 graduate student supported. Dates: 08/1/2009-08/1/2012. Amount: $280,000. **Share: $140,000**.
- **3**. Title: *Support of Stockpile Stewardship Program*. Sponsor: Lawrence Livermore National Laboratory. PI: Jim Morel. Co-PI(s): **R. Arróyave**, Yongmei Jin, Bojan Popov, Marvin Adams, Jean-Luc Guermond, Bani Mallick, Nancy Amato, Lawrence Rauchwerger, Tahir Cagin, Amine Benzerga. 2 graduate students supported. Dates: 07/2008-09/2011. Amount: $2,933,514. **Share: $210,000**.
- **2**. Title: *Collaborative Research: Solid-Liquid Interactions during Transient Liquid Phase Bonding*. Sponsor: NSF-CMMI. PI: **R. Arróyave**. 4 graduate and 2 undergraduate students supported. Dates: 06/2008-06/2011 (no-cost extension requested). **Amount: $518,942**.
- **1**. Title: *Computational and Experimental Design of Novel CoNiGa High Temperature Shape memory Alloys.* Sponsor: NSF-DMR. PI: **R. Arróyave**. Co-PI(s): Ibrahim Karaman. 1 graduate student supported. Dates: 06/2008-06/2013. Amount: $345,000. **Share: $145,000.**

Internal Grants

- **5**. Title: *Use of Large Introductory Classes to Propagate Active Teaching Methodologies Throughout Undergraduate Curricula*. Sponsor: TAMU COE. PI: P. Shamberger. Co-PI(s): R. Arroyave, M. Radovic, T. Hartwig. Dates: 09/01/2014-09/01/2016. Amount: $50,000. **Share: $15,000**.
- **4**. Title: *SEED Program: Materials Genomics of Phase Transforming Multi-functional Materials*. Sponsor: TAMU COE-TEES, VPR. PI: **R. Arróyave**. Co-PI(s): E. Dougherty, I. Karaman, R. Aramayo. 1 graduate student. Dates: 09/01/2014-09/01/2016. Amount: $250,000. Share: **$150,000**
- **3**. Title: *Collaborative Research: Diffusion of Indium in Metal/Dielectric/InGaAs Nanofilms*. Sponsor: TAMU-CONACyT Program. PI: **R. Arróyave**. Co-PI: A. Herrera-Gomez. 1 graduate student. Dates: 09/201108/2012. Amount: $24,000. **Share: $12,000**.
- **2**. Title: *Collaborative Research: Thermal Stability and Mass Transport in Nanofilms*. Sponsor: TAMU-CONACyT Program. PI: **R. Arróyave**. Co-PI: A. Herrera-Gomez 1 graduate student supported. Dates: 3/11/20083/10/2009. Amount: $24,000. Share: $12,000.

Funding (continued)

- **1**. Title: *Collaborative Research: Computational Modeling and Experimental Verification of Solidification and Microstructural Evolution of Al-Si-Sr Alloys*. Sponsor: TAMU-CONACyT Program. PI: G. Trapaga. Co-PI(s): Yongmei Jin, **R. Arróyave**. 1 graduate student supported. Dates: 09/01/2007-08/31/2008. Amount: $24,000. **Share: $8,000**.

Invited Talks

- As of January, 2016, R. Arróyave has given 49 (20 international) invited talks.
- **49. Arróyave, R.**; Benzerga, A.; Lagoudas, D.; Karaman, I. *The Texas A&M/IIMEC Summer School in Computational Materials Science* Symposium: Curricular Innovations and Continuous Improvement of Academic Programs (and Satisfying ABET along the Way): The Elizabeth Judson Memorial Symposium. Materials Science & Technology 2016, Salt Lake City, Utah, October 23-27th, 2016.
- **48. Arróyave, R.**; Talapatra, A.; Duong, T.; Son, W.; Gao, H.; Radovic, M. *Intrinsic Alloying Behavior in M and A Sublattices in 211 and 312 MAX Phases Insights from* Ab Initio *Calculations.* Symposium: Materials Design, New Compositions and Composites 41st International Conference & Exposition on Advanced Ceramics and Composites, ICACC 2017, Daytona Beach, FL, January 22nd-27th, 2017.
- **47. Arróyave, R.**; Singh, N.; Talapatra, A.; Duong, T.; Karaman, I.; Entel, P. *Insights into Magneto-Structural-Configurational Couplings in Ferromagnetic Shape Memory Alloys from Electronic Structure Calculations.* International Conference on Ferromagnetic Shape Memory Alloys (ICFSMA 2016), Sendai, Japan, Sept. 05-09th, 2016.
- **46. Arróyave, R.** *A Hierarchical Multi-scale Computational Materials Science Approach to the Understanding of the Discontinuous Precipitation in U-Nb Alloys.* Los Alamos National Laboratory, May 18th, 2016.
- **45. Arróyave, R.** *Getting Cited: a Brief Tutorial on Scientific Writing.* Graduate Track; SHPE Annual Conference, Baltimore, MD, Nov 11-15th, 2015.
- **44. Arróyave, R.**; *From Thermodynamics and Kinetics to Materials Design: Application to the Development of Advanced Steels.* ASM International - Oak Ridge National Laboratory Educational Symposium on Computational Thermodynamics and Materials Design, Oak Ridge, TN, April 16th, 2015.
- **43. Arróyave, R.**; Li, S.; Wang, C. J.; Villarreal, R.; Jozaghi, T.; Karaman, I. *CALPHAD-based Alloy Design: Application to Advanced Steels.* Symposium: CALPHAD-Based ICME Research for Materials Genomic Design. TMS Annual Meeting, Orlando, FL, March 15-19th, 2015.
- **42. Arróyave, R.** ; *Parameter Identification in Phase-Field Models of Microstructure Evolution: Tuning Models to Discover Phenomena.* American Mechanics Symposium (Amerimech). Austin, TX, December 10-12th, 2014.
- **41. Arróyave, R.** *Getting Published: a Brief Tutorial on Scientific Writing.* Graduate Track; SHPE Annual Conference, Detroit, MI, Nov 5-9th, 2014.
- **40. Arróyave, R.** ; Park, M. S.; Gibbons, S. L. *Towards the Materials Genome of Pb-free Interconnects: Contributions from Phase Field Modeling.* Symposium: Pb-free Solders and Advanced Interconnecting Materials. MS&T 2014, Pittsburgh, PA, October 12-16th, 2014.
- **39. Arróyave, R.** ; *High-throughput Tools for the Discovery of Heusler Alloys.* NIST Workshop on First Principles Phase Stability Repositories. August 6-8th, 2014.
- **38. Arróyave, R.**; *Computer-Aided Design and Development of Materials.* Graduate Seminar, College of Engineering, Universidad de Nuevo León. Monterrey, NL, México, July, 23rd, 2014.

Invited Talks (continued)

- **37. Arróyave, R.**; *The Past, Present and Future of Materials Science and Materials Development.* Plenary Seminar, U-ERRE (Universidad Regiomontana). Monterrey, NL, México, July, 14^{th}, 2014.
- **36. Arróyave, R.** ; *Phase Stability in Multi-layered Thin Films.* Condensed Matter Physics Seminar. Department of Physics, Texas A&M University. College Station, TX, April 18^{th}, 2014.
- **35. Arróyave, R.**; Junkaew, A.; B. Ham; X. Zhang. *Phase Stability in Multi-layered Thin Films.* Invited Talk, 3^{rd} International Symposium on Nano-science and Nanomaterials . Ensenada, México, March 10-14th, 2014.
- **34. Arróyave, R.**; Gibbons, E. G.; Li, S.; Malak, R. *Solving Inverse Problems in Phase Stability: A Design Theoretic Approach.* Symposium: Hume-Rothery Award Symposium: Thermodynamics and Kinetics of Engineering Materials. TMS Annual Meeting, San Diego, CA, February 16-20^{th}, 2014.
- **33. Arróyave, R.**; Junkaew, A.; Duong, T. *Computational Phase Stability Research and Education in Energy Materials: Some Examples in Hydrogen Storage and Nuclear Materials.* Symposium: Computational Modeling and Simulation of Advanced Materials for Energy Applications. TMS Annual Meeting, San Diego, CA, February 16-20^{th}, 2014.
- **32. Arróyave, R.**; Li, S.; Gibbons, S.; Karaman, I.; Malak, R.; Galvan, E.; Rivera Diaz del Castillo, P. *From Computational Materials Science to Computer-Aided Materials Design: Optimization of Multi-component, Multi-phase TRIP Steels.* Graduate Seminar, North Carolina State University. Raleigh, NC, November 8^{th}, 2013.
- **31. Arróyave, R.**; Li, S.; Gibbons, S.; Karaman, I.; Malak, R.; Galvan, E.; Rivera Diaz del Castillo, P. *Search and Optimization Tools for the Design of Multi-component and Multi-phase Materials.* Symposium: Material Data and Software Tools Needed to Make MGI and ICME a Reality . Materials Science & Technology 2013, Montreal, Canada, October 27^{th}-31^{st}, 2013.
- **30. Arróyave, R.**; *Ferromagnetic Shape Memory Alloys from an Ab Initio Perspective.* Cambridge University, Cambridge, United Kingdom, August 28^{th}, 2013.
- **29. Arróyave, R.**; *Optimization of Mechanical Performance of Multi-component, Multi-phase Alloys: Application to TRIP Steels.* Delft University, Delft, Netherlands, August 30^{th}, 2013.
- **28. Arróyave, R.**; Singh, N.; Gruner, M.; Entel, P. *Alloying, Configurational, Thermal and Magnetic Effects on the Phase Stability of Ferromagnetic Shape Memory Alloys: Perspectives from Ab Initio Calculations.* XXII International Materials Research Congress. MRS International. Canc'un, México, August 11-15^{th},2013.
- **27. Arróyave, R.;** Shi, S.-Y.; Wang, C.; Zhu, R.; Rivera-Díaz-del-Castillo, P. E. J.; Karaman, I.; Malak, R.; Galvan, E. *An optimization-based Framework for the Design of Advanced Multi-component, Multi-phase Materials: Application to TRIP-assisted Steels* . Materials by Design Workshop, Los Alamos National Laboratory, July 16-18^{th}, 2013.
- **26. Arróyave, R.;** Shi, S.-Y.; Zhu, R.; Rivera-Diaz-del-Castillo, P. E. J.; Karaman, I. *Computer-Aided Design of Multi-phase Alloys: Application to TRIP Steels.* CENIM (National Center of Metallurgical Research), Madrid, Spain, June 3-4^{th}, 2013.
- **25. Arróyave, R.;** Shi, S.-Y.; Zhu, R.; Rivera-Diaz-del-Castillo, P. E. J.; Karaman, I. *New Approaches to the Computer-Aided Design of Multi-Phase Multi-Component Structural Alloys.* TKM-2013, International Workshop on Materials Design Process: Thermodynamics, Kinetics and Microstructure Control, IMDEA, Madrid, Spain, June 3-4^{th}, 2013.
- **24. Arróyave, R.** *From it to bit: The Application of Computational Materials Science in the Development of Advanced Materials.* . Graduate Seminar Series, Texas Tech University. Lubbock, Texas, April 22^{nd}, 2013.

Invited Talks (continued)

- **23.** Park, M. S.; **Arróyave, R.** *Investigation of Intermetallic Compounds Formation Evolution in Pb-free Soldering: Simulation and Critical Experiments.* Symposium: Pb-Free Soldering. Materials Science & Technology 2012, Pittsburgh, Pennsylvania, October 7-11th, 2012.
- **22. Arróyave, R.** *Understanding Solid/Liquid Interfacial Interactions: Phase Field Modeling of Soldering Reactions.* Research Seminar. EMPA, Zurich, Switzerland, July 25th, 2012.
- **21. Arróyave, R.** *Computational and Experimental Optimization of Performance of Multi-component Multi-Phase Structural Alloys: TRIP Steels.* Research Seminar. ENSAM-Metz, Metz, France, July 23rd, 2012.
- **20. Arróyave, R.** *Ab Initio Investigation and Thermodynamic Modeling of Shape Memory Alloys.* Graduate Seminar. Materials Science and Engineering Department, Michigan Technological University, Houghton, MI, September 9th, 2011.
- **19. Arróyave, R.** *Big Challenges and Opportunities in Practical Computational Materials Science.* Seminar. Institute for Computational and Engineering Sciences, University of Texas, Austin, TX, July 27th, 2011.
- **18. Arróyave, R.** *Using Computational Materials Science to Develop Advanced Materials.* Research Seminar. Engineering Enrichment Experience (E3 Program) at Texas A&M University, College Station, TX, June 7th, 2011.
- **17. Arróyave, R.** *From it to bit; Or the Application of Computational Materials Science to the Development of Novel Materials.* A series of seminars offered at Chancaya, Hacettepe, Middle East Technical and Bilkent Universities from May 9-12th, 2011 in Ankara, Turkey.
- **16. Arróyave, R.** *Ab Initio Thermodynamics and Elastic Properties of Structural Materials at Finite Temperatures.* NSF Workshop on Challenges and Opportunities for Research in Multiscale Modeling in Mechanics and Materials (M^4). Co-chairs: Glaucio Paulino and Clark Cooper, NSF. NSF CMMI Grantees Conference, January 4th-5th, 2011.
- **15. Arróyave, R.** *Ab Initio Investigation and Thermodynamic Modeling of Co-Ni-Ga and Co-Ni-Al Shape Memory Alloys.* Special Workshop on Shape Memory Alloys. Istanbul, Turkey, June 19-24th, 2010.
- **14. Arróyave, R.** *Development of an Integrated Framework for the Prediction of Thermodynamic, Structural and Kinetic Properties of Alloys by using Ab Initio Methods.* Symposium:Discovery and Optimization of Materials through Computational Design. MS&T 2009, Pittsburgh, PA, October 25-29th, 2009.
- **13. Arróyave, R.** *Ab Initio Investigation of Shape Memory Alloys.* Institute of Applied Mathematics and Computational Science (IAMCS); Workshop on Multi-functional Materials. College Station, TX, September 30th-October 1st, 2009.
- **12. Arróyave, R.** (Williams, M. E.) *Implementing an Open Source Integrated Framework for Ab Initio Thermodynamics using Python as a Glue Language*Symposium: Open Source Tools for Materials Research and Engineering: Session I. TMS 2009, San Francisco, CA, February 15-19th, 2009.
- **11. Arróyave, R.** *The Importance of Computational Modeling in Materials Science.* Keynote Talk, INGENIA Engineering Conference, Instituto Tecnológico y de Estudios Superiores de Monterrey, Campus Edo. de México, México City, October 31st, 2008.
- **10. Arróyave, R.** *Thermodynamic Stability of Materials: Integration of Finite-Temperature Ab Initio Methods and CALPHAD Modeling.* Symposium: Discovery and Optimization of Materials through Computational Design. MS&T 2008, Pittsburgh, PA, October 5-9th, 2008.

Invited Talks (continued)

- **9. Arróyave, R.** *MSEN 681 Graduate Seminar: "Application of Density Functional Theory Methods to the Prediction of Thermodynamic, Structural and Kinetic Properties of Metallic Systems".* Texas A&M University, Department of Mechanical EngineeringCollege Station, TX, Nov. 9^{th}, 2007.
- **8. Arróyave, R.** *Multi-scale Materials Modeling for Alloy Design.* Centro de Investigación y Estudios Avanzados del IPN, Unidad Querétaro. Querétaro, México, Oct. 4^{th}, 2007.
- **7. Arróyave, R.** *MEEN 681 Graduate Seminar: "Applications of Computational Thermodynamics in Materials Modeling and Design".* Texas A&M University, Department of Mechanical EngineeringCollege Station, TX, Sep. 12^{th}, 2007.
- **6. Arróyave, R.** *Computational Materials Design.* University of Texas, Pan-American, Edinburg, TX, Feb. 16^{th}, 2007.
- **5. Arróyave, R.** *Application of Computational Thermodynamics to the Solution of Practical Problems in Materials Science.* Centro de Investigación de Materiales Avanzados, Segundo Congreso CIMAV. Chihuahua, México, Oct. 26-27^{th}, 2005.
- **4. Arróyave, R.** *From Quantum Mechanics to the Processing of Materials, Application to the Grain Refining of the Mg-Zn-Zr System.* Centro de Investigación y Estudios Avanzados del IPN, Unidad Querétaro. Querétaro, México, Mar. 10th 2005. Centro de Investigación y Estudios Avanzados del IPN, Unidad Saltillo. Saltillo, México, Mar. 11^{th}, 2005.
- **3. Arróyave, R.** *Seminar on Computational Thermodynamics and Kinetics of Materials.* Centro de Investigación y Estudios Avanzados del IPN, Unidad Querétaro. Querétaro, México, Mar. 8-9^{th} 2005.
- **2. Arróyave, R.** *Thermodynamic and Kinetic Aspects of Ceramic-Metal Joints.* Materials Science Seminar. Centro de Investigación y Estudios Avanzados del IPN, Unidad Querétaro. Querétaro, México, Jul. 28^{th}, 2003.
- **1. Arróyave, R.** *Joining Complex Oxide Ceramics to Metals.* Materials Science Seminar at New Mexico Institute of Technology. Socorro, NM. Jan. 10^{th} 2003.

Affiliations

2008-present • American Society for Engineering Education (ASEE)
2004-present • The Mineral, Metals and Materials Society (TMS)
• The Materials Research Society (MRS)
2002-present • ASM International

Service

Department and University

2015 • Member, MSEN Undergraduate Curriculum Committee
2016 • Member, Texas A&M University, High Performance Research Computing Allocation Committee
2015 • Member, Texas A&M University, High Performance Research Computing Director Search Committee
• Member, Department of Materials Science, Computational Materials Faculty Search Committee
2014 • Chair, Department of Materials Science, Computational Materials Faculty Search Committee
2013-present • Founding Faculty, Department of Materials Science and Engineering

Service (continued)

2012-present
- Member, Center for Teaching Excellence Faculty and Student Advisory Board, Texas A&M University
- Member, Faculty Senate Committee on Workplace Climate and Diversity Committee, Texas A&M University
- Member, Faculty Senate, Texas A&M University
- Member, Faculty Development Subcommittee, College of Engineering Strategic Plan, Texas A&M University

2010-present
- Chair, Curriculum Committee, Materials Science and Engineering, Texas A&M University

2008-2009
- Member, Admissions Committee, Materials Science and Engineering Program, Texas A&M University

2008-present
- Advisor, Materials Advantage Chapter, Texas A&M University

Editorial Work

2016-present
- Associate Editor, Materials Letters
- Associate Editor, Journal of Materials Science

2015-present
- Associate Editor, Journal of Phase Equilibria and Diffusion

2014
- Special Issue Co-editor, Physica Status Solidi B, *Ferroic Glasses: Magnetic, Polar and Strain Glass*. October, 2014.

2013
- Special Issue Editor, JOM, *Recent Advances in Ab Initio Thermodynamics of Materials*. November, 2013.

2012
- Special Issue Co-editor, JOM, *Gas-alloy Interactions at Elevated Temperatures*. December, 2012.

Professional Societies

2017-present
- Chair, Functional Materials Division, TMS

2015-present
- Member, Professional Development Committee, TMS

2014-present
- Vice-chair, Alloy Phase Diagram Committee, ASM.
- Vice-chair, Functional Materials Division (FMD), TMS.

2007-present
- Member, Alloy Phases Committee, EMPMD Division, TMS.

2012-2014
- Chair, Alloy Phases Committee, EMPMD Division, TMS

2010-2012
- Vice-chair, Alloy Phases Committee, EMPMD Division, TMS

2007-present
- Member, Alloy Phase Diagram Committee, ASM International

2012-2014
- Secretary, Alloy Phase Diagram Committee, ASM International

2008-2010
- Member, John Bardeen Award Committee, EMPMD Division, TMS

2008-2011
- Representative of Electronic, Magnetic & Photonic Materials Division (EMPMD) to Education Committee of The Minerals, Metals and Materials Society (TMS)

2008-present
- Member, Chemistry and Physics of Materials Committee, TMS

2010-present
- Member, Integrated Computational Materials Engineering Committee, EMPMD Division, TMS

2011-2013
- Member, Education Committee, EMPMD Division, TMS

Conference Organization

2016-2018
- Lead Organizer, CALPHAD , Querétaro, México, May 27^{th}-June 1^{st}, 2018.

Service (continued)

2016
- Co-Chair, Symposium: Computational Thermodynamics and Kinetics; Conference: TMS Annual Meeting, San Diego, February 26^{th} - March 2^{nd}, 2016

2015
- Chair, Symposium: Frustrated Ferroic Materials; Conference: TMS Annual Meeting, Orlando, FA, March 15-19^{th}, 2015.
- Co-Organizer, Symposium: Micromechanics of Structurally Inhomogeneous Materials: An FMD Symposium in Honor of Armen Khachaturyan ; Conference: TMS Annual Meeting, Orlando, FA, March 15-19^{th}, 2015.
- Co-Organizer, Symposium: Hume-Rothery Award Symposium: Multicomponent Alloy Metallurgy, the Bridge from Materials Science to Materials Engineering ; Conference: TMS Annual Meeting, Orlando, FA, March 15-19^{th}, 2015.
- Co-Organizer, TMS Middle East-Mediterranean Materials Congress on Energy and Infrastructure Systems (MEMA 2015), Doha, Qatar, January 11-15^{th}, 2015.

2011
- Chair, Symposium: Computational Thermodynamics and Kinetics; Conference: TMS Annual Meeting, San Diego, CA, February 27^{th}-March 3^{rd}, 2011.

2009,2013
- Chair, Symposium: Phase Stability, Diffusion Kinetics and Their Applications (PSDK-IV); Conference: Materials Science and Technology, Pittsburgh, PA, October 25-29^{th}, 2009 and Montreal, Canada, October 27-31^{st}

2009-2013
- Co-Organizer, Symposium: Computational Thermodynamics and Kinetics; Conference: TMS Annual Meeting.

2009
- Co-Organizer, Round Table, The Gibbs Project; Conference: TMS Annual Meeting, 2009. San Francisco, CA, February 15-19^{th}, 2009.

2007-2016
- Co-Organizer, Symposium: Phase Stability, Diffusion Kinetics and Their Applications (PSDK-II-X); Conference: Materials Science and Technology.

Reviewer

2002-present
- Journal Reviewer: Acta Materialia; Applied Physics Letters; CALPHAD; Computational Materials Science; Inorganic Chemistry; Intermetallics; Journal of Alloys and Compounds; Journal of Applied Physics; Journal of Chemistry and Physics of Solids; Journal of Electronic Materials; Journal of Intelligent Materials and Structures; Journal of Materials Chemistry; Journal of Metals; Journal of Physics: Condensed Matter; Journal of the American Welding Society; Journal of the European Ceramic Society; Materials Science and Engineering A; Materials Chemistry and Physics; Mathematics and Computer Simulations; Metallurgical and Materials Transactions A; Metallurgical and Materials Transactions B; MRS Proceedings; Physica B; Physical Review B; Philosophical Magazine; Physical Review Letters.

2008-present
- NSF Panelist

2009-present
- TAMU-CONACyT Proposals Reviewer

2010
- External Reviewer, Austrian Science Fund

2013
- External Reviewer, Swiss National Science Foundation

Invited Participation/Organization in/of Workshops

July 2016
- Co-Organizer, Workshop on Interdisciplinary Frontiers of Designing Engineering Material Systems. Texas A&M University, College Station, TX, July 18-19^{th}

June 2015
- Invited to Participate in 'Support for Rise of Data in Materials Research' Workshop, College Park, MD, June 29-30^{th}, 2015.

August 2014
- Invited to Participate in NIST Workshop on First Principles Phase Stability Repository, August 6-8^{th}, 2014.

Service (continued)

July 2013 • Invited to Participate in Materials Design Workshop. Los Alamos National Laboratory, July 16-18th, 2013.

June 2013 • Invited to Participate in International Workshop on Materials Design Process: Thermodynamics, Kinetics and Microstructure Control, IMDEA, Madrid, Spain, June 3-4th, 2013.

September 2011 • Invited to Participate in First Annual Workshop on Nuclear Materials Compatibility. Thermodynamics Round Table. Golden, Colorado, September 12-15th, 2011.

January 2011 • NSF Workshop on Challenges and Opportunities for Research in Multiscale Modeling in Mechanics and Materials (M^4). NSF CMMI Grantees Conference, Atlanta, GA, January 4th-5th, 2011.

Other Professional Service

2014-2015 • , Member, Study Group, "Modeling Across Length Scales: A Roadmapping Study for Development of Models, Computer Codes, and Personnel Integration for Connecting Materials Simulations Across Length Scales". Led by TMS, Sponsored by NIST. Group consists of 15 world-renowned experts on computational materials science.

Conferences

• As of December, 2016, 79 contributed and invited talks by students as well as 57 conference talks as author or co-author (excluding talks by students).

Conference Talks by/with Students

• **79.** Son, W.; Gao, H.; Talapatra, A.; Duong, T.; Radovic, M.; **Arróyave, R.**. *Computational and Experimental Approach to Structural, Mechanical and Thermodynamic Properties of $Ti_3(Si_xAl_{1-x})C_2$.*-**Invited**. Materials Design, New Composition and Composites. 41st International Conference & Exposition on Advanced Ceramics and Composites, ICACC 2017, Daytona Beach, FL, January 22nd-27th, 2017.

• **78.** Duong, T.;Talapatra, A.; Son, W.; Radovic, M.; **Arróyave, R.**. *First-principles-based Evaluation of Ti_2AlC-Cr_2AlC Phase Diagram.* Symposium: Materials for Extreme Environments: Ultrahigh Temperature Ceramics (UHTCs) and Nano-laminated Ternary Carbides and Nitrides (MAX Phases). 41st International Conference & Exposition on Advanced Ceramics and Composites, ICACC 2017, Daytona Beach, FL, January 22nd-27th, 2017.

• **77.** Son, W.;Talapatra, A.;Duong, T.; Radovic, M.; **Arróyave, R.** *Effect of A Element on Mechanical Properties of $Ti_3(Si_xAl_{1-x})C_2$.* Symposium: Computational Design of Ceramics and Glasses. Materials Science & Technology 2016, Salt Lake City, Utah, October 23-27th, 2016.

• **76.** Duong, T.; Talapatra, A.;Son, W.; **Arróyave, R.**; Radovic, M.; *On the Calculation of $(Ti,Cr)_2AlC$ Phase Diagram: A First-Principles Approach.* Symposium: Computational Design of Ceramics and Glasses. Materials Science & Technology 2016, Salt Lake City, Utah, October 23-27th, 2016.

• **75.** Talapatra, A.; Duong, T.; Son, W.; Radovic, M.; **Arróyave, R.** *Effect of M Site Alloying on the Solid-Solution Behaviour of $(Ti,V,Zr,Hf)_2AlC$ MAX Phases Using High-Throughput Ab-Initio Methods.* Symposium: Computational Design of Ceramics and Glasses. Materials Science & Technology 2016, Salt Lake City, Utah, October 23-27th, 2016.

Conferences (continued)

- **74.** Elwany, A.; **Arróyave, R.**; Karaman, I.; Ma, J.; Tapia, G.; Franco, B.; Karayagiz, K. *Integrated Process Monitoring Physics-based Modeling Approach for Uncertainty Quantification in Metal-based Additive Manufacturing* . Symposium: Additive Manufacturing: In-situ Process Monitoring, Defect Detection and Control. Materials Science & Technology 2016, Salt Lake City, Utah, October 23-27th, 2016.
- **73.** Morgan, Z. J.; Jin, Y. M.; Attari, V.; **Arróyave, R.**; *Coupled Charge Conduction and Mass Diffusion* . Symposium: Emerging Interconnect and Pb-free Materials for Advanced Packaging Technology. Materials Science & Technology 2016, Salt Lake City, Utah, October 23-27th, 2016.
- **72.** Attari, V.; **Arróyave, R.**; Morgan, Z. J.; Jin, Y. M. *Computational Study of Low Volume Solder Interconnects for 3D Integrated Circuit Packaging.* Symposium: Emerging Interconnect and Pb-free Materials for Advanced Packaging Technology. Materials Science & Technology 2016, Salt Lake City, Utah, October 23-27th, 2016.
- **71.** Ma, J.; Franco, B.; Karayagiz, K.; Tapia, G.; Elwany, A.; **Arróyave, R.**; Karaman, I. *Spatially Tailored Stimulus Response in Shape Memory Alloys.* Symposium: Additive Manufacturing of Composites and Complex Materials. Materials Science & Technology 2016, Salt Lake City, Utah, October 23-27th, 2016.
- **70.** Karayagiz, K.; Johnson, L.; Franco, B.; Tapia, G.; Elwany, A.; Karaman, I.; **Arróyave, R.** *A Coupled Thermal and Precipitation Modeling for Selective Laser Melting Process.* Symposium: Additive Manufacturing of Shape Memory, Superelastic Alloys and Multifunctional Materials. Materials Science & Technology 2016, Salt Lake City, Utah, October 23-27th, 2016.
- **69.** Tapia, G.; Johnson, L.; Franco, B.; Karayagiz, K.; Elwany, A.; **Arróyave, R.**; Ma, J.; Karaman, I. *Bayesian Calibration of a Physics-based Precipitation Model for the Additive Manufacturing of Shape Memory Alloys.* Symposium: Additive Manufacturing of Shape Memory, Superelastic Alloys and Multifunctional Materials. Materials Science & Technology 2016, Salt Lake City, Utah, October 23-27th, 2016.
- **68.** Franco, B.; Tapia, G.; Karayagiz, K.; Ma, J.; Elwany, A.; **Arróyave, R.**; Karaman, I. *The Effect of Microstructure on the Shape Memory Behavior in Selective Laser Melted Ni-rich NiTi Alloys.* Symposium: Additive Manufacturing of Shape Memory, Superelastic Alloys and Multifunctional Materials. Materials Science & Technology 2016, Salt Lake City, Utah, October 23-27th, 2016.
- **67.** Tapia, G.; Johnson, L.; Karayagiz, K.; Franco, B.; Elwany, A.; **Arróyave, R.**; Ma, J.; Karaman, I. *Bayesian Calibration of a Physics-based Precipitation Model for the Additive Manufacturing of Shape Memory Alloys.* Symposium: Solid Free-Form Fabrication Symposium, Austin, TX, August 8-10th, 2016.
- **66.** Karayagiz, K.; Johnson, L.; Franco, B.; Tapia, G.; Elwany, A.; Ma, J.; Karaman, I.; **Arróyave, R.** *A Coupled Thermal and Precipitation Modeling for Selective Laser Melting Process.* Symposium: Solid Free-Form Fabrication Symposium, Austin, TX, August 8-10th, 2016.
- **65.** Franco, B.; Tapia, G.; Karayagiz, K.; Ma, J.; Elwany, A.; **Arróyave, R.**; Karaman, I. *The Effect of Microstructure on the Shape Memory Behavior in Selective Laser Melted Ni-rich NiTi Alloys.* Symposium: Solid Free-Form Fabrication Symposium, Austin, TX, August 8-10th, 2016.
- **64.** Ma, J.; Tapia, G.; Franco, B.; Karayagiz, K.; Elwany, A.; **Arróyave, R.**; Karaman, I. *Spatially Tailored Stimulus Response in Shape Memory Alloys.* Symposium: Solid Free-Form Fabrication Symposium, Austin, TX, August 8-10th, 2016.

Conferences (continued)

- **63.** Honarmandi, P.; **Arróyave, R.** *Bayesian Calibration of a Physical Model for Plastic Flow Behavior of TRIP Steels.* Symposium: Computational Methods for Uncertainty Quantification, Model Validation, and Stochastic Predictions. TMS Annual Meeting, Nashville, TN, February 14-17th, 2016.
- **62.** Duong, T.; Talapatra, A.;Son, W.; Gao, H.; Radovic, M.; **Arróyave, R.** *How ICME and MGI Fruition Benefits the MAX Community: A Case Study on the Calculation of the (Ti,Cr)$_2$AlC Phase Diagram.* Symposium: Ceramic Genome and Integrated Materials Computational Engineering I. 40th International Conference and Exposition on Advanced Ceramics and Composites (ICACC). Daytona Beach, Florida, January 24-28th, 2016.
- **61.** Son, W.; Duong, T.; Talapatra, A.;Gao, H.; Radovic, M.; **Arróyave, R.** *Effect of M-A Bonds on the Mechanical Properties in MAX Phases.* Symposium: Materials for Extreme Environments: Ultrahigh Temperature Ceramics (UHTCs) and Nano-laminated Ternary Carbides and Nitrides (MAX Phases). 40th International Conference and Exposition on Advanced Ceramics and Composites (ICACC). Daytona Beach, Florida, January 24-28th, 2016.
- **60.** Gao, H.; Son, W.; Duong, T.; Talapatra, A.;**Arróyave, R.**; Radovic, M. *Experimental Study of Physical and Mechanical Properties of Ti$_3$(Al, Si)C$_2$ Solid Solutions.* Symposium: Materials for Extreme Environments: Ultrahigh Temperature Ceramics (UHTCs) and Nano-laminated Ternary Carbides and Nitrides (MAX Phases). 40th International Conference and Exposition on Advanced Ceramics and Composites (ICACC). Daytona Beach, Florida, January 24-28th, 2016.
- **59.** Talapatra, A.;Duong, T.; Son, W.; Gao, H.; **Arróyave, R.**; Radovic, M. *A High-throughput Combinatorial Approach to the Exploration of the Effect of M-site Alloying on the Solid Solution Behavior of Ti$_2$AlC MAX Phase.* Symposium: Materials for Extreme Environments: Ultrahigh Temperature Ceramics (UHTCs) and Nano-laminated Ternary Carbides and Nitrides (MAX Phases). 40th International Conference and Exposition on Advanced Ceramics and Composites (ICACC). Daytona Beach, Florida, January 24-28th, 2016.
- **58.** Talapatra, A.; **Arróyave, R.**; Entel, P.; Valencia, J. I.; Romero, A. H. *An ab-initio study of the factors affecting phase selection during the martensitic transformation in Co$_2$2NiGa Heusler alloy.* Symposium: Mechanics of Nanoscale phenomena & Multi-functional Material: Computational Materials with Emphasis on Phase Transformation. SES 2015. College Station, TX, October 25-28th, 2015.
- **57.** Son, W.; Duong, T.; Talapatra, A.; Gao, H.; Radovic, M.; **Arróyave, R.** *Ab-Initio Investigation of the Elastic Properties of Ti$_3$Si$_X$Al$_{1-X}$C^2 Solid Solutions.* Symposium: Ultra High Performance Metals, Metal Alloys, Intermetallics, and Metal Matrix Composites for Aerospace and Defense Applications. Materials Science & Technology 2015, Columbus, OH, October 4-8th, 2015.
- **56.** Johnson, L.; **Arróyave, R.** *Coupling Precipitation Simulations and Mesh Adaptive Direct Search for Precipitation Heat Treatment Optimization in Shape Memory Alloys.* Symposium: Data and Tools for Materials Discovery and Design. Materials Science & Technology 2015, Columbus, OH, October 4-8th, 2015.
- **55.** Chaudhary, N.; **Arróyave, R.**; Karaman, I.; Youssef, S.; Dima, A.; Sauceda, D.; Dougherty, E.; Qian, X.; Ren, S. *An Informatics Approach to Prediction of Stackning Fault Energies in Austenitic Stainless Steels.* Symposium: Data and Tools for Materials Discovery and Design. Materials Science & Technology 2015, Columbus, OH, October 4-8th, 2015.
- **54.** Sauceda, D.; **Arróyave, R.**; Youssef, S.; Dima, A.; Chaudhary, N.; Karaman, I,; Aramayo, R.; Perez, R. *Materials Curation Project: Introduction.* Symposium: Data and Tools for Materials Discovery and Design. Materials Science & Technology 2015, Columbus, OH, October 4-8th, 2015.

Conferences (continued)

- **53.** Duong, T; Hackenberg, R. E.; Volz, H. M.; Llobet, A.; Smith, A. I.; King, G.; Landa, A.; Gibbons, S.; Bajaj, S.; Ruban, A.; Vitos, L.; Turchi, P. E. A.; **Arróyave, R.**; *A Hierarchical Computational Thermodynamic and Kinetic Approach to the Discontinuous Precipitation in U-Nb.* International Conference on Solid-Solid Phase Transformation in Inorganic Materials, Whistler, Canada, July 2, 2015.
- **52.** Valencia, J. I.; Romero, A. H.; Talapatra, A.; **Arróyave, R.** *An ab-initio Study of the Factors Affecting Phase Selection during the Martensitic Transformation in Co_2NiGa Heusler Alloy.* Calphad XLIV, Loano, Italy, May 31 - June 5, 2015
- **51.** **Arróyave, R.**; Gibbons, S.; Galvan, E.; Malak, R. *The Inverse Phase Stability as a Constraint Satisfaction Problem.* 3^{rd} World Congress on ICME (ICME 2015), Colorado Springs, CO, May 31^{st}-June 4^{th}, 2015.
- **50.** **Arróyave, R.**; Li, S.; Zhu, R.; Karaman, I. *ICME Approaches to Design Advanced Steels: Application to Transformation Induced Plasticity and Alumina Forming Stainless Steels.* 3^{rd} World Congress on ICME (ICME 2015), Colorado Springs, CO, May 31^{st}-June 4^{th}, 2015.
- **49.** **Arróyave, R.**; Li, S.; Zhu, R.; Karaman, I. *Alloy Design Strategies through Computational Thermodynamics and Kinetics Approaches.* TMS Middle East - Mediterranean Materials Congress on Energy and Infrastructure Systems (MEMA 2015), Doha, Qatar, Jan 11-15^{th}, 2015.
- **48.** Duong, T.; **Arróyave, R.**. *Multiscale Modeling of Discontinuous Precipitation in U-Nb.* TMS Middle East - Mediterranean Materials Congress on Energy and Infrastructure Systems (MEMA 2015), Doha, Qatar, Jan 11-15^{th}, 2015.
- **47.** Cáceres-Díaz, L. A; García-Herrera, J. E.; Ruiz-Luna, H.; Alvarado Orozco, J. M.; Lau, H.; Stiewe, C.; Boldrick, M. S.; **Arróyave, R.**; Trápaga-Martínez, G.; Muñoz Salaña, J. M. *Effects of Ternary Alloying Elements Additions on the Structural and Mechanical Properties of B2 NiAl-X Intermetallics.* XXII International Materials Research Congress. MRS International. Canc'un, México, August 11-15^{th},2013.
- **46.** Li, S.; **Arróyave, R.;** *A Computational Strategy for the Design of TRIP Steels.* Invited Talk. Department of Metallurgy and Materials Science, University of Cambridge, Cambridge, U. K., July 16^{th}, 2013.
- **45.** Talapatra, A.; **Arróyave, R.;** *The B2-B19'-BCO Transformation in Ni-Ti: An Ab-Initio Investigation.* Symposium: Phase Transformation and Microstructural Evolution. TMS Annual Meeting, San Antonio, TX, March 3-7^{th}, 2013.
- **44.** Park, M. S.; Gibbons, S.; **Arróyave, R.;** *Two-Dimensional Simulation of Intermetallic Compound Growth during the Lead-Free Soldering under the Influence of Electromigration.* Symposium: Pb-free Solders and Emerging Interconnect and Packaging Technologies. TMS Annual Meeting, San Antonio, TX, March 3-7^{th}, 2013.
- **43.** Thawabi, H.; Singh, N.; **Arróyave, R.;** *Modeling of Magnetic and Structural Phase Transformations in Co-Ni-Al and Co-Ni-Ga Ferromagnetic Shape Memory Alloys FSMAs.* Symposium: Magnetic Materials for Energy Applications-III. TMS Annual Meeting, San Antonio, TX, March 3-7^{th}, 2013.
- **42.** Duong, T.; Landa, A.; Turchi, P.; Bajaj, S.; **Arróyave, R.;** *Thermodynamic Reassessment of U-Nb System.* Symposium: Computational Thermodynamics and Kinetics. TMS Annual Meeting, San Antonio, TX, March 3-7^{th}, 2013.
- **41.** Junkaew, A.; Ham, B.; Zhang, X.; **Arróyave, R.;** *Pseudomorphic Growth in Mg/Nb Multilayered Thin Films.* Symposium: Computational Thermodynamics and Kinetics. TMS Annual Meeting, San Antonio, TX, March 3-7^{th}, 2013.

Conferences (continued)

- **40.** Gibbons, S.; **Arróyave, R.;** Li, S. *Hybrid Genetic Algorithm and Mesh Adaptive Direct Search Algorithm Approach for the Thermodynamic Assessment of Multi-component Alloys.* . Symposium: Computational Discovery of Novel Materials. TMS Annual Meeting, San Antonio, TX, March 3-7th, 2013.
- **39.** Li, S.; Zhu, R.; Karaman, I.; **Arróyave, R.;** *A Genetic Algorithm Approach to Design the Micro-Structure for TRIP-Assisted Steel.* Symposium: Computational Discovery of Novel Materials. TMS Annual Meeting, San Antonio, TX, March 3-7th, 2013.
- **38.** Li, S.; Zhu, R.; Karaman, I.; Rivera-Diaz-Del-Castillo, P. E. J.; **Arróyave, R.;** *An Evolutionary Approach for the Alloy and Heat Treatment Optimization of Low Alloyed TRIP-ssisted Steels.* . Symposium: Recent Developments in High Strength Steels for Energy Applications. Materials Science & Technology 2012, Pittsburgh, Pennsylvania, October 7-11th, 2012.
- **37.** Zhu, R. Li, S.; Karaman, I.; **Arróyave, R.;** *Re-Visiting the Phase Constitution Effect on the Mechanical Response of Low Alloyed TRIP-assisted Steel.* . Symposium: Recent Developments in High Strength Steels for Energy Applications. Materials Science & Technology 2012, Pittsburgh, Pennsylvania, October 7-11th, 2012.
- **36.** Park, M. S.; **Arróyave, R.;** *Investigation of Intermetallic Compounds Formation Evolution in Pb-free Soldering: Simulation and Critical Experiments.* . Symposium: Pb-Free Soldering. Materials Science & Technology 2012, Pittsburgh, Pennsylvania, October 7-11th, 2012.
- **35.** Singh, N.; Gibbons, S.; Duong, T.; Junkaew, A.; Talapatra, A.; Li, S.; Thawabi, H.; **Arróyave, R.;** *Characterization of Impurity Effects on Structural Properties of NiTi Alloys.* . Symposium: Phase Stability, Diffusion, Kinetics and their Applications (PSDK-VII). Materials Science & Technology 2012, Pittsburgh, Pennsylvania, October 7-11th, 2012.
- **34.** Talapatra, A.; **Arróyave, R.;** *Investigation of the Energetics of Structural Transformations in Shape Memory Alloys.* . Symposium: Phase Stability, Diffusion, Kinetics and their Applications (PSDK-VII) . Materials Science & Technology 2012, Pittsburgh, Pennsylvania, October 7-11th, 2012.
- **33.** Duong, T.C.; Bajaj, S.; Landa, A.; Turchi, P.E. A.;**Arróyave, R.;** *Density Functional Study of Uranium-Niobium System.* . Poster Session. Materials Science & Technology 2012, Pittsburgh, Pennsylvania, October 7-11th, 2012.
- **32.** Li, S.; Zhu, R.; Karaman, I.; **Arróyave, R.;** *Thermodynamic and Kinetic Investigation of the Two-Stage Heat Treatment of TRIP-Assisted Steels.* . Symposium: Recent Developments in High Strength Steels for Energy Applications. Materials Science & Technology 2012, Pittsburgh, Pennsylvania, October 7-11th, 2012.
- **31.** Singh, N.;**Arróyave, R.;** *Magnetocaloric Effects in Fe Doped NiMnGa Alloys.* . Symposium: Phase Stability, Diffusion, Kinetics and their Applications (PSDK-VII). Materials Science & Technology 2012, Pittsburgh, Pennsylvania, October 7-11th, 2012.
- **30.** Cáceres Díaz, L. A.; Alvarado Orozco, J. M.; **Arróyave, R.;** Singh, N.; García Herrera, J. E.; Mora García, A. G.; Ortíz Merino, J. L.; Koenitzer, D.; Muñoz Salaña, J. M. *Effects of Thermal Exposure on The Structural Stability of B2-(Ni,Pt)Al Bond Coat Systems.* . Symposium: Advanced Structural Materials. XXI International Materials Research Congress, Cancun, México, August 12-17th, 2012.
- **29.** Park, M. S.; Hudspeth, K.; Gibbons, S. L.; **Arróyave, R.**. *Multiphase-field Simulations of Evolution of Intermetallic Compound in Soldering Systems.* CALPHAD Meeting. Berkeley, CA. June 3-8th, 2012.
- **28.** Li, S.; Zhu, R.; Karaman, I.; Rivera-Diaz-Del-Castillo, P. E. J.; **Arróyave, R.**. *The Theoretical Model for Maximizing Austenite Volume Fraction in Steel Alloy.* CALPHAD Meeting. Berkeley, CA. June 3-8th, 2012.

Conferences (continued)

- **27.** Junkaew, A.; Ham, B.; Zhang, X.; **Arróyave, R.**. *Thermodynamic Implications in Mg/Nb Multi-layered Thin Films for Hydrogen Storage Applications.* CALPHAD Meeting. Berkeley, CA. June 3-8th, 2012.
- **26.** **Arróyave, R.**; Singh, N.. *First Principles Investigations of Magnetic Shape Memory Alloys.* CALPHAD Meeting. Berkeley, CA. June 3-8th, 2012.
- **25.** Olivos, E.; Miranda, A. L.; Singh, N.; **Arróyave, R.;**; Romero, A. H.. *Magnetic Characterization of Crystalline Systems under Pressure from First Principles*. Fourth Workshop Mexico-Chile on Magnetism in Nanosciences and its Applications. Mexico City, México. March 19-23th, 2012.
- **24.** Li, S.; Zhu, R.; Karaman, I.; **Arróyave, R.;**. *A Genetic Algorithm Approach to Maximize Austenite Volume Fraction in TRIP Steels*. Symposium: Computational Thermodynamics and Kinetics. 2012 TMS Annual Meeting, Orlando, FL, March 12-26th, 2012.
- **23.** Thawabi, H.; Singh, N.; **Arróyave, R.;**. *Modeling Magnetic and Structural Phase Transformations in Co-Ni-Al Ferromagnetic Shape Memory Alloys*. Symposium: Magnetic Materials for Energy Applications. 2012 TMS Annual Meeting, Orlando, FL, March 12-26th, 2012.
- **22.** Singh, N.; **Arróyave, R.;**. *Effect of Atomic Ordering on the Magnetic Behavior of Co2NiGa alloys*. Symposium: Shape Memory Alloys. Materials Science and Technology 2011, Columbus, Ohio, October 16-20th, 2011.
- **21.** Zhu, R.; Li, S.; Karaman, I.; **Arróyave, R.;**. *On the Multi-Phase Microstructure Design of a Low Alloy TRIP-Assisted Steel through Computational and Experimental Methodology*. Symposium: Steel Product Metallurgy and Applications. Materials Science and Technology 2011, Columbus, Ohio, October 16-20th, 2011.
- **20.** Cáceres Díaz, L. A.; Alvarado Orozco, J. M.; **Arróyave, R.;** Singh, N.; García Herrera, J. E.; Mora García, A. G.; Ortíz Merino, J. L.; Koenitzer, D.; Muñoz Salaña, J. M. *Experimental and Theoretical Studies of the Structural and Mechanical Properties Evolution of β-(Ni,Pt)Al Bond Coats as a Function of Isothermal Treatments at 1100 C*. Symposium: Advances in Computational Materials Science. XX International Materials Research Congress, Cancun, México, August 14-19th, 2011.
- **19.** Junkaew, A.; Ham, B.; Zhang, X.; **Arróyave, R.** *Energetics and Microstructures in Mg/Nb Multilayers.* Symposium: Hydrogen Storage Materials: Theory and Experiments. TMS Annual Meeting, San Diego, CA, February 26th-March 3rd, 2011.
- **18.** Bajaj, S.; Landa, A.; Soderlind, P.; Turchi, P.; **Arróyave, R.** *CALPHAD and DFT Assessment of Metallic Alloy Fuel Materials.* Symposium: Materials for the Nuclear Renaissance II. TMS Annual Meeting, San Diego, CA, February 26th-March 3rd, 2011.
- **17.** Park, M. S.; **Arróyave, R.** *Phase-field Simulations of Microstructure and Crystal Orientation Evolution of Intermetallic Compound (Cu_6Sn_5) during Early Stages of Lead-free Soldering.* Symposium: Pb-Free Solders and Other Materials for Emerging Interconnect and Packaging Technologies. TMS Annual Meeting, San Diego, CA, February 26th-March 3rd, 2011.
- **16.** Chivukula, A.; **Arróyave, R.**; Basu, S.; Radovic, M. *On the Thermodynamic Stability of the Crystal Structure and Morphology in Ti_3AlC.* Symposium: Nanolaminated Ternary Carbides and Nitrides (MAX Phases). Materials Science and Technology Conference, Houston, TX, October 17th-22nd, 2010.
- **15.** Park, M. S.; **Arróyave, R.** *Formation and Growth of Intermetallic Compound (Cu_6Sn_5) at Early Stages in Lead-Free Soldering.* Symposium: Pb-Free Solders and Emerging Interconnect and Packaging Technologies. Materials Science and Technology Conference, Houston, TX, October 17th-22nd, 2010.

Conferences (continued)

- **14.** Bajaj, S.; Sevik, C.; Garay, A.; Cagin, T.; Turchi, P.; **Arróyave, R.** *Thermodynamic Study of the Neptunium-Zirconium System.* Symposium: Materials Solutions for the Nuclear Renaissance. Materials Science and Technology Conference, Houston, TX, October 17^{th}-22^{nd}, 2010.
- **13.** Junkaew, A.; Ham, B.; Zhang, X.; **Arróyave, R.** *Investigation of Structural and Thermodynamic Properties in Mg/Nb Multilayers.* Symposium: Clean Energy: Fuel Cells, Batteries, Renewables - Materials, Processing and Manufacturing. Materials Science and Technology Conference, Houston, TX, October 17^{th}-22^{nd}, 2010.
- **12.** Chivukula, A.; Dogan, E.; Karaman, I.; **Arróyave, R.** *An Analysis of the Alloying Effect on the Martensitic Transformation of Co_2NiGa Using First-Principles.* Symposium:Phase Stability, Diffusion, Kinetics and Their Applications. Materials Science and Technology Conference, Houston, TX, October 17^{th}-22^{nd}, 2010.
- **11.** Bajaj, S.; Garay, A.; Landa, A.; Söderlind, P,; Turchi, P.; **Arróyave, R.** *Thermodynamic Study of the Neptunium-Zirconium System.* NuMat 2010, Karlsruhe, Germany, October 4-7^{th}, 2010.
- **10.** Fernandes-Eleno, L. T.; Chivukula, A.; **Arróyave, R.**; Schön, C. G. *Metastable BCC Phase Diagram in the Co-Ni-Ga System*. Discussion Meeting on Thermodynamics of Alloys (TOFA-2010), Porto, Portugal,September 12-16^{th}, 2010.
- **9.** Park, M. S.; **Arróyave, R.** *Computational Investigations of Intermetallic Compound Formation and Growth in Cu/Sn Soldering*. Discussion Meeting on Thermodynamics of Alloys (TOFA-2010), Porto, Portugal,September 12-16^{th}, 2010.
- **8.** Bajaj, S.; **Arróyave, R.** *Thermodynamic Study of the Neptunium-Zirconium System.* Symposium:The Vasek Vitek Honorary Symposium on Crystal Defects, Computational Materials Science and Applications. TMS Annual Meeting, Seattle, WA, February 15-18^{th}, 2010.
- **7.** Park, M.-S.; **Arróyave, R.** *Formation and Growth of Intermetallic Compound Cu_6Sn_5 at Early Stages in Lead-Free Soldering.* Symposium:Pb-free Solders and Emerging Interconnect and Packaging Technologies. TMS Annual Meeting, Seattle, WA, February 15-18^{th}, 2010.
- **6.** Garay, A.;Trapaga, G.; **Arróyave, R.** *Thermodynamic Study of the Al-Si-Sr System.* Materials Science and Technology Conference, Pittsburgh, PA, October 25-29^{th}, 2009.
- **5.** Chari, A.; Garay, A.; **Arróyave, R.** *Thermodynamic Modelling of Ni-Ga System through Combined CALPHAD and Ab Initio Approach.* Symposium: Phase Stability, Diffusion Kinetics and Their Applications (PSDK-IV). Materials Science and Technology Conference, Pittsburgh, PA, October 25-29^{th}, 2009.
- **4.** Garay, A.; Trápaga, G.; **Arróyave, R.** *Determination of the Ground State of the Al-Si-Sr System by First-principles Calculations.* XVIII International Materials Research Congres 2009, Cancún, México, August 17-21^{th}, 2009.
- **3.** Park, M.-S.; **Arróyave, R.** *Multi-phase Field Simulation of Intermetallic Compound Growth during Lead Free Soldering* Symposium: Pb-Free Solders and Emerging Interconnect and Packaging Technologies: Microstructure, Modeling and Test Methods. TMS Annual Meeting, San Francisco, CA, February 15-19^{th}, 2009.
- **2.** Park, M.-S.; **Arróyave, R.** *Phase Field Simulation of the Morphology of Eutectic Solidification in a Binary Alloy Containing Encapsulated Impurities.* Symposium: Discovery and Optimization of Materials through Computational Design. Materials Science and Technology Conference, Pittsburgh, PA, October 5-9^{th}, 2008.
- **1.** Williams, M. E.; **Arróyave, R.** *Ab Initio Thermodynamic Properties of High-Temperature Cubic Intermetallics at Finite Temperatures.* Symposium: Phase Stability, Diffusion Kinetics and Their Applications. Materials Science and Technology Conference, Detroit, Michigan, September 16-20^{th}, 2007.

Conferences (continued)

Conference Talks

- **58.** Chang, C.-N.; Pardo, M.; Semma, B.; Fowler, D.; **Arróyave, R.**; Shamberger, P. J. *Data-Enabled Discovery and Design of Energy Materials (D^3EM): Structure of an Interdisciplinary Materials Design Graduate Program.* Symposium: Today's Teaching and Learning in Materials Science- Challenges and Advances. MRS Annual Fall Meeting. Boston, MA, Nov. 28^{th}-Dec. 2^{nd}, 2016
- **57.** **Arróyave, R.**; Talapatra, A.; Singh, N.; Entel, P. *Alloying, Configurational, Thermal and Magnetic Effects on the Phase Stability of Ferromagnetic Shape Memory Alloys: Perspectives from Ab Initio Calculations.* Symposium: Mechanics of Nanoscale phenomena & Multi-functional Material: Computational Materials with Emphasis on Phase Transformation. SES 2015. College Station, TX, October 25-28^{th}, 2015.
- **56.** Entel, P.; Gruner, M. E.; Zhang, H.; **Arróyave, R.**; Talapatra, A.; Singh, N.; Sokolovskiy, V. V.; Buchelnikov, V. D.; Ogura, M. *First-principles and Monte Carlo Simulations of Magnetocaloric Materials* EMN 2015, San Sebastian, Spain, September 1-4^{th}, 2015.
- **55.** Entel, P.; Sokolovskiy, V.; **Arróyave, R.**; Buchelnikov, V.; Gruner, M.; Uebayashi, K.; Singh, N.; *Large Magnetocaloric Effects in Magnetic Intermetallics: First-principles and Monte Carlo Studies* ESOMAT 2015, Antwerp, Belgium, September 14-18^{th}, 2015.
- **54.** Shamberger, P.; Jung, E.; Zhou, Y.; **Arróyave, R.**; Radovic, M. *Psychometric Analysis of the Materials Concept Inventory (MCI).* First Annual Mid Years Engineering Experience (MYEEC) Conference: From Slump to Jump!. College Station, TX, March 22-24^{th}, 2015.
- **53.** **Arróyave, R.**. *Synergistic Computational and Microstructural Design of Next Generation High-temperature Austenitic Stainless Steels* The National Energy Technology Laboratory's 2015 Crosscutting Technology Research Review Meeting, Pittsburgh, PA, April 27-30^{th}, 2015.
- **52.** Entel, P.; **Arróyave, R.**; Singh, N.; Gruner, M.; Grunebohm, A.; Sokolovskiy, V.; Buchelnikov, V. *First-Principles Calculation of Frustrated Ferroic Materials Ni-Co-Mn-(Ga, In, Sn)* Symposium: Frustrated Ferroic Materials. TMS Annual Meeting, Orlando, FL, March 15-19^{th}, 2015.
- **51.** Singh, N.; Gruner, M. E.; Entel, P.; **Arróyave, R.**. *Modeling Spin Glass Behavior in Shape Memory Alloys.* Symposium: Frustrated Ferroic Materials. TMS Annual Meeting, Orlando, FL, March 15-19^{th}, 2015.
- **50.** **Arróyave, R.**. *Phase Field Modelling of Microstructure Evolution in Solder Interconnects.* Symposium: Micromechanics of Structurally Inhomogeneous Materials: An FMD Symposium in Honor of Armen Khachaturyan. TMS Annual Meeting, Orlando, FL, March 15-19^{th}, 2015.
- **49.** Monroe, J.; Raymond, J. E.; Xu, X.; Kainuma, R.; Chumlyakov, Y. I.; **Arróyave, R.**; Karaman, I. *Multiple Ferroic Glasses via Ordering in a Single Material Composition.* Symposium: Frustrated Ferroic Materials. TMS Annual Meeting, Orlando, FL, March 15-19^{th}, 2015.
- **48.** **Arróyave, R.**; Li, S.; Wang, C. J.; Villarreal, R.; Jozaghi, T.; Karaman, I. *CALPHAD-based Alloy Design: Application to Advanced Steels.* Symposium: CALPHAD-Based ICME Research for Materials Genomic Design. TMS Annual Meeting, Orlando, FL, March 15-19^{th}, 2015.
- **47.** Entel, P.; **Arróyave, R.**; Singh, N.; Sokolovskiy, V.; Buchelnikov *Calculation of Electronic Structure and Field Induced Magnetic Collapse in Ferroic Materials*. TMS Middle East - Mediterranean Materials Congress on Energy and Infrastructure Systems (MEMA 2015), Doha, Qatar, Jan 11-15^{th}, 2015.
- **46.** **Arróyave, R.** *Coupled Structural and Magnetic Transformations in Smart Heusler Alloys: A Modeling Approach*. Engineering Research Symposium; SHPE Annual Conference, Detroit, MI, Nov 5-9^{th}, 2014.

Conferences (continued)

- **45.** Galvan, E.; Malak, R.; Gibbons, S. L.; **Arróyave, R.** *Constraint Satisfaction Approach to the Design of Multi-Component Multi-phase Alloys*. ASME International Design Engineering Technical Conference & Computers and Information in Engineering Conference (IDETC), Buffalo, NY, August 17-20th, 2014.
- **44. Arróyave, R.** ; *Parameter Identification in Phase-Field Models of Microstructure Evolution: Tuning Models to Discover Phenomena.* American Mechanics Symposium (Amerimech). Austin, TX, December 10-12th, 2014.
- **43. Arróyave, R.** ; Park, M. S.; Gibbons, S. L. *Towards the Materials Genome of Pb-free Interconnects: Contributions from Phase Field Modeling.* Symposium: Pb-free Solders and Advanced Interconnecting Materials. MS&T 2014, Pittsburgh, PA, October 12-16th, 2014.
- **42. Arróyave, R.**; A. Junkaew; B. Ham; X. Zhang. *Phase Stability in Multi-layered Thin Films.* Invited Talk, 3rd International Symposium on Nano-science and Nanomaterials . Ensenada, México, March 10-14th, 2014.
- **41. Arróyave, R.**; Gibbons, E. G.; Li, S.; Malak, R. *Solving Inverse Problems in Phase Stability: A Design Theoretic Approach.* Symposium: Hume-Rothery Award Symposium: Thermodynamics and Kinetics of Engineering Materials. TMS Annual Meeting, San Diego, CA, February 16-20th, 2014.
- **40. Arróyave, R.**; Junkaew, A.; Duong, T. *Computational Phase Stability Research and Education in Energy Materials: Some Examples in Hydrogen Storage and Nuclear Materials.* Symposium: Computational Modeling and Simulation of Advanced Materials for Energy Applications. TMS Annual Meeting, San Diego, CA, February 16-20th, 2014.
- **39. Arróyave, R.**; Li, S.; Gibbons, S.; Karaman, I.; Malak, R.; Galvan, E.; Rivera Diaz del Castillo, P. *Search and Optimization Tools for the Design of Multi-component and Multi-phase Materials.* Symposium: Material Data and Software Tools Needed to Make MGI and ICME a Reality . Materials Science & Technology 2013, Montreal, Canada, October 27th-31st, 2013.
- **38. Arróyave, R.**; Li, S. *Evolutionary Approaches for the Design of Multi-phase Multi-component Steel Alloys.* SHPE Research Symposium. SHPE Annual Conference. Indianapolis, October 31st-Novemberrd, 2013.
- **37. Arróyave, R.**; Singh, N.; Gruner, M.; Entel, P. *Alloying, Configurational, Thermal and Magnetic Effects on the Phase Stability of Ferromagnetic Shape Memory Alloys: Perspectives from Ab Initio Calculations.* XXII International Materials Research Congress. MRS International. Canc'un, México, August 11-15th, 2013.
- **36. Arróyave, R.;** Shi, S.-Y.; Wang, C.; Zhu, R.; Rivera-Díaz-del-Castillo, P. E. J.; Karaman, I.; Malak, R.; Galvan, E. *An Evolutionary Approach to the Design of Transformation Induced Plasticity (TRIP)-Aided Steels.* Second World Congress on ICME, Salt Lake City, Utah, July 7-11th, 2013.
- **35. Arróyave, R.;** Shi, S.-Y.; Zhu, R.; Rivera-Díaz-del-Castillo, P. E. J.; Karaman, I. *New Approaches to the Computer-Aided Design of Multi-Phase Multi-Component Structural Alloys.* TKM-2013, International Workshop on Materials Design Process: Thermodynamics, Kinetics and Microstructure Control, IMDEA, Madrid, Spain, June 3-4th, 2013.
- **34. Arróyave, R.;** Li, S.-Y.; Wang, C.; Zhu, R.; Rivera-Díaz-del-Castillo, P. E. J.; Karaman, I. *An Evolutionary Approach to the Design of Transformation Induced Plasticity (TRIP)-Aided Steels.* CALPHAD Meeting, San Sebastián, Spain, May 26-31st, 2013.
- **33.** Santamarta, R.; Pons, J.; Evirgen, A.; **Arróyave, R.;** Karaca, H.; Karaman, I.; Noebe, R. *Characteristics of a New Precipitate Phase in Ni-rich Ni-Ti-Hf and Ni-Ti-Zr High Temperature Shape Memory Alloys.* Symposium: Physical and Mechanical Metallurgy of Shape Memory Alloys. TMS Annual Meeting, San Antonio, TX, March 3-7th, 2013.

Conferences (continued)

- **32. Arróyave, R.** *Ab Initio Thermodynamics and Elastic Properties of Structural Materials at Finite Temperatures.* NSF Workshop on Challenges and Opportunities for Research in Multiscale Modeling in Mechanics and Materials (M^4). Co-chairs: Glaucio Paulino and Clark Cooper, NSF. NSF CMMI Grantees Conference. Atlanta, GA, January 4-5th, 2011.
- **31. Arróyave, R.**; Junkaew, A.; Garay, A.; Chari, A.; Yao, C.-W. *Thermodynamics, structural properties and transformation behavior of CoNiGa Alloys from First Principles.* Symposium:Computational Thermodynamics and Kinetics. TMS Annual Meeting, Seattle, WA, February 15-18th, 2010.
- **30. Arróyave, R.** *Ab Initio Investigation and Thermodynamic Modeling of Co-Ni-Ga and Co-Ni-Al Shape Memory Alloys*Special Workshop on Shape Memory Alloys, Istanbul Turkey, June 19-24th, 2010.
- **29. Arróyave, R.**;Chari, A.; Chivukula, A.; Junkaew, A. *Ab Initio Investigation and Thermodynamic Modelling of Co-Ni-Ga and Co-Ni-Al Shape Memory Alloys* International Conference of Materials Science, Cancun, Mexico, August 15-22th, 2010.
- **28. Arróyave, R.** *Development of an Integrated Framework for the Prediction of Thermodynamic, Structural and Kinetic Properties of Alloys by using Ab Initio Methods.*Symposium:Discovery and Optimization of Materials through Computational Design. Materials Science and Technology Conference, Pittsburgh, PA, October 25-29th, 2009.
- **27. Arróyave, R.**; Williams, M. E. *Implementing an Open Source Integrated Framework for Ab Initio Thermodynamics using Python as a Glue Language*-**Invited.** Symposium: Open Source Tools for Materials Research and Engineering: Session I. TMS Annual Meeting, San Francisco, CA, February 15-19th, 2009.
- **26. Arróyave, R.** *Thermodynamic Stability of Materials: Integration of Finite-Temperature Ab Initio Methods and CALPHAD Modeling*-**Invited.** Symposium: Discovery and Optimization of Materials through Computational Design. Materials Science and Technology Conference, Pittsburgh, PA, October 5-9th, 2008.
- **25. Arróyave, R.**; Garay, A. M.; Williams, M. E.; Trapaga, G. *Ab Initio Investigation of the Finite-Temperature Thermodynamic Properties of Strontium Silicides.* Symposium: Phase Stability, Diffusion Kinetics and Their Applications (PSDK-III). Materials Science and Technology Conference, Pittsburgh, PA, October 5-9th, 2008.
- **24. Arróyave, R.**; Liu, Z. K.; Schmid-Fetzer *Application of Ab Initio Finite Temperature Thermodynamics to CALPHAD Modeling.*CALPHAD XXXVI Meeting. State College, PA, May 5-10th, 2007.
- **23.** Mantina, M.; Wang, Y.; **Arróyave, R.**; Wolverton, C.; Chen, L. Q.; Liu, Z. K. *Calculating Diffusion Coefficients via First-Principles Methods.*Symposium: Diffusion in Advanced Materials and Processing: Atomistic and Multiscale Simulations. TMS Annual Meeting, Orlando, Florida, February 26-March 1st, 2007.
- **22. Arróyave, R.**; Shin, D.; Prins, S.; Shang, S.; Wang, T.; Yang, M.; Liu, Z. K. *Thermodynamic Modeling of Random Mixing using First-Principles Methods: An Application of Special Quasirandom Structures.* Symposium: Phase Stability, Diffusion and Their Applications. Materials Science and Technology Conference, Cincinnati, Ohio, October 15-19th, 2006.
- **21. Arróyave, R.**; Williams, J.; Fischer, D.; Eagar, T. W. *Using Computational Thermodynamics in the Development of Lead-FreeSolder Alloys.* Symposium: Lead-Free Soldering: It is Here to Stay. Materials Science and Technology Conference, Cincinnati, Ohio, October 15-19th, 2006.

Conferences (continued)

- **20.** Mantina, M.; **Arróyave, R.**; Wang, Y.; Wolverton, C.; Chen, L.-Q.; Liu, Z. K. *Calculating Impurity Diffusion Coefficients via First-Principles Methods.* Symposium: Phase Stability, Diffusion and Their Applications. Materials Science and Technology Conference, Cincinnati, Ohio, October 15-19th, 2006.
- **19.** Mantina, M.; **Arróyave, R.**; Wang, Y.; Wolverton, C.; Chen, L.-Q.; Liu, Z. K. *Calculating Self-Diffusion Coefficients via First-Principles Methods.* Symposium: Diffusion in Advanced Materials and Processing. Materials Science and Technology Conference, Cincinnati, Ohio, October 15-19th, 2006.
- **18.** **Arróyave, R.**; Prins, S.; Liu, Z. K. *First-principles thermodynamic properties of the stable binary B2 phases in the Al-Ni-Ru-Ir-Pd System.* Symposium: Computational Thermodynamics and Phase Transformations. TMS Annual Meeting, San Antonio, Texas, March 12-16th, 2006.
- **17.** **Arróyave, R.**; Ohno, M.; Liu, Z. K.; Schmid-Fetzer, R. *Finite-Temperature Thermodynamic Properties of Intermetallics in the Mg-Ca-Sn System via First-Principles Methods.* Symposium: Magnesium Technology 2006. TMS Annual Meeting, San Antonio, Texas, March 12-16th, 2006.
- **16.** **Arróyave, R.**; Williams, J; Eagar, T. W. *Thermodynamic models for the Bi-Ga-In-Sn-Zn lead-free system; Symposium on Lead Free Solder Implementation.* Symposium: Lead Free Alloys Design. TMS Annual Meeting, San Antonio, Texas, March 12-16th, 2006.
- **15.** **Arróyave, R.**; Shin, D.; van de Walle, A.; Liu, Z. K. *The Mg-Zn-Zr System: From First Principles to Grain Refining, An Integrated Approach to Materials Design.* Symposium: Materials Design Approaches and Experiences II. TMS Annual Meeting, San Antonio, Texas, March 12-16th, 2006.
- **14.** Liu, Z. K.; Curtarolo, S.; Kolmogorov, A.; **Arróyave, R.**; Shin, D. *Integrating First-Principles Calculations and Thermodynamic Modelling*. Symposium: Hume-Rothery Symposium on Alloy Theory. TMS Annual Meeting, San Antonio, Texas, March 12-16th, 2006.
- **13.** Prins, S.; **Arróyave, R.**; Liu, Z. K. *Study of Defects Structures in B2 Phases via First-Principles Calculations.* Symposium: Point Defects in Materials. TMS Annual Meeting, San Antonio, Texas, March 12-16th, 2006.
- **12.** Shin, D.; Golumbfskie, W.; **Arróyave, R.**; Liu, Z. K. *CALPHAD/First-Principles Hybrid Approach: The study of Phase Equilibria and Solidification Behavior of the Al-Ni-Y System.* Symposium: Simulation of Aluminum Shape Casting Processing. TMS Annual Meeting, San Antonio, Texas, March 12-16th, 2006.
- **11.** Golumbfskie, W. J; **Arróyave, R.**; Shin, D. W.; Liu, Z. K. *Combining First-Principles and CALPHAD: Al-Ni-Y Phase Diagram Prediction.* CALPHAD XXXIV, Maastricht, The Netherlands, May 22-27th, 2005.
- **10.** Prins, S.; **Arróyave, R.**; Liu, Z. K. *The use of first principle Calculations for the Thermodynamic Assessment of B2 in the Al-Ni-Ru System.* , CALPHAD XXXIV, Maastricht, The Netherlands, May 22-27th, 2005.
- **9.** **Arróyave, R.**; Liu, Z. K. *Thermodynamic Model of the Mg-Zn-Zr System and its Application to the Grain Refinement of Mg-Zn-Zr Alloys.* Symposium: Magnesium Technology 2005. TMS Annual Meeting, San Francisco, California, February 13-17th, 2005.
- **8.** **Arróyave, R.**; Prins, S.; Liu, Z. K. *B2 Phases and their Defect Structures: Part II. Ab initio Vibrational and Electronic Free Energy in the Al-Ni-Pt-Ru System.* Symposium: Intermetallics: An Integrative Approach. MRS Fall Meeting, Boston Massachusetts, November 29-December 2nd, 2004.

Conferences (continued)

- **7.** Prins, S.; **Arróyave, R.**; Jiang, C.; Liu, Z. K. *B2 Phases and their Defect Structures: Part I. Ab initio Enthalpy of Formation and Enthalpy of Mixing in the Al-Ni-Pt-Ru System.* Symposium: Intermetallics: An Integrative Approach. MRS Fall Meeting, Boston Massachusetts, November 29-December 2nd, 2004.
- **6. Arróyave, R.**; Liu, Z. K. *Integration of Multiscale Materials Simulation and Design: Ab Initio Methods and CALPHAD Approach*.Gordon Research Conference, Physical Metallurgy, Holderness School, New Hampshire, July 25-30th, 2004.
- **5. Arróyave, R.**; Eagar, T.W. *Thermodynamic Assessment of the Ag-Cu-Ti System.* Symposium: Computational Thermodynamics and Phase Transformations. TMS Annual Meeting, Charlotte, North Carolina, March 14-18th, 2004.
- **4. Arróyave, R.**; Eagar, T. W. *Modeling of Coupled Ti-oxide Growth in Ceramic/Metal Interfaces using Phase-Field Methods.* CALPHAD XXXII, Quebec, Canada May 25-30th, 2003.
- **3. Arróyave, R.**; Eagar, T. W.; Larson, H. *Joining $LaMO_3$ Perovskite Ceramics to Nickel-based Super Alloys using Liquid Brazing/TLPB Techniques*.225th ACS National Meeting in Fuel Symposia, New Orleans, March 23-27th, 2003.
- **2. Arróyave, R.**; Eagar, T. W. *The Use of Thermodynamic and Kinetic Tools to Understand Ceramic/Metal Joining.* University Welding Research Conference for Defense Applications, Columbus, Ohio, August 6-7th, 2002.
- **1. Arróyave, R.**; Kaufman, L.; Eagar, T. W. *Thermodynamic Assessment of the Zr-O System.* CALPHAD XXXI, Stockholm, Sweden, May 5-6th, 2002.

Research Group

Postdoctoral Scholars

- **4.** Thien Duong, 2016-present
- **3.** Anjana Talapatra, 2016-present
- **2.** Navdeep Singh, 2011-2013
- **1.** Min Soo Park, 2009-2014

PhD Students

- **16.** Luke Johnson, PhD (12/2020-expected), *Design of Alloys for Additive Manufacturing*
- **15.** Ruben Villarreal, PhD (12/2020-expected), *Transformation Paths in VO_2 through Ab Initio Methods*
- **14.** Frank Greenhalt, PhD (12/2019-expected), *Heusler Strain Glasses*
- **13.** Woongrak Son, PhD (12/2019-expected), *Ab Initio Investigation of MAX Phases Solid Solutions*
- **12.** Vahid Attari, PhD (12/2019-expected), *Phase Field Modeling of Low Volume Solder Interconnects*
- **11.** Pejman Honarmandi, PhD (12/2018-expected), *Uncertainty Quantification and Propagation in Physical Materials Models*
- **10.** Kubra Karayagiz, PhD (12/2018-expected), *Phase Field Models of Rapid Solidification during Additive Manufacturing*
- **9.** Emilia Olivos, PhD (12/2016-expected), *Ab Initio Investigation in Fe-Mn-Ga Heusler Systems*
- **8.** Sean Gibbons, PhD (05/2016), *Austenite Grain Refinement and ε-Carbide Precipitation Optimization in Ultra-High-Strength Steel Alloy ES-1*

Research Group (continued)

- **7.** Thien Duong, PhD (12/2015), *Integrated Computational Materials Science and Engineering for The Research and Development of Gen-IV Metallic Fuels: Application to Uranium-Niobium*
- **6.** Anjana Talapatra, PhD (12/2015), *Ab Ab Initio Investigation of Thermoelastic Phase Transformations in Transition Metal Alloys*
- **5.** Chung-Hau Hsu, PhD (05/2013), *Manipulation of Thermal Phonons*
- **4.** Shengyen Li, PhD (08/2013), *Genetic Algorithm Optimization of Advanced High Strength Steels*
- **3.** Anchalee Junkaew, PhD (12/2013), *Mg-based Nano-layered Thin Films for Hydrogen Storage*
- **2.** Andres Garay, PhD (12/2010), *First-Principles Investigation of the Al-Si-Sr System*, CINVESTAV, Mexico
- **1.** Min Soo Park, PhD (12/2009), *Phase-Field Models for Solidification and Solid/Liquid Interactions*

MS Students

- **9.** Vinay Akula, MS (05/2017-expected), *Project: Deployment of the Materials Data Curation System*
- **8.** Nayan Chaudhary, MS (08/2016), *A Machine Learning Approach to the Prediction of Stacking Fault Energies in Austenitic Steels*
- **7.** Ramaranjan Ruj, MS (05/2016-expected), *Project: Development and Deployment of MS Galaxy Materials Informatics System*
- **6.** Luke Johnson, MS (12/2015), *A Computational Framework for the Prediction of Multistage Heat Treatments in Age Hardened Alloys*
- **5.** Chung Wang, MS (12/2014), *Study of Alumina in Stainless Steels*
- **4.** Hassan Thawabi, MS (05/2013), *Ab-initio First Principles Modeling of Structural and Magnetic Phase Transformations in Co-Ni-Al Based Shape Memory Alloys*
- **3.** Arpita Chari, MS (08/2011), *Computational Thermodynamics of CoNiGa High Temperature Shape Memory Alloys*
- **2.** Saurabh Bajaj, MS (12/2010), *First-Principles and CALPHAD Study of the Np-Zr System*
- **1.** Michael E. Williams, MS (05/2008), *Ab Initio Elastic and Thermodynamic Properties of High-Temperature Intermetallics at Finite Temperatures*

BS Students

- **8.** Anas Abu-Odeh, BS (05/2017), *Project: Data Curation of Stacking Fault Energies*
- **7.** Daniel Sauceda, BS (05/2017), *Project: Materials Data Curation System*
- **6.** Miguel Reyes, BS (05/2012), *Project: Lead-free Solders*
- **5.** Kyle Hudspeth, BS (05/2013), *Project: Implementing Micromechanics in Phase-Field Models*
- **4.** Malcolm Stephenson, BS (05/2011), *Project: Experimental Work on Lead-Free Soldering*
- **3.** Colton Shannon, BS (05/2011), *Project: Experimental Work on Lead-Free Soldering*
- **2.** Ramon Silva, BS (05/2010), *Project: Computational Investigation of Elastic Properties of Metals and Ceramics*
- **1.** Stephen Smith, BS (05/2009), *Project: Development of Numerical Schemes for Microstructure Modeling*

Research Group (continued)

Visiting Students

- **4.** Emilia Olivos, MS/PhD (2013/2014), Institution: CINVESTAV, Mexico, *Ab Initio Investigation in Fe-Mn-Ga Heusler Alloys*
- **3.** Oussama Hattab, MS (06/2011), Institution: Tunisian Polytechnic University, Tunisia, *Elastic Constants of Shape Memory Alloys*
- **2.** Alberto Caceres Diaz, MS (12/2011), Institution: CINVESTAv, Mexico, *Investigation of Phase Transformation in B2 Bond Coat Materials*
- **1.** Andres Garay, PhD (08/2010), Institution: CINVESTAV, Mexico, *Project: Eutectic Modification in Al-Si-Sr Ternary Alloys*