

119 Engineering/Physics Bldg  
Department of Mechanical Engineering  
Texas A & M University  
College Station, TX 77843-3123  
Ph: (979) 845-5416 rarroayave@tamu.edu

## Raymundo Arróyave, Ph. D.

### 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

- 2006-...      • **Assistant Professor of Mechanical Engineering, Member of Materials Science and Engineering Faculty**  
*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)*

### Teaching Experience

- Spring 2008      • **Instructor, Thermodynamics in Materials Science (MEEN 489/689-MSEN 689 )**  
*Texas A & M University, (College Station, TX )*  
Graduate Level Course
- 2007-...      • **Instructor, Introduction to Materials Science and Engineering (MEEN 222 )**  
*Texas A & M University, (College Station, TX )*  
Undergraduate Level Course-U2
- Spring 2007      • **Instructor, Numerical Methods for Mechanical Engineers (MEEN 357 )**  
*Texas A & M University, (College Station, TX )*  
Undergraduate Level Course-U3
- Spring 2005      • **Teaching Assistant, Computational Thermodynamics (MatSE597C )**  
*Pennsylvania State University, (University Park, PA)*  
Instructor: Prof. Zi-Kui Liu

## Teaching Experience (continued)

- 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

- 2006-2007 • Young Leaders Professional Development Award, EPMD Division. (Formerly known as the Young Leaders Internship Award). The Mineral, 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

### *Refereed Journals*

- 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
- Powell IV, A. C.; **Arróyave, R.** *Open Source Tools for Materials and Process Modeling*. JOM (2008), 60(5), pp.32-37
- Kozlov, A.; Ohno, M.; **Arróyave, R.**; Liu, Z.-K.; Schmid-Fetzer, R. *Phase Equilibria and Thermodynamics of the Mg-Ca-Sn System Part I. Thermodynamic Modeling of Ternary Mg-Sn-Ca Phase Equilibria*. Intermetallics (2008), 16(2), pp.299-315
- 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
- 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.
- 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.
- Shin, D.; **Arróyave, R.**; Liu, Z.-K. *Thermodynamic Modeling of the Hf-Si-O System*. CALPHAD (2006), 30(4), pp.375-386.
- **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
- 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.
- 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
- **Arróyave, R.**; Liu, Z.-K. *Thermodynamic Modelling of the Zn-Zr System*. CALPHAD, (2006), 30(1), pp. 1-13.

## Publications (continued)

- Golumbskie, 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.
- Venimadhava, 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  $\text{Na}_x\text{CoO}_2$  Thin Films*. Applied Physics Letters (2005), 87(17), pp. 172104 1-3.
- **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.
- **Arróyave, R.**; Shin D.; Liu, Z.-K. *Modification of the Thermodynamic Model for the Mg-Zr System*. CALPHAD (2005), 29(3), pp. 230-238.
- 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.
- **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.
- **Arróyave, R.**; Eagar, T.W. *Thermodynamic Assessment of the Ag-Cu-Ti System*. TMS Letters (2004), 1(5), pp. 87-88.
- 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.
- **Arróyave, R.**; Eagar, T. W. *Metal Substrate Effects on the Thermochemistry of Active Braze Interfaces*. Acta Materialia, (2003) 51(16), pp. 4871-4880.
- **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.
- **Arróyave, R.**; Kaufman, L.; Eagar, T. W. *Thermodynamic Modeling of the Zr-O system*. CALPHAD(2002), 26(1), pp. 95-118.
- 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.

## Refereed Journals, Submitted

- Mantina, M; Wang, Y.;**Arróyave, R.**;Shang, S.; Chen, L. Q.; Liu, Z.-K. *First-principles Approach to Transition States of Diffusion*. Physical Review Letters (2008), Submitted
- Park, M.-S.; **Arróyave, R.** *A Phase-Field Model of the Eutectic Solidification of Binary Alloy containing Encapsulated Impurities*. Computational Materials Science (2008), Submitted
- Williams, M. E.; Liu, Z.-K.; **Arróyave, R.** *First-Principles Thermodynamic and Elastic Properties of B2 NiAl, RuAl and IrAl at Finite Temperatures*. Intermetallics (2008), Submitted
- Garay, A.; Trapaga, G.; Liu, Z.-K.;**Arróyave, R.** *Thermodynamic Modelling of the Si-Sr System*. CALPHAD (2008), Submitted
- Garay, A.; Williams, M. E.; Trapaga,**Arróyave, R.** *Thermodynamics, Lattice Stability and Defect Structure of Strontium Silicides via First-Principles Calculations*CALPHAD (2008), Submitted

## Conference Proceedings

- 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 (2009). Submitted

## Publications (continued)

- 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 NaXCoO<sub>2</sub> Thin Films*. Materials Research Society Symposium Proceedings (2006), 886 (Materials and Technologies for Direct Thermal-to-Electric Energy Conversion), pp. 64-74
- **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.
- 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.
- **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.
- **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.
- **Arróyave, R.**; Eagar, T.W.; Larson, H. *Joining LaMO<sub>3</sub> Perovskite Ceramics to Nickel-based Super Alloys using Liquid Brazing/TLPB Techniques*. Fuel Chemistry Division Preprints, (2003), 48(1), pp. 247-250.
- 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.

## Invited Talks

- *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.
- *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.
- *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 Engineering College Station, TX, Nov. 9th, 2007
- *Multi-scale Materials Modeling for Alloy Design*. Centro de Investigación y Estudios Avanzados del IPN, Unidad Querétaro. Querétaro, México, Oct. 4th 2007.
- *MEEN 681 Graduate Seminar: "Applications of Computational Thermodynamics in Materials Modeling and Design"*. Texas A&M University, Department of Mechanical Engineering College Station, TX, Sep. 12th, 2007
- *Computational Materials Design*. University of Texas, Pan-American Edinburg, TX, Feb. 16th, 2007
- *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. 26-27th, 2005.

## Invited Talks (continued)

- *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. 11th 2005.
- *Seminar on Computational Thermodynamics and Kinetics of Materials.* Centro de Investigación y Estudios Avanzados del IPN, Unidad Querétaro. Querétaro, México, Mar. 8-9th 2005.
- *Thermodynamic and Kinetic Aspects of Ceramic-Metal Joints.* Materials Science Seminar. Centro de Investigación y Estudios Avanzados del IPN, Unidad Querétaro. Querétaro, México, Jul. 28th 2003.
- *Joining Complex Oxide Ceramics to Metals.* Materials Science Seminar at New Mexico Institute of Technology. Socorro, NM. Jan. 10th 2003.

## Affiliations

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

## Service

### *Professional*

- 2002-... • Journal Reviewer: CALPHAD; Intermetallics; Journal of Alloys and Compounds; Journal of the American Welding Society; Journal of Metals; Materials Science and Engineering A; Metallurgical and Materials Transactions B; Metallurgical Transactions A; MRS Proceedings.
- 2008-... • NSF Review Panel
- Member, Admissions Committee, Materials Science and Engineering Program, Texas A&M University
- Representative of Electronic, Magnetic & Photonic Materials Division (EMPMD) to Education Committee of The Minerals, Metals and Materials Society (TMS)
- Member, Chemistry and Physics of Materials Committee, TMS
- 2008-2011 • Member, John Bardeen Award Committee, EMPMD Division, TMS
- 2007-... • Member, Alloy Phases Committee, EMPMD Division, TMS
- 2007-2010 • Member, Alloy Phase Diagram Committee, ASM International
- 2007-... • Co-Organizer, Symposium: Phase Stability, Diffusion Kinetics and Their Applications (PSDK-II-...); Conference: Materials Science and Technology, 2007-...

### *Department and University*

- 2008-... • Member, Admissions Committee, Materials Science and Engineering Program, Texas A& University
- Advisor, Materials Advantage Chapter, Texas A& University

## Conferences

- **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. MS&T 2008, Pittsburgh, PA, October 5-9th, 2008.
- **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. MS&T 2008, Pittsburgh, PA, October 5-9th, 2008.
- **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). MS&T 2008, Pittsburgh, PA, October 5-9th, 2008.
- **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. MS&T 2007, Detroit, Michigan, September 16-20th, 2007.
- **Arróyave, R.; Liu, Z.-K.; Schmid-Fetzer** *Application of Ab Initio Finite Temperature Thermodynamics to CALPHAD Modeling.* CALPHAD XXXVI Meeting. State College, PA, May 5th-10th, 2007.
- **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. 2007 TMS Annual Meeting, Orlando, Florida, February 26-March 1st, 2007.
- **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 2006, Cincinnati, Ohio, October 15-19th, 2006.
- **Arróyave, R.; Williams, J.; Fischer, D.; Eagar, T. W.** *Using Computational Thermodynamics in the Development of Lead-Free Solder Alloys* Symposium: Lead-Free Soldering: It is Here to Stay. Materials Science and Technology 2006, Cincinnati, Ohio, October 15-19th, 2006.
- **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 2006, Cincinnati, Ohio, October 15-19th, 2006.
- **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 2006, Cincinnati, Ohio, October 15-19th, 2006.
- **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. 2006 TMS Annual Meeting, San Antonio, Texas, March 12-16th, 2006.
- **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. 2006 TMS Annual Meeting, San Antonio, Texas, March 12-16th, 2006.
- **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. 2006 TMS Annual Meeting, San Antonio, Texas, March 12-16th, 2006.
- **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. 2006 TMS Annual Meeting, San Antonio, Texas, March 12-16th, 2006.

## Conferences (continued)

- 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. 2006 TMS Annual Meeting, San Antonio, Texas, March 12-16th, 2006.
- Prins, S.; **Arróyave, R.**; Liu, Z. K. *Study of Defects Structures in B2 Phases via First-Principles Calculations*. Symposium: Point Defects in Materials. 2006 TMS Annual Meeting, San Antonio, Texas, March 12-16th, 2006.
- Shin, D.; Golombfskie, 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. 2006 TMS Annual Meeting, San Antonio, Texas, March 12-16th, 2006.
- Golombfskie, 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.
- 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.
- **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. 2005 Annual TMS Meeting, San Francisco, California, February 13-17th, 2005.
- **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.
- 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.
- **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.
- **Arróyave, R.**; Eagar, T.W. *Thermodynamic Assessment of the Ag-Cu-Ti System*. Symposium: Computational Thermodynamics and Phase Transformations. 2004 Annual TMS Meeting, Charlotte, North Carolina, March 14-18th, 2004.
- **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.
- **Arróyave, R.**; Eagar, T. W.; Larson, H. *Joining LaMO<sub>3</sub> 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.
- **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.
- **Arróyave, R.**; Kaufman, L.; Eagar, T. W. *Thermodynamic Assessment of the Zr-O System*. CALPHAD XXXI, Stockholm, Sweden, May 5-6th, 2002.

## 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; computational materials design.

### *Teaching*

- Thermodynamics; Kinetics; Computational Methods in Materials Science; Phase Transformations; Materials Design.

## Collaborations

- Tahir Cagin, Texas A&M, USA  
Stefano Curtarolo, Duke University, USA  
Thomas W. Eagar, MIT, USA  
Jeff Froyd, Texas A&M, USA  
Alberto Herrera-Gomez, CINVESTAV, México  
Yongmei Jin, Texas A&M, USA  
Zi-Kui Liu, Pennsylvania State University, USA  
Miladin Radovic, Texas A&M, USA  
Rainer Schmid-Fetzer, TU Clausthal, Germany  
Gerardo Trápaga Martínez, CINVESTAV, México  
Axel van de Walle, Northwestern University, USA

## Students

- Michael E. Williams, M. Sc. 2008  
Andres Garay, PhD  
Anchalee Junkaew, PhD  
Min Soo Park, PhD  
Chun-Wei Yao, PhD  
Arpita Chari, M. Sc.  
Saurabh Bajaj, M. Sc.  
Kevin SMith, B. Sc.  
Ramon Silva, B. Sc.