Sergiy Kalnaus
Curriculum Vitae

Oak Ridge National Laboratory
Computational Engineering and Energy Sciences
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EDUCATION

Ph.D., Mechanical Engineering 2009
University of Nevada, Reno, NV

M.S., Mechanical Engineering 1998
Kharkiv State Polytechnic Institute, Kharkiv, Ukraine

B.S., Mechanical Engineering 1996
Kharkiv State Polytechnic Institute, Kharkiv, Ukraine

RESEARCH EXPERIENCE

Oak Ridge National Laboratory 2009 to present

Project title: Safe Fire Resistant Electrolyte (SAFIRE) (DOE, ARPA-e) 2014

- Development of shear thickening electrolyte for Li-ion batteries.

Project title: CAEBAT - Computer Aided Engineering for Electric Drive Vehicle Batteries (DOE, VTP) 2012-2014

- Development of predictive battery design tools for optimizing cost, performance and life.

Project title: Tough solid electrolytes for Li and Li-ion batteries (LDRD, ORNL) 2010-2013

- Simulations of effective mechanical and electrical properties of novel composite electrolytes for Li-ion batteries.

Project title: Intercalation kinetics and ion mobility in electrode materials for advanced lithium-ion batteries (DOE, VTP) 2009-2012

- Electrochemical Strain Microscopy (ESM) investigation of lithium ion kinetics in thin film cathode materials.
- Effect of mechanical damage on ion mobility in Li-ion battery cathode materials.
- Coupled kinetic, thermal and mechanical modeling of Focused Ion Bean (FIB) micro-machined electrodes of cathode materials for Li-ion batteries.

Project title: In-situ characterization of fatigue behavior of electrodes (DOE, VTP) 2009-2011

- Prediction of stress development and fracture of active electrode material particles in Li-ion battery based on experimental Acoustic Emission (AE) data.

Department of Mechanical Engineering, 2004-2009
University of Nevada, Reno

Project title: Development of a novel approach for fatigue life prediction of structural materials (DOD) 2005-2008

- Extensive experimental study on fatigue behavior of metallic materials, mainly austenitic stainless steels. Experiments involving multiaxial fatigue with different fracture modes as well as crack growth experiments.
- Development of multiaxial fatigue models based on the experimental results.
- Experimental study and modeling of cyclic plasticity properties of stainless steels.
- Crack growth rate modeling with constant and variable loading conditions.

Project title: Environmental effects on the incubation time characteristics in stress-corrosion cracking (ONR) 2008-2010

- Environmentally assisted cracking and fatigue of high-strength alloys.

Research Assistant 2007

- Experimental investigation of fatigue properties of nano-composite materials.

RESEARCH INTERESTS

- Diffusion-stress coupling and degradation of materials for energy storage
- Composite materials for energy storage
- Fatigue and fracture of materials
- Stress-corrosion and corrosion fatigue
- Constitutive relations for inelastic deformation

TEACHING EXPERIENCE

Courses Taught

Applied Numerical Methods 2007-2008

Department of Mechanical Engineering, University of Nevada, Reno.
Developed and taught the course. Prepared and delivered lectures and exams.

Dynamics 2008

Department of Mechanical Engineering, University of Nevada, Reno.
Developed and taught the course. Prepared and delivered lectures and exams.

Teaching Assistant

Advanced Mechanics 2007
Department of Mechanical Engineering, University of Nevada, Reno.
Developed and conducted the lab section of the course.

Computational Methods for Engineering 2005
Department of Mechanical Engineering, University of Nevada, Reno.
Conducted the computer lab section of the course.

Design Synthesis 2004
Department of Mechanical Engineering, University of Nevada, Reno.
Conducted study sessions and performed grading of the projects.

Awards

Teaching Recognition Award, University of Nevada, Reno 2007

Student Mentoring

Sarah J. Newman. Volkswagen Distinguished Scholars Program, ORNL 2010

TEACHING INTERESTS

- Energy storage
- Numerical methods for engineers
- Continuum mechanics
- Mechanical behavior of materials (elastic, inelastic, fatigue and creep)
- Strength of materials

PROFESSIONAL AFFILIATIONS

- American Society of Mechanical Engineers (ASME)
- Electrochemical Society (ECS)
- Society for Industrial and Applied Mathematics (SIAM)
- Materials Research Society (MRS)

REVIEW SERVICES

ASM Journal of Engineering Materials and Performance, International Journal of Fatigue, International Journal of Plasticity, Ionics, Solid State Ionics, Metallurgical and Materials Transactions (MMT) A, MMT E, ASME Journal of Engineering Materials and Technology, Journal of Power Sources.

JOURNAL PUBLICATIONS

- Allu, S., Kalnaus, S., Elwasif, W., Simunovic, S., Turner, J.A., Pannala, S., 2014, "A New Open Computational Framework for Highly-Resolved Coupled Three-Dimensional Multiphysics Simulations of Li-ion Cells," *Journal of Power Sources*, **246**, pp. 876-886.
- Kalnaus, S., Tenhaeff, W.E., Sakamoto, J., Sabau, A.S., Daniel, C., Dudney, N.J., 2013, "Analysis of Composite Electrolytes with Sintered Reinforcement Structure for Energy Storage Applications," *Journal of Power Sources*, **241**, pp. 178-185.
- Mohanty, D., Sefat, A.S., Kalnaus, S., Li, J., Meisner, R.A., Payzant, E.A., Abraham, D.P., Wood, D.L., and Daniel, C., 2013, "Investigating Phase Transformation in Li1.2Co0.1Mn0.55Ni0.15O2 Lithium-ion Battery Cathode During High-Voltage Hold (4.5 V) via Magnetic, X-ray Diffraction and Electron Microscopy Studies," *Journal of Materials Chemistry A*, **1**(20), pp. 6249-6261.
- Mohanty, D., Kalnaus, S., Meisner, R., Li, J., Payzant, E.A., Rhodes, K., Wood, D., and Daniel, C., 2013, "Structural Transformations in a $Li_{1.2}Co_{0.1}Mn_{0.55}Ni_{0.15}O_2$ Lithium-ion Battery Cathode During High-Voltage Hold," *RSC Advances*, **3**(20), pp. 7479-7485.
- Mohanty, D., Kalnaus, S., Meisner, R., Li, J., Rhodes, K., Abraham, D., Daniel, C., and Wood, D., 2013, "Structural Transformation of a Lithium-Rich $Li_{1.2}Co_{0.1}Mn_{0.55}Ni_{0.15}O_2$ Cathode During High-Voltage Cycling Resolved by in-situ X-Ray Diffraction," *Journal of Power Sources*, **229**, pp. 239-248.
- Weng, L., Zhang, J., Kalnaus, S., Feng, M., and Jiang, Y., 2013, "Corrosion Fatigue Crack Growth of AISI 4340 Steel," *International Journal of Fatigue*, **48**, pp. 156-164.
- Park, J., Kalnaus, S., Han, S., Lee, Y.K., Less, G.B., Dudney, N.J., Daniel, C., and Sastry, A.M., 2012 "In-situ Atomic Force Microscopy Studies on Lithium (de)Intercalation-Induced Morphology Changes in Li_xCoO_2 Micro-Machined Thin Film Electrodes," *Journal of Power Sources*, **222**, pp. 417-425.
- Balke, N., Kalnaus, S., Daniel, C., Jesse, S., and Kalinin, S.V., 2012, "Local Detection of Activation Energy for Ionic Transport in Lithium Cobalt Oxide," *Nano Letters*, **12**(7) pp. 3399-3403.
- Balke, N., Eliseev, E.A., Jesse, S., Kalnaus, S., Daniel, C., Dudney, N.J., Morozovska, A.N., and Kalinin, S.V., 2012, "Three-Dimensional Vector Electrochemical Strain Microscopy," *Journal of Applied Physics*, **112**, 052020.
- Kalnaus, S., Sabau, Tenhaeff, W.E., Dudney, N.J., and Daniel, C., 2012, "Design of Composite Polymer Electrolytes for Li-ion Batteries Based on Mechanical Stability Criteria," *Journal of Power Sources*, **201**, pp. 280-287.
- Kalnaus, S., Sabau, A.S., Newman, S., Tenhaeff, W.E., Daniel, C., and Dudney, N.J., 2011, "Effective Conductivity of Particulate Polymer Composite Electrolytes Using Random Resistor Network Method," *Solid State Ionics*, **199-200**, pp. 44-53.

- Guo, S., Jesse, S., Kalnaus, S., Balke, N., Daniel, C., and Kalinin, S.V., 2011, "Direct Mapping of ion Diffusion Times on $LiCoO_2$ Surfaces with Nanometer Resolution," *Journal of the Electrochemical Society*, **158**(8), pp. A982 – A990.

- Kalnaus, S., Rhodes, K., and Daniel, C., 2011, "A Study of Lithium ion Intercalation Induced Fracture of Silicon Particles Used as Anode Material in Li-ion Battery," *Journal of Power Sources*, **196**, pp. 8116-8124.

- Zhang, J., Kalnaus, S., Behrooz, M., and Jiang, Y., 2010, "Effect of Loading History on Stress Corrosion Cracking of 7075-T651 Aluminum Alloy in Saline Aqueous Environment," *Metallurgical and Materials Transactions A*, **42A**(2), pp. 448-460.

- Kalnaus, S., Zhang, J., and Jiang, Y., 2010, "Stress-Corrosion Cracking of AISI 4340 Steel in Aqueous Environments," *Metallurgical and Materials Transactions A*, **42A**(2), pp. 434-447.

- Kalnaus, S., Fan, F. Jiang, Y., and Vasudevan, A.K., 2009, "An Experimental Investigation of Fatigue Crack Growth of Stainless Steel 304L," *International Journal of Fatigue*, **31**, pp. 840-849.

- Fan, F., Kalnaus, S., and Jiang, Y., 2008, "Modeling of Fatigue Crack Growth of Stainless Steel 304L," *Mechanics of Materials*, **40**, pp.961-973

- Kalnaus, S., and Jiang, Y., 2008, "Fatigue of AL6XN Stainless Steel," ASME *Journal of Engineering Materials and Technology*, **130**(3), 031013 (12 pp.)

- Kalnaus, S., Fan, F., Vasudevan, A.K., and Jiang, Y., 2008, "An Experimental Investigation on Fatigue Crack Growth of AL6XN Stainless Steel," *Engineering Fracture Mechanics*, **75**(8) pp. 2002-2019.

- Kalnaus, S., Jiang, Y., 2006, "Fatigue Life Prediction of Copper Single Crystals Using a Critical Plane Approach," *Engineering Fracture Mechanics*, **73**(6), pp. 684-696.

- Serhovets, O.I., Fesenko, A.V., Ushakov, A.N., and Kalnaus, S., 2002, "Mathematical Modeling of Part Shaping Error in Automatic Cycle Grinding," *Bulletin of Kharkiv Technical Agricultural University*, **10** pp. 174-179. (In Ukrainian)

- Serhovets, O.I., Fesenko, A.V., Ushakov, A.N., and Kalnaus, S., 2001, "Dynamic Parameters Modeling for Infeed Grinding," *Bulletin of Engineering Academy of Ukraine*, **3**(1) pp. 404-406. (In Ukrainian)

- Kalnaus, S., and Lavinski, V.I., 2000, "Conjugation of Temperature and Deformation Fields During Wave Propagation in Thermo-Elastic Layer," *New Technologies in Manufacturing*, **1** pp. 122-128. (In Russian)

CONFERENCE PROCEEDINGS/PRESENTATIONS

- Kalnaus, S., Sabau, A., Tenhaeff, W., Daniel, C., Dudney, N., 2012, "Analysis of Composite Polymer Electrolytes for Li Battery Applications," Spring 2012 MRS Meeting, San Francisco, CA, USA.
- Kalnaus, S., Arruda, T., Balke, N., Bei, H., Daniel, C., Kalinin, S.V., Dudney, N., 2012, "Effect of Local Mechanical Damage on Li-ion Mobility," Spring 2012 MRS Meeting, San Francisco, CA, USA.
- Balke, N., Jesse, S., Kalnaus, S., Daniel, C., Dudney, N., Kalinin, S.V., "Nanoscale Probing of Anisotropic Ionic Transport," Spring 2012 MRS Meeting, San Francisco, CA, USA.
- Jesse, S., Balke, N., Dudney, N., Kalnaus, S., Daniel, C., Kalinin, S.V., "Local Probing of Activation Energy of Ionic Transport," Spring 2012 MRS Meeting, San Francisco, CA, USA.
- Tenhaeff, W., Herbert, E., Pharr, G., Kalnaus, S., Newman, S., Sabau, A., Daniel, C., Yu, X., Hong, K., Dudney. N.J., 2010 "Characterizing the Electrochemical and Mechanical Properties of Glass and Polymer Electrolytes and Predicting the Effective Conductivity of Their Composite Structures by Random Resistor Networks." Fall 2010 MRS Meeting, Boston, MA, USA.
- Kalnaus, S., Sabau, A., Tenhaeff, W., Newman, S., Dudney, N.J., Daniel. C., 2010 "Effective Conductivity and Percolation Threshold of Polymer Composite Electrolyte by Random Resistor Networks." Fall 2010 MRS Meeting, Boston, MA, USA.
- Kalnaus, S., Rhodes, K., Daniel, C., 2010 "Lithium ion Intercalation Induced Stress and Fracture of Active Electrode Material." Fall 2010 MRS Meeting, Boston, MA, USA.
- Tenhaeff, W., Herbert, E., Pharr, G., Yu, X., Hong, K., Kalnaus, S., Sabau, A., Perry, K., More, K., Deng, S., Mays, J., Dudney, N.J., 2010, "Electrochemical and Mechanical Characterization of Composite Nanostructures of Solid Glass and Polymer Electrolytes." Fall 2010 MRS Meeting, Boston, MA, USA.
- Kalnaus, S., Park, J., Han, S., Lee, Y.K., Less, G., Sastry, A.M., Dudney, N.J., Daniel C., 2010, "Investigation of Lithium Insertion/Extraction Induced Morphology Changes in Micro-Machined Specimens of Li ion Battery Cathode Material." Fall 2010 218th ECS Meeting, Las Vegas, NV, USA.
- Daniel, C., Rhodes, K., Kalnaus, S., 2010, "Probing Mechanical Degradation in Energy Storage Applications." International Workshop on SPM in Energy Application 2010, Oak Ridge, TN, USA.

- Rhodes, K., Kalnaus, S., Daniel, C., Dudney, N.J., Lara-Curzio, E., 2010, "In-situ Acoustic Emission Spectroscopy Combined with Stress Analysis." Energy Storage Beyond Lithium Ion: Computational Perspective, 2010, Argonne National Lab, USA.
- Daniel, C., Kalnaus, S., Dudney, N.J., 2010, "Intercalation Induced Mechanical Strain in Micro-Machined Li-ion Battery Electrodes." First European Energy Conference 2010, Barcelona, Spain
- Kalnaus, S., and Jiang, Y., 2009, "A Study of Fatigue Behavior of AISI 4340 VM," International Symposium PLASTICITY 2009, St Thomas, Virgin Islands, USA.
- Kalnaus, S., Fan, F., and Jiang, Y., 2007, "Fatigue and Cyclic Plasticity Properties of a Super-Austenitic Stainless Steel," *Proceedings of PVP 2007*, ASME Pressure Vessels and Piping Division Conference, 2007, San Antonio, TX, USA.
- Kalnaus, S., and Jiang, Y., 2006, "Fatigue Life Prediction of Copper Single Crystals Using a Critical Plane Approach," 9th International Fatigue Congress FATIGUE 2006, Atlanta, GA, USA.

PATENTS

Method and Apparatus for In-Situ Drying Investigation and Optimization of Slurry Drying Methodology. B.L. Armstrong, C. Daniel, J.Y. Howe, J.O. Kiggans, A.S. Sabau, S. Kalnaus, D.L. Wood III. US Patent Office Application Number: 13/656020. (2012)