Raj Kiran Koju

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Specialties: High performance computing, Computational physics, GB segregation and diffusion, Deformation, LAMMPS, Machine Learning, Data analysis and visualization, Time-series analysis.

Research experiences:

George Mason University, Advisor: Yuri Mishin

- Atomistic study of thermal stability of immiscible Cu-Ta alloys through shear-coupling and capillary driven grain boundary motion.

- Analyzed formation mechanisms of immiscible precipitates, phases, interface behavior and micro-structural evolution under intense heating.

- Investigation of creep mechanisms in a thermally stable nanocrystalline Cu-Ta alloys.

- Atomistic study of grain boundary segregation and diffusion across tilt and twist boundaries in Al-Mg alloy.

- Atomistic modeling of solute drag effect in Cu-Ag alloys.

- Atomic scale investigation of recrystallization and grain growth dynamics during severe plastic deformation of Al.

- Developed parallel MPI code for understanding texture orientation and grain evolution during deformation.

- Development of machine learning potential for Cu using neural network (NN) and physically-informed neural network (PINN) models.

- MD simulations using accelerated dynamics method.

Publications:

1. B.C. Hornbuckle, C. Kale, **R.K. Koju**, S. Srinivasan, K. Darling, Y. Mishin, K.N. Solanki "Stress-driven grain refinement in a microstructurally stable NC binary alloy", **in review, Scripta Materialia**

2. **R.K. Koju**, Y. Mishin "Atomistic study of grain-boundary segregation and grain-boundary diffusion in Al-Mg alloys", **in review, Acta Materialia, Manuscript ID: A-20-2575**

3. C. Kale, S. Srinivasan, B.C. Hornbuckle, **R.K. Koju**, K. Darling, Y. Mishin, K.N. Solanki "An experimental and modeling investigation of tensile creep resistance in a stable nanocrystalline alloy", Acta Materialia, **199**, 141-154 (2020).

4. **R.K. Koju**, Y. Mishin "Direct atomistic modeling of solute drag by moving grain boundaries", Acta Materialia, **198**, 111-120 (2020).

5. **R.K. Koju**, Y. Mishin: "Relationship between grain boundary segregation and grain boundary diffusion in Cu-Ag alloys", Physical Review Materials **4**, 073403 (2020) (**Selected as Editor's Suggestion**).

6. M. Rajagopalan, K. Darling, C. Kale, S. Turnage, **R.K. Koju**, B. Hornbuckle, Y. Mishin, K.N. Solanki "Nanotechnology enabled design of a structural material with extreme strength as well as thermal and electrical properties", Materials Today **31**, 10-20 (2019).

7. **R.K. Koju**, K.A. Darling, K.N. Solanki and Y. Mishin: "Atomistic modeling of capillary-driven grain boundary motion in Cu-Ta alloys", Acta Materialia **148**, 311-319 (2018).

8. M. Rajagopalan, K. Darling, S. Turnage, **R.K. Koju**, B. Hornbuckle, Y. Mishin, K.N. Solanki: "Microstructural evolution in a nanocrystalline Cu-Ta alloy: A combined in-situ TEM and atomistic study", Materials and Design **113**, 178-185 (2017).

9. **R.K. Koju**, K. A. Darling, L. J. Kecskes and Y. Mishin: "Zener pinning of grain boundaries and structural stability of immiscible alloys", JOM **68**, 1596-1604 (2016).

10. **R.K. Koju**, B. Aryal, S. R. Shahi: "Photometry of Betelgeuse from the National Observatory, Nagarkot, Nepal", Scientific World **10**, 7-12 (2012).

Presentations: Presentations marked with * is poster, † is contributed talk and ‡ is invited talk.

1. ‡ R.K. Koju, **Y. Mishin** "Interaction of moving grain boundaries with solutes in alloys", TMS 2020, San Diego, California.

2. ‡ **R.K. Koju** "Kinetic stabilization of nanocrystalline alloys studied by atomistic simulations", Naval Research Lab (NRL), 2019

3. * **R.K. Koju**, K.N. Solanki, K. A. Darling, Y. Mishin: "Deformation mechanisms of nanocrystalline Cu-Ta alloys", TMS 2019, San Antonio, Texas.

4. ‡ K. A. Darling, K.N. Solanki, R.K. Koju, **Y. Mishin**: "The Mechanisms of Thermal Stability and Strength of Nanocrystalline Immiscible Alloys", TMS 2018, Phoenix, Arizona.

5. * **R.K. Koju**, M. Rajagopalan, K. A. Darling, L. J. Kecskes, K. N. Solanki, Y. Mishin: "Interaction of grain boundaries with nano-clusters in immiscible Cu-Ta alloys", TMS 2017, San Diego, California.

6. ‡ R.K. Koju, K. A. Darling, L. J. Kecskes, **Y. Mishin**: "Zener pinning of grain boundary migration in immiscible nano-crystalline alloys", TMS 2016, Nashville, Tennessee.

7. † **R.K. Koju**, B. Aryal: "Dust structures around Pulsars at D < 1 kpc", International conference on Astrophysics and Cosmology 2012, Tribhuvan Univeristy, Kathmandu, Nepal.

Education:

Ph.D. in Physics   December 2019

George Mason University, Fairfax, VA

Thesis: "Atomistic Scale Investigation of Thermal Stability, Cluster Dynamics and Microstructural Evolution of Immiscible Cu-Ta Alloys"

Advisor: Yuri Mishin

Central Department of Physics, University Campus, Tribhuvan University

Thesis: "Study of visual flux emitted from the outer layer of red super giant Betelgeuse observed from national observatory, Nagarkot, Nepal"

Advisor: Binil Aryal

Scholarships:

- Presidential Scholarship, George Mason University (2012-2015)

- Scholarship for M.Sc. thesis, B.P. Koirala Memorial Planetarium Observatory and Science Museum Development Board, Ministry of Science & Technology, Government of Nepal (2010)

- Merit Scholarship, Kathmandu Institute of Science and Technology (KIST) (2002)

Workshops/Trainings:

1. LAMMPS Workshop and Symposium, University of New Mexico, Albuquerque, (August 13-15, 2019)

2. XSEDE Big Data Workshop, Office of Research Computing, George Mason University, Fairfax (December 4-5, 2018)

3. XSEDE GPU Programming Using OpenACC", Office of Research Computing, George Mason University, Fairfax (November 6, 2018)

4. Artificial Intelligence for Material Science, NIST, Gaithersburg (August 07-08, 2018)

5. Atomistic Simulations for Industrial Needs, National Cybersecurity Center of Excellence, Rockville (August 01-03, 2018)

6. XSEDE HPC Summer Hybrid Computing Workshop, Office of Research Computing, George Mason University, Fairfax (June 4-7, 2018)

7. XSEDE OpenMP workshop, Office of Research Computing, George Mason University, Fairfax (August 15, 2017)

Skills:
Parallel programming: OpenMP, MPI, OpenACC
Languages: C/C++, Python, Matlab, R, Bash shell, Awk
Operating Systems: Linux (openSUSE, Fedora, Ubuntu), MacOS
Softwares: LAMMPS, OVITO, Latex
Basic knowledge of Github, Java, HTML

References:

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