

Predicting atomic arrangements, structural and transport properties of multicomponent alloys

Dr. Ganesh Balasubramanian Lehigh University February 13, 2018 --- 4:10 p.m. --- WH 303

<u>Abstract</u>

Propulsion systems such as gas turbine engines require materials that are resistant to high temperature degradation by rapid oxidation, poor mechanical strength, microstructure and phase transformations. On one hand, conventional alloy strength decreases as temperature increases above 70% the absolute melting temperature; on the other hand, high temperature applications now require alloys beyond the traditional Fe, Ni, Co superalloys with superior mechanical strength in addition to good oxidation and corrosion resistance. Hence, the design and development of refractory metallic alloys that possess improved reactive, structural and transport properties for harsh environments are required to facilitate improved efficiency at lower operating costs. A possible solution is to consider refractory multi-principal element alloys (MPEAs) that are concentrated solid solutions containing several elements in comparable proportions. MPEAs composed of elements with high melting temperatures can be potentially engineered for high mechanical strength, and by inclusion of stable oxide forming elements can offer good oxidation resistance. We will present findings from first principle calculations and molecular simulations illustrating the effects of mixing multiple elements on the crystallographic structure of these alloys, as well as the resulting structural and transport properties that are strongly dependent on the material phase and composition. Finally, we will share a design strategy to computationally explore several elemental combinations in these alloys with a view to potentially tailoring the composition and structure to achieve desired material properties.

<u>Biography</u>

Ganesh Balasubramanian is an Assistant Professor of Mechanical Engineering & Mechanics at Lehigh University. Previously, he was an Assistant Professor of Mechanical Engineering and (by courtesy) of Materials Science and Engineering at Iowa State University. He received his BME degree in Mechanical Engineering from Jadavpur University (India) in 2007, his PhD in Engineering Mechanics from Virginia Tech in 2011, and was a postdoctoral research associate in Theoretical Physical Chemistry at TU Darmstadt (Germany) till fall of 2012. His research and teaching interests are in advanced energy and structural materials, nanoscale transport and mechanics, and multi-scale engineering. Some of his recognitions include the ASEE Outstanding New ME Educator award, AFRL Summer Faculty Fellowship, Miller Faculty Fellowship at Iowa State, the Graduate Man of the Year and Liviu Librescu Scholarship at Virginia Tech, and Young Engineering Fellowship from the Indian Institute of Science.

> Refreshments served at 3:45 p.m. outside Whitaker 303 Attendance is required of all full-time MSE Graduate Students. --- Seminars Open to Visitors ---