

Local Chemical Ordering in Complex Liquids

1. **Research Title:** Local Chemical Ordering in Complex Liquids
2. **Individual Sponsor:**

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3. **Academic Area/Field and Education Level**

Materials Science, Physics, Computer Science (MS, PhD level)

4. **Objectives:** Derive the local ordering in complex molten engineering alloys (e.g. Ni-based superalloys) in order to predict critical conditions for defect formation during advanced casting of single crystal airfoils.
5. **Description:** Nickel-base single crystals are critical to the operation of high performance turbine engines used in aerospace as well terrestrial applications. In recent years grain defect formation in turbine airfoils during directional solidification has become an increasingly important problem due to the higher levels of refractory alloying additions and the increasing size and complexity of single-crystal castings required for new aircraft engines. These (freckle) defects occur when convection instabilities form in the molten channels between primary dendrites in the solidification zone. Predictions for the critical processing parameters require density, viscosity as well as thermal conductivity. Modern electronic structure methods (Ab-initio Molecular Dynamics) have shown that molten alloy density is relatively insensitive to chemical ordering. However, predications for viscosity (and diffusion) require derivation of the chemical short range order. While this can be quite challenging hybrid Monte-Carlo / Molecular Dynamics approaches offer a viable pathway for extracting this information. With a proper representation of short range order AIMD methods can then be used to predict viscosity and other materials properties related to kinetics. This provides a way forward to more advanced predictions for freckle formation are for commercial as well as exploratory alloys.
6. **Research Classification/Restrictions:** This research topic is basic research and will be published in the open literature.
7. **Eligible Research Institutions:** Indicate to what organizations this topic should be provided



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