An Molecular Dynamics Investigation of the Shear Rate Dependency of the Thermophysical Properties for Molten Fe-C

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Metal-based additive manufacturing is highly dependent on a comprehensive understanding of the fluid dynamics and heat transfer characteristics present within the melt pool. A significant component of the fluid dynamics generated within the melt pool involves surface tension gradients induced by extreme temperature gradients caused by the incident laser heat source. The resulting Marangoni convection is a complex physical phenomenon that is governed primarily by the thermophysical properties of the melt pool's constituent compenents. Typical computational modeling approaches treat these thermophysical properties as either: a) constant, b) temperature-dependent, or c) a two-phase solution that accounts for characteristics caused by a "mushy zone". In this investigation, an additional characteristic of the thermophysical properties for a melt pool is now considered: a shear rate dependency. Using non-equilibrium molecular dynamics simulations, the shear viscosity, heat capacity, and density of molten Fe-C is investigated over a range of shear rates and temperatures. The results obtained from these molecular dynamics simulations are compared with previous results obtained by the presenter for pure molten Fe. Based on the results obtained, a map of thermophysical properties values is presented for use in future computational modeling investigations.