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Thermal Conductivity within Nanoparticle Powder Beds MARK WILSON, Computational Materials and Data Science, Sandia National Laboratories, Albuquerque, NM 87185, MICHAEL CHANDROSS, Materials Science and Engineering Center, Sandia National Laboratories, Albuquerque, NM 87185 — Non-equilibrium molecular dynamics is utilized to compute thermal transport properties within nanoparticle powder beds. In the realm of additive manufacturing of metals, the electronic contribution to thermal conduction is critical. To this end, our simulations incorporate the two temperature model, coupling a continuum representation of the electronic thermal contribution and the atomic phonon system. The direct method is used for conductivity determination, wherein thermal gradients between two different temperature heat flux reservoirs are calculated. The approach is demonstrated on several example cases including 304L stainless steel. The results from size distribution variations of mono/poly-disperse systems are extrapolated to predict values at the micron length scale, along with bulk properties at infinite system sizes. Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.

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