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Melting and stress response of metallic alloys using molecular dynamics[1] JUANA MORENO, Louisiana State University, SARAH BARTLEY, Agnes Scott College and Louisiana State University — Selective laser melting of powdered metals holds the promise of revolutionizing additive manufacturing. However, there are many unanswered questions about how the initial conditions of the melting and the composition of the powder determine the final alloy properties. In this study, we will run molecular dynamics simulations with an embedded-atom potential. Using different melting conditions for a range of compositions of NiAl alloys, we will explore the formation of different phases, grain structures, and segregation of impurities to interfaces and grain boundaries. We will identify the most promising structures and study their stress response to better understand the appearance of dislocations and the interaction between dislocations and interfaces in nanoscale metallic samples. We will apply uniaxial compression and nanoindentation to explore dislocation starvation and hardening and how the strength of the structure depends on diverse deformation process such as grain rotation, twinning, and stress-driven grain coarsening.

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