Nickel and iron based alloys are widely used as raw materials in 3D printing or additive manufacturing process. In direct metal laser sintering (DMLS) process, a primary 3D printing technique for metals, metallic powders are sintered to a desired shape by heat energy from a laser beam.

This study presents a molecular dynamics study to simulate the sintering process and resultant mechanical properties of 3D printed metal parts. The model will elucidate and quantify the diffusion process during 3D printing of nickel and iron powders. Further, to study the mechanical properties of the sintered nickel parts, uniaxial tensile test simulations will be performed on the parts sintered at different heating rates. The calculated diffusion activation energy for nickel is 7.91 KJ/mole in the nickel particle core region; and 8.55 KJ/mole on the surface area, respectively, which agrees well with the experimentally measured data from literature. Uniaxial tensile test simulation results show that a higher heating rate will increase the mechanical strength of sintered material.