

## Molecular Dynamic Simulation of Cold Spray Process

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**Abstract :** Cold Spray (CS) process is deposition of solid particles over a substrate above a certain critical impact velocity. Unlike thermal spray processes, CS process does not melt the particles thus retaining their original physical and chemical properties. These characteristics make CS process ideal for various engineering applications involving metals, polymers, ceramics and composites. The bonding mechanism involved in CS process is extremely complex considering the dynamic nature of the process. Though CS process offers great promise for several engineering applications, the realization of its full potential is limited by the lack of understanding of the complex mechanisms involved in this process and the effect of critical process parameters on the deposition efficiency. The goal of this research is to understand the complex nanoscale mechanisms involved in CS process. The study uses Molecular Dynamics (MD) simulation technique to understand the material deposition phenomenon during the CS process. Impact of a single crystalline copper nanoparticle on copper substrate is modelled under varying process conditions. The quantitative results of the impacts at different velocities, impact angle and size of the particles are evaluated using flattening ratio, von Mises stress distribution and local shear strain. The study finds that the flattening ratio and hence the quality of deposition was highest for an impact velocity of 700 m/s, particle size of 20 Å and an impact angle of 90°. The stress and strain analysis revealed regions of shear instabilities in the periphery of impact and also revealed plastic deformation of the particles after the impact. The results of this study can be used to augment our existing knowledge in the field of CS processes.

**Keywords :** cold spray process, molecular dynamics simulation, nanoparticles, particle impact

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