**Proceedings of the Canadian Society for Mechanical Engineering International Congress 2021**
**CSME Congress 2021**
**June 27-30, 2021, Charlottetown, PE, Canada**

# Influence of forcefield selection on the formation of viable nanocrystalline copper structures using the Melt Cool method

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ABSTRACT

The influence of forcefield selection on the development of a viable nanocrystalline structure using Molecular Dynamics (MD) is of utmost importance as researchers identify enhanced methods for creating realistic microstructures. One such method for creating nanocrystalline structures which possess realistic microstructures with randomized defects is the Melt Cool method. The simulation process involves annealing the starting single crystal structure to temperatures which exceed the melting point of the metal, followed by a rapid quench and equilibration to room temperature which allows for the formation of nanocrystalline grains. However, the influence forcefields have on the formation of viable structures is not discussed in currently available studies found in literature. Many studies fail to demonstrate the effect various forcefield fitting parameters have on the formation of viable structures using the Melt Cool method. Therefore, there is a deficiency of valuable information available for researchers working in the forcefield development. Moreover, a disservice is not only given to forcefield development, but also future research on more complicated nanocrystalline materials. As such, the current investigation was performed to highlight the influence forcefield selection has on the formation of viable nanocrystalline structures of pure copper. It was shown that the forcefield has a direct impact on the formation of said structures and it is of utmost importance to provide valuable data for the development of future forcefields.

Word count: 222