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Influence of isotropy on mechanical properties of nanocrystalline iron

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ABSTRACT

The influence of isotropy on the prediction of mechanical properties for nanocrystalline metals using Molecular Dynamics (MD) is highly ignored in currently available studies found in literature. Many of these studies grossly ignore the isotropic nature of macroscopic metals when attempting to simulate a bulk nanocrystalline material. Moreover, said studies provide no substantial justification for the selection of the number of grains utilized. This is of utmost importance since there may not be a statistically significant number of grains to provide aggregate properties of a simulated bulk material due to the anisotropic nature of many metallic single crystals. As such, these studies unknowingly influence the prediction of mechanical properties such as elastic modulus, Poisson's ratio, and maximum stress. Therefore, the current investigation was performed to obtain reliable mechanical properties of nanocrystalline pure iron of a simulated bulk material through the use of MD. The current investigation provides a thorough guideline for obtaining an isotropic structure prior to obtaining mechanical properties while simultaneously highlighting the inaccuracies of currently available investigations found in literature.

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