# Plastic deformation mechanism in gradient nanoscale grained iron via atomistic model coupled with crystal plasticity finite element simulations

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**Abstract:** Gradient nanocrystalline with enhancing strength-ductility synergy would been used in applications of advanced coatings of bulk material. Accurate characterization of mechanical properties of gradient nanocrystalline plays key role in widespread use of gradient nanocrystalline. In this study, the plastic deformation of gradient nanocrystalline iron under uniaxial tension is investigated via molecular dynamics and crystal plasticity finite element analysis, and compared with the relevant experimental results. The result from molecular dynamics simulation shows that the partial dislocation is dominated the plastic deformation of small grains; and the full dislocation, deformation twinning and grain boundary migration control that of large grains. Result from crystal plasticity finite element shows that the gradient stress and plastic strain in gradient nanocrystalline iron are found. The gradient strain plasticity is usually caused by a non-uniform deformation, such as twisting, bending and indention. Gradient microstructure induces gradient plastic strain, resulting in strengthening iron. Based on the above results, it reveals that the grain boundary migration, dislocation emission, deformation twinning govern the deformation of gradient nanocrystalline, and the reasonable distribution of grain size and position could effectively improve the strengthening and hardening of gradient nanocrystalline.

**Keywords:** Gradient nanocrystalline; Plastic deformation mechanism; Molecular dynamics; Crystal plasticity finite element;