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Mechanical behavior of Ni and Ni_3Al free-standing and matrix-embedded nanoparticles at different temperatures

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Nano-composite materials represent a tremendous opportunity for improving mechanical properties and/or multi-physics coupling. Nevertheless, the understanding of their deformation mechanisms is still limited, especially at lower scales. Few studies have already investigated the mechanical behavior of free-standing nanoparticles at room temperature (see [1-3] for instance).

In the present work, we investigate both free-standing and matrix-embedded nanoparticle behavior thanks to molecular dynamics simulations. Uniaxial compressions are performed on 20nm-sized nanoparticles after relaxation and thermalization. The impact of the force field model is first studied in order to discuss the modelling representativeness of mechanical testing in molecular dynamics.

The Ni_3Al nanoparticle mechanical behavior is then investigated through a large spectrum of temperatures. The plastic deformation mechanisms are analyzed in details both for free-standing and Ni matrix-embedded nanoparticles. The effect of nanoparticle shape, crystallographic orientation or temperature on plasticity mechanisms and yield stress are discussed.

References:

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