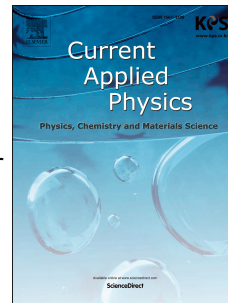


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Structural Properties of β -Fe₂O₃ Nanorods Under Compression and Torsion: Molecular Dynamics Simulations

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Abstract

In recent years, one-dimensional (1D) magnetic nanostructures, such as magnetic nanorods and chains of magnetic nanoparticles have received great attentions due to the breadth of applications. Especially, magnetic nanorods has been opened an area of active research and applications in medicine, sensors, optofluidics, magnetic swimming, and microrheology since they possess the unique magnetic and geometric features. This study focuses on the molecular dynamisc (MD) simulations of an infinitely long crystal β -Fe₂O₃ nanorod. To elucidate the structural properties and dynamics behavior of β -Fe₂O₃ nanorods, MD simulation is a powerful technique. The structural properties such as equation of state and radial distribution function of bulk β -Fe₂O₃ are performed by lattice dynamics (LD) simulations. In this work, we consider three main mechanisms affecting on deformation characteristics of a β -Fe₂O₃ nanorod: 1) temperature, 2) the rate of mechanical compression, and 3) the rate of mechanical torsion.

Keywords: β -Fe₂O₃, Nanorod, Molecular Dynamics, Compression, Torsion.

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