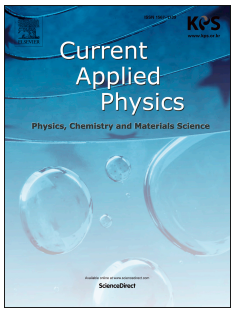
Accepted Manuscript



Structural properties of β-Fe_2O_3 nanorods under compression and torsion: Molecular dynamics simulations

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PII: S1567-1739(18)30216-5

DOI: 10.1016/j.cap.2018.07.019

Reference: CAP 4801

To appear in: *Current Applied Physics*

Received Date: 28 March 2018

Revised Date: 30 June 2018

Accepted Date: 25 July 2018

Please cite this article as: M.E. Kilic, S. Alaei, Structural properties of β-Fe_2O_3 nanorods under compression and torsion: Molecular dynamics simulations, *Current Applied Physics* (2018), doi: 10.1016/j.cap.2018.07.019.

Structural Properties of $\beta-Fe_2O_3$ 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 $\beta-Fe_2O_3$ nanorod. To elucidate the structural properties and dynamics behavior of $\beta-Fe_2O_3$ nanorods, MD simulation is a powerful technique. The structural properties such as equation of state and radial distribution function of bulk $\beta-Fe_2O_3$ are performed by lattice dynamics (LD) simulations. In this work, we consider three main mechanisms affecting on deformation characteristics of a $\beta-Fe_2O_3$ nanorod: 1) temperature, 2) the rate of mechanical compression, and 3) the rate of mechanical torsion.

Keywords: $\beta-Fe_2O_3$, Nanorod, Molecular Dynamics, Compression, Torsion.

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