Structural Properties of Copper Nanorods under Strain: Molecular Dynamics Simulations

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Abstract

Structural properties of copper nanorods generated from low-index surfaces (100), (110), (111) under uniaxial strain have been investigated. Classical molecular dynamics simulations at various temperatures have been performed using an atomistic potential. It has been found that uniaxial strain shows cross section geometry dependent characteristics. The nanorods generated from (100) and (110) surfaces are relatively stronger against uniaxial strain than the nanorods generated from (111) surface.

Introduction

Copper nanorods and nanowires applications generally involve their magnetic and high conductive properties [1]. The excellent electrical conductivity and low cost of copper makes it ideal for applications in magnetic recording media, medical sensors and contrast enhancement agent for MRI [2]. A novel and interesting usage is the making of transparent-conductive films which can be used in flat panel displays, touchscreens and solar cells [3]. With their low cost compared to the currently used Indium Tin Oxide (ITO) and their flexibility, copper nanorods can greatly change the development of flexible displays, light emitting diodes and thin film solar cells.

Uniform arrays of copper 1D structures can be produced using simple liquid-solid reactions. Methods for obtaining different axial grown nanorods are present [4,5].

Methods of Calculation

In these atomistic level computer simulations the Erkoc empirical model potential was used [6]. The potential energy function (PEF) is formed from pair interactions, which contains many-body effects. The total energy of the system is expressed as the linear combination of two two-body functions [7]:

$$\mathbf{\Phi} = D_{21}\phi_{21} + D_{22}\phi_{22}$$

where ϕ_{21} and ϕ_{22} are the two-body energies

$$\phi_{2k} = \sum_{i<j} U_{ij}^{(2k)} \quad , \ \mathrm{k=1,2}$$

The two body interactions are defined as:

$$U_{ij}^{(2k)} = A_k r_{ij}^{-\lambda_k} e^{-\alpha_k r 2_{ij}} \quad , \ \mathrm{k=1,2}$$

Two sets of parameters are used (repulsive, attractive). The molecular dynamics time step is 0.9×10^{-15}. The velocities and positions of the particles are calculated using the velocity summed form of Verlet algorithm.

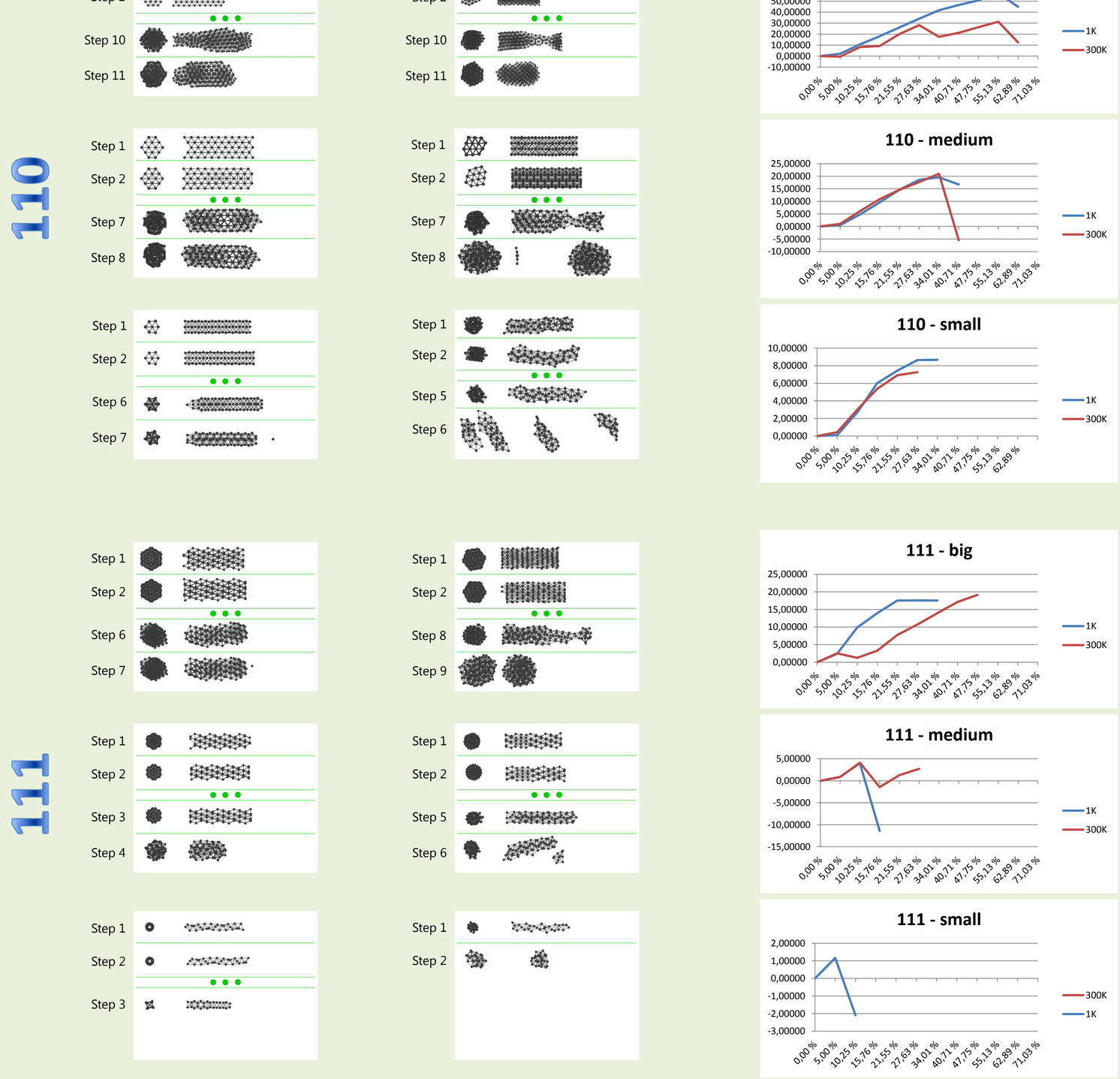
The simulations for the nanorods are repeated at the temperatures 1K and 300K for all the rods. A minimum of 100.000 steps are repeated as a minimum for the systems to reach equilibrium.

Periodic boundaries are used in the related cross section direction. After each relaxation, the system is elongated by 5% and MD steps are repeated for the system to reach equilibrium again.

Conclusions

It has been shown that uni-axial strain shows cross-section geometry dependent characteristics. The nanorods generated from (100) and (110) surfaces are relatively stronger against uniaxial strain with respect to the nanorods generated from (111) surfaces. These results could help future researches for copper nanorods applications for their mechanical strength properties.

Results



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