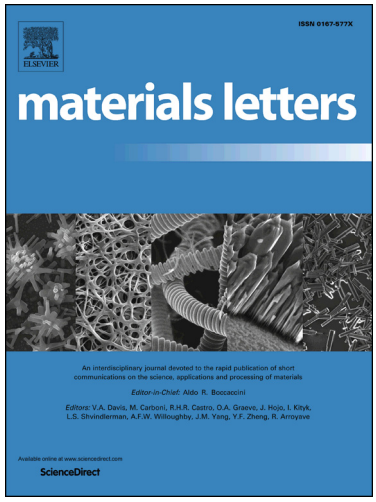

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PII: S0167-577X(18)30849-8
DOI: https://doi.org/10.1016/j.matlet.2018.05.094
Reference: MLBLUE 24394

To appear in: *Materials Letters*

Received Date: 15 April 2018
Revised Date: 18 May 2018
Accepted Date: 21 May 2018

Please cite this article as: L. Zhang, C. Lu, A.K. Tieu, Nonlinear elastic response of single crystal Cu under uniaxial loading by molecular dynamics study, *Materials Letters* (2018), doi: https://doi.org/10.1016/j.matlet.2018.05.094

Nonlinear elastic response of single crystal Cu under uniaxial loading by molecular dynamics study

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Abstract: Molecular dynamics simulations were carried out to study the mechanical response of single crystal Cu with various orientations under uniaxial loading. Cu shows a high degree of elastic anisotropy as a function of the crystal orientations, and the yield stress varies significantly with the crystal orientations and the loading directions. An obvious nonlinear stress-strain response was observed at the elastic deformation stage under applied loading, namely elastic hardening and elastic softening. This nonlinear elastic behavior is derived from the potential energy between atoms and can play a significant role in yield stress and yield asymmetry of crystals under tension and compression.

Keywords: Molecular dynamics; Elastic properties; Nonlinear response; Yield asymmetry

1. Introduction

Compression/tension (C/T) asymmetry in strength is an important phenomenon of materials when the grain sizes are reduced. The C/T asymmetry has been widely reported in the previous experiments in the ultrafine and nanocrystalline metals and alloys [1-7]. Atomistic simulations predict a similar asymmetry in the strength of metals when the grain sizes are down to nanometer scale [8-16]. For example, Tschopp et al. [9, 10] performed molecular dynamics (MD) simulations to investigate the C/T asymmetry property in single crystal Cu with different orientations. It was found that the yield strength shows a higher value in compression than in tension in almost all the studied cases. By using polycrystal samples, Lund et al. [11, 12] investigated nanocrystalline Ni with grain size near the amorphous limit (2~4 nm), the C/T strength difference was found to be in the order of 30%. Dongare et al. [15] studied the macroscopic deformation behavior of nanocrystalline Cu with a grain size of 6 nm, and they reported a similar stress asymmetry of the simulation samples. The above experimental and computational-based studies have revealed a ubiquitous higher compressive