

Author's Accepted Manuscript

Molecular dynamics simulation for orientation dependence of deformations in monocrystalline AlN during nanoindentation

Henggao Xiang, Haitao Li, Jingjing Chen, Sha Sun, Qibin Li, Bo Yang, Xianghe Peng



www.elsevier.com/locate/ceri

PII: S0272-8842(18)30603-5
DOI: <https://doi.org/10.1016/j.ceramint.2018.03.051>
Reference: CER117688

To appear in: *Ceramics International*

Received date: 24 January 2018
Revised date: 7 March 2018
Accepted date: 7 March 2018

Cite this article as: Henggao Xiang, Haitao Li, Jingjing Chen, Sha Sun, Qibin Li, Bo Yang and Xianghe Peng, Molecular dynamics simulation for orientation dependence of deformations in monocrystalline AlN during nanoindentation, *Ceramics International*, <https://doi.org/10.1016/j.ceramint.2018.03.051>

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting galley proof before it is published in its final citable form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Molecular dynamics simulation for orientation dependence of deformations in monocrystalline AlN during nanoindentation

Henggao Xiang^a, Haitao Li^{a,b*}, Jingjing Chen^c, Sha Sun^a, Qibin Li^a, Bo Yang^a, Xianghe Peng^{a,b*}

^aCollege of Aerospace Engineering, Chongqing University, Chongqing 400044, China

^bChongqing Key Laboratory of Heterogeneous Material Mechanics, Chongqing University, Chongqing, 400044, China

^cSchool of Information and Electrical Engineering, Ningde Normal University, Fujian Ningde 352100, China

htli@cqu.edu.cn

xhpeng@cqu.edu.cn

*Corresponding authors. College of Aerospace Engineering, Chongqing University, Chongqing 400044, China. Tel.: +86 2365103755; fax: +86 2365102521.

Abstract

Molecular dynamics simulations were performed for the nanoindentations using a virtual cylindrical indenter on monocrystalline aluminum nitride (AlN) with the indentation surface orientations of $[0001]$, $[10\bar{1}0]$, $[\bar{1}2\bar{1}0]$ and $[\bar{1}01\bar{2}]$, respectively, to investigate the orientation dependence of the material. Vashishta potential was used to model the interactions between Al-Al, N-N, and Al-N atoms in the specimens. Simulation results indicated that the deformation mechanism varies with surface orientations at the initial inelastic stage. In the specimens with the surface orientations

Download English Version:

<https://daneshyari.com/en/article/7887122>

Download Persian Version:

<https://daneshyari.com/article/7887122>

[Daneshyari.com](https://daneshyari.com)