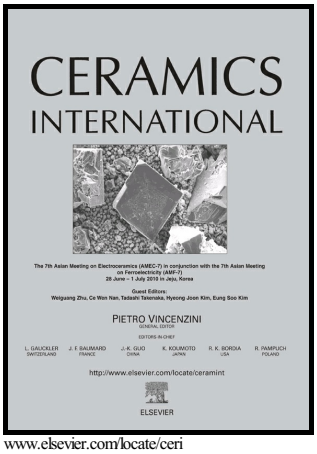
# Molecular dynamics simulation for orientation dependence of deformations in monocrystalline AlN during nanoindentation

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: CERI17688

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

# 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*]

[a]*College of Aerospace Engineering, Chongqing University, Chongqing 400044, China*

[b]*Chongqing Key Laboratory of Heterogeneous Material Mechanics, Chongqing University, Chongqing, 400044, China*

[c]*School 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