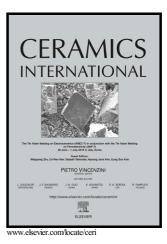
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Molecular dynamics simulation for orientation dependence of deformations in monocrystalline AlN during nanoindentation

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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], $[10\overline{10}]$, $[\overline{12}\overline{10}]$ and $[\overline{1012}]$, 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

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