

Molecular Dynamics Study on the Effects of Surface Notches on Plastic Deformation Behavior of Magnesium Nanopillars

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Abstract: In this study, molecular dynamics simulations were performed to study the uniaxial compression deformation of magnesium nanopillars with square and triangular surface notches. The generation and evolution process of internal defects of magnesium nanopillars was analyzed in detail. The results indicated that the triangular notches had little effect on the deformation behavior of magnesium nanopillars, and the governing mechanism of plastic deformation was the initiation and motion of pyramidal dislocations. As for magnesium nanopillars with square notches, the initial plastic deformation was mainly caused by the pyramidal slip. After the notches were closed, $\{10\bar{1}1\} \langle 10\bar{1}2 \rangle$ twins were observed, the expansion of twins and the interaction between twins and dislocations had an important influence on the plastic deformation behavior.

Keywords: Molecular dynamics; magnesium; surface notches; plastic deformation