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<AT>Orientation and strain rate dependent tensile behavior of single crystal titanium nanowires by molecular dynamics simulations

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Molecular dynamics simulation was employed to study the tensile behavior of single crystal titanium nanowires (NWs) with $[11\bar{2}0]$, $[\bar{1}100]$ and [0001] orientations at different strain rates from $10^8$ $s^{-1}$ to $10^{11}$ $s^{-1}$. When strain rates are above $10^{10}$ $s^{-1}$, the state transformation from HCP structure to amorphous state leads to super plasticity of Ti NWs, which is similar to FCC NWs. When strain rates are below $10^{10}$ $s^{-1}$, deformation mechanisms of Ti NWs show strong dependence on orientation. For $[11\bar{2}0]$ orientated NW, $\{10\bar{1}1\}$ compression twins (CTs) and the frequently activated transformation between CTs and deformation faults lead to higher plasticity than the other two orientated NWs. Besides, tensile deformation process along $[11\bar{2}0]$ orientation is insensitive to strain rate. For $[\bar{1}100]$ orientated NW, prismatic <*a*> slip is the main deformation mode at $10^8$ $s^{-1}$. With strain rate increases, more types of dislocations are activated during plastic deformation process. For [0001] orientated NW, $\{10\bar{1}2\}$ extension twinning is the main deformation mechanism, inducing the yield stress of [0001] orientated NW, which has the highest strain rate sensitivity. The number of initial nucleated twins increases while the saturation twin volume fraction decreases nonlinearly with strain rate increases.

<KWD>Keywords: Molecular dynamics; Single crystal titanium nanowires; Strain rate; Orientation; Plastic deformation mechanisms

## <H1>1. Introduction

Metallic nanowires (NWs) have attracted much attention because of their magic structures, conductance, and large potential in the applications of nano/micro electro-mechanical systems [1-5]. The high surface area to volume ratio and low defect density endue the nanostructures with unique mechanical properties, which are different from its bulk materials [6,7]. The surface effects have great influence on the mechanical properties at the nanoscale because the surface atoms have a coordination number deficiency. Therefore, it is extremely important to know the deformation behavior of metallic NWs before applications. The mechanical behavior and properties of NWs are not well established due to the complexities of mechanical testing at the nanoscale level. In recent years, molecular dynamics (MD) simulations have been employed as an important tool to investigate the mechanical properties and deformation mechanisms of NWs. Current literatures are mainly focused on mechanical properties of face-centered cubic (FCC) and body-centered cubic structure (BCC) typed metal NWs, such as Cu [8-10], Ag [11-14], Ni [15,16], Pt [17,18], W