



Full length article

# Competing mechanisms between dislocation and phase transformation in plastic deformation of single crystalline yttria-stabilized tetragonal zirconia nanopillars



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## ABSTRACT

Molecular dynamics (MD) is employed to investigate the plastic deformation mechanisms of single crystalline yttria-stabilized tetragonal zirconia (YSTZ) nanopillars under uniaxial compression. Simulation results show that the nanoscale plastic deformation of YSTZ is strongly dependent on the crystallographic orientation of zirconia nanopillars. For the first time, the experimentally explored tetragonal to monoclinic phase transformation is reproduced by MD simulations in some particular loading directions. Three distinct mechanisms of dislocation, phase transformation, and a combination of dislocation and phase transformation are identified when applying compressive loading along different directions. The strength of zirconia nanopillars exhibits a sensitive behavior depending on the failure mechanisms, such that the dislocation-mediated deformation leads to the lowest strength, while the phase transformation-dominated deformation results in the highest strength.

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## 1. Introduction

Zirconia ( $ZrO_2$ ) has three polymorphs, i.e., monoclinic ( $m$ ), tetragonal ( $t$ ) and cubic ( $c$ ) phases. At room temperature, only the low symmetry monoclinic phase is thermodynamically stable, and around 1480 K, the first-order martensitic transition to the tetragonal phase would be triggered, and further converted to the higher symmetry cubic fluorite phase at 2573 K [1]. Prior to 1970s, pure monoclinic zirconia was of very limited interest due to the crumbling (e.g. fracture, crack) of the ceramic components commonly observed during cooling from the tetragonal phase, which is accompanied by a volume expansion of ~4% [2]. In contrast, the high-temperature phases of zirconia, i.e., tetragonal and cubic, have excellent mechanical, thermal, chemical and dielectric properties including high-strength, low thermal conductivity, high corrosion resistant, and high ionic conductivity, which lead zirconia to a wide range of industrial, technological and medical applications. Currently zirconia is employed as, for example, catalytic support medium [3], electrolyte in solid oxide fuel cells at low temperature [4,5], thermal barrier coating [6], nuclear waste confinement [7], one of the leading candidates for

alternative gate dielectrics [8], and in shape memory [9,10] and dental applications [11].

In general, the stabilization of high symmetry polymorphous of zirconia, i.e.,  $t$ - and  $c$ - $ZrO_2$ , at room temperature can be achieved by doping a variety of oxide additions [12], one of which is yttria ( $Y_2O_3$ ), or by reducing the grain size to nanometer scale [13,14]. The  $t$ - $ZrO_2$  grains have been observed to be size-stabilized below 200 nm [15], while  $c$ - $ZrO_2$  was stated to be stable at a few nanometers scale [16].

The discovery, that the martensitic tetragonal-to-monoclinic ( $t \rightarrow m$ ) transformation in zirconia can be controlled to serve as the source of transformation plasticity, heralded new visions for the high-performance applications of zirconia [2]. Transformation toughening of zirconia was first reported by Garvie, Hannink and Pascoe in 1975 [17]. Yttria-stabilized tetragonal zirconia (YSTZ) presents a stress-induced phase transformation of tetragonal to stable monoclinic form, which is accompanied by a volumetric expansion to close crack tips and superimposes compressive stresses on the existing stress field, hence, makes the material more resistant to crack propagation [17]. During the past decades, considerable efforts have been devoted to study  $t \rightarrow m$  phase transformation behavior of stabilized zirconia. This transition not only is of intrinsic interest, but is also important because it has been suggested that the reverse transition, i.e., from the monoclinic to

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tetragonal phase, should be related to the recognition of the potential shape memory and superelastic ceramics [9,10].

Theoretically, transformation-induced plasticity and transformation toughening require a reliable determination of the strain field in the stress-activated transformation zone [2], and this, in turn, requires a detailed understanding of transformation crystallography. Thus, several phenomenological theories have been developed based on the crystallographic characteristics. For example, the crystallographic theory [18], which describes the structural change by a homogeneous lattice deformation, was applied to calculate the strains associated with formation of individual units of monoclinic product in a tetragonal matrix. In addition, a generalized theory of martensite crystallography [19,20] was employed to provide the quantitative data that is essential for developing a credible, comprehensive understanding of the transformation toughening process.

Experimentally, the  $t \rightarrow m$  phase transformation has been studied mainly by optical methods or transmission electron microscopy (TEM) [21]. Both the positive (transformation toughening) and negative consequences (low temperature degradation, microcracking) of this transformation have been investigated. By annealing in water, the polycrystalline yttria-doped tetragonal  $\text{ZrO}_2$  on the surface of the sintered body was observed to transform to the monoclinic phase, accompanied by microcracking [22]. In addition, using Raman spectroscopy, atomic force microscopy (AFM) and optical microscopy, catastrophic cracks were detected during phase transformation in zirconia films due to the change of circumferential stress. In turns, such cracks were found to lead to breakaway oxidation of zircaloy [23]. The phase composition and structure of zirconia single crystal doped with  $\text{Y}_2\text{O}_3$  was studied by X-ray diffraction analysis and TEM, in which twinning hierarchy was observed to facilitate the elastic stress relaxation [1]. On the other hand, under high-pressure torsion a  $t \rightarrow m$  phase transformation with a coherent interface occurred. Once the monoclinic phase reached the saturation level, nanograins of high dislocation density but with no twins were formed [24]. With a small amount of  $\text{Al}_2\text{O}_3$  doped in 3.0 mol%  $\text{Y}_2\text{O}_3$ -stabilized tetragonal zirconia polycrystal, the cubic phase regions were formed and the grain-growth rate was enhanced by the diffusion-enhanced effect of  $\text{Al}_2\text{O}_3$ -doping [25]. It is now generally recognized that the size of grains has a strong effect on the transformation toughening. Alternatively, fracture toughness of nanocrystalline zirconia was measured by nano-indentation methods, and it was found that the larger the tetragonal grains the greater propensity to undergo martensitic transformation into stable monoclinic structure, consequently enhance the toughness of material [26]. Recently, to overcome the shortcomings of bulk zirconia ceramics that tend to crack when undergo martensitic transition, a fine-scale structure with few crystal grains was fabricated. Such oligo crystalline structures were found to be capable of superelastic cycles and robust shape memory by virtue of reduction of internal mismatch stress during phase transition [9,10,27].

Recently, computer simulations have become uniquely powerful tools for addressing issues of phase transition at atomistic and micro scales. Indeed, important insights have already come from simulations; for example, first-principle [28] and *Ab initio* calculations [29] have been performed to look into the structural and electronic properties of pure zirconium and yttria-stabilized cubic zirconia. More recently, elastic phase field models were proposed [30,31] with an attempt to study the effect of external stress on martensitic phase transformation and transformation toughening. Such model was demonstrated to be capable of predicting the transformation zone and stress field around crack tips [32], as well as the pseudoelasticity behavior exhibits in shape memory application [33]. Despite the tremendous capabilities of phase field

modeling in predicting microstructure evolutions at the mesoscale [34], it does not explicitly deal with the behavior of the individual atoms, which is essentially important for an in-depth understanding of the physics of phase transformation in zirconia. Moreover, hybrid Monte Carlo-molecular dynamics simulations [35] were carried out to study defect distributions near tilt grain boundaries in nanocrystalline YSTZ. Very recently, a new approach that adapted the first-principle model has been reported to analysis the superplastic behavior of fine-grained YSTZ polycrystal [36]. With the advantages of offering tight control on composition and microstructure, as well providing valuable atomistic information of structure evolutions, molecular dynamics (MD) technique has been widely used as a powerful computational tool for studying the mechanisms of plastic deformation [37–39] and stabilization [40], thermal transport [41–44], diffusion of oxygen ions [45–48], and cubic-to-tetragonal phase transition [49] of zirconia. However, MD simulations of YSTZ are by now mainly concentrated on polycrystalline structure and the cubic polymorph of zirconia. To understand how the texture affects the mechanical properties, one should first examine mechanical properties of single crystals and interpret the deformation processes involved. However, the fundamental understanding of  $t \rightarrow m$  transformation behavior at atomic level is less investigated up to this time, and to the best of our knowledge and despite its significance,  $t \rightarrow m$  phase transition in single crystalline YSTZ has not been investigated so far.

In addition to  $t \rightarrow m$  martensitic phase transformation, other microstructural features, such as dislocation, can also play a pivotal role in determining the mechanical properties of material. Dislocation migration, as one of the dominated deformation mechanisms of cubic zirconia, has been extensively studied. And dislocations were found to preferentially occur on cube planes, such as {100}, {110} and {111} planes [50]. For tetragonal zirconia, a ferroelastic behavior preceding dislocation plasticity [50] was reported experimentally. Under tension loading, a tetragonal single crystal forms containing residual defects. Although the dislocation pile-ups activity at the interface between grains in nanocrystalline cubic zirconia [51,52] are receiving much attention, there are relatively fewer studies on dislocation behavior of single crystalline tetragonal zirconia, especially under compressive loading.

For size-limited single crystals, as one traverses to the nanometer scale, phase transition and dislocation nucleation behavior becomes ultra-difficult to capture for the present *in situ* nanoscale tomography compared to the bulk parent material. In addition, the accurate orientation control of material, which is particularly important for anisotropic crystals, arises another challenging issue for experiments. For example, in a very recently work by Zeng et al. [53], a study on martensite mechanics was conducted by using micro-scale YSTZ specimens; the results indicated that the stress-induced martensitic transformation in zirconia-based shape memory ceramics depends on the orientation of tetragonal crystals. However, the detailed evolution of phase transformation and dislocation motion during plastic deformation is very hard to capture by the current experimental techniques. Apparently, a lack of ground understanding of the atomistic deformation mechanisms in materials severely limits our ability to design nanomaterials with desired mechanical properties. Therefore, atomistic computer simulation, which has been demonstrated to be successful in modeling phase transition and dislocation behavior regarding orientation effect under compression [37,39], is ideally suited to provide valuable atomistic information of zirconia.

In this study, MD simulation is applied to the single crystalline yttria-stabilized tetragonal zirconia (YSTZ) nanopillars to investigate the behavior of  $t \rightarrow m$  phase transformation and dislocation migration under uniaxial compression. The aim of the study is to systematically explore the atomistic deformation mechanisms of

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