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Peridynamic simulations of the tetragonal to monoclinic phase transformation in zirconium dioxide

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ABSTRACT

Whether present as a manufactured stabilised ceramic, or as an oxide layer on zirconium alloys, mechanical degradation in zirconia is influenced by the tetragonal to monoclinic phase transformation. Peridynamic theory was implemented within the Abaqus finite element framework to understand how the tetragonal to monoclinic phase transformation can itself cause fracture in zirconia. In 2D these simulations represent a single grain, transforming via an isometric dilational expansion, surrounded by a homogenous monoclinic oxide. The effect of transformation time, applied bi-axial pressure, and the fracture strain were assessed using the change in strain energy and the amount of damage in the oxide surrounding the transformed grain. Reducing the applied compressive stress or applying a tensile stress reduces the transformation strain energy. The introduction of a fracture strain leads to damage in the surrounding oxide region largely in the form of cracks, and reduces the transformation strain energy further by reducing the constraint on the transforming grain. The extent of the fracture, and reduction in constraint on the transformed grain, is more significant with the application of a biaxial tensile pressure.

1. Introduction

Whether used as an engineering ceramic, or present as an oxide layer grown thermally on zirconium alloys, zirconium dioxide demonstrates distinctive behaviours that centre on the tetragonal to monoclinic phase transformation. In either system the mechanisms for room temperature stabilisation, and potentially destabilisation, are the same. The addition of doping elements to manufactured zirconia has been shown to stabilise the tetragonal phase at room temperature [16,66]. A number of these elements are present as alloying elements in commercial zirconium alloys [3–4,28,34,40]. Recent work using X-ray absorption near edge spectroscopy XANES) [32], and density functional theory DFT) [6], has indicated that solid solution tin incorporated into the oxide layer should be present in both Sn^{2+} and Sn^{4+} oxidation states. The reduction of tin in zirconium-niobium alloys has been shown to produce oxide layers with a lower tetragonal phase fraction [22,67]. A proposed theory behind this mechanism is that introducing a doping element with a lower valence state than Zr^{4+} may stabilise the presence of oxygen vacancies, which in turn distort the lattice and make the tetragonal phase more energetically favourable [21,29,31,60]. As zirconium alloys oxidise entirely due to the inward migration of oxygen ions [13], there should be an increasing concentration of oxygen vacancies approaching the metal-oxide interface from the oxide surface [14,45,70]. This could be a contributing factor to the increased tetragonal phase fraction close to the metal-oxide interface [50].

The tetragonal phase of zirconia has been proven to be stabilised by the application of compressive hydrostatic pressure [25]. Zirconia thin films can experience residual biaxial compressive stresses of the order of MPa to GPa, whether the material is applied as a coating [59,65], or formed during thermal oxidation [2,33,50,51,56,57,71]. It is possible to destabilise the tetragonal phase by applying a tensile hydrostatic stress e.g. ahead of an advancing crack tip [12]. In engineering ceramics this mechanism is referred to as transformation toughening because of the resulting retardation of crack growth by the tetragonal to monoclinic phase change and its associated increase in volume [10,20,35]. Oxides formed on zirconium alloys in autoclave and reactor undergo a transition and acceleration in the corrosion kinetics that has previously been linked with the formation of a network of lateral cracks close to the metal-oxide interface [9,56,69].

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Exposure of manufactured zirconia to moist environments up to ~400 °C has been shown to cause the tetragonal phase to transform to monoclinic, this phenomenon is referred to as low temperature, or hydrothermal, degradation [12,18,29,60]. These conditions are very similar to those experienced by oxidising zirconium alloys in nuclear reactors or autoclaves, and these oxide films also demonstrate a continuous reduction in tetragonal phase fraction and degradation in the protective character of the oxide layer [50,51,56,57,71]. In both cases a key issue is the ingress of oxygen containing species. The tetragonal to monoclinic phase transformation is known to generate cracks [12,35], as a consequence of the ~6% volumetric expansion and ~16% shear strain upon transformation [52]. Nano-scale cracks associated with this phase transformation have also been observed using transmission electron microscopy TEM) in oxides formed on zirconium alloys [8]. In either scenario these cracks could create fast ingress routes for oxygen containing species, reducing the protective nature of the oxide film, or accelerating the rate of hydrothermal degradation. A fundamental challenge then is in understanding exactly how this phase transformation leads to crack formation.

Whether the transformation occurs in sintered zirconia, or in the zirconia oxide layer grown on zirconium alloys, there are numerous factors that impact the extent of transformation induced fracture. Typically these factors occur simultaneously and make a systematic, quantitative experimental assessment highly challenging. As such, this research aims to improve understanding by applying the peridynamics approach in a simulated study of a single grain phase transformation induced fracture in zirconia.

Previously, finite element analysis has been used to simulate the tetragonal to monoclinic phase transformation [52]. This work highlighted how relaxation of the in-plane biaxial compressive stress, or the application of a triaxial tensile stress, could destabilise the tetragonal phase. The volumetric expansion and shear strain associated with the transforming grain induced very high levels of stress in the surrounding oxide layer. However, these simulations did not include fracture. The result was that the transformation strain energy was artificially very high, and information on the likely crack formation was limited. Simulation of fracture in FEM is difficult due to the strong mesh dependence and requirement for crack branching criteria. XFEM offers improved results, but still has the problem that the use of classical partial differential equations leads to singularities at crack surfaces and tips [5]. At a singularity, as the distance to the crack tip tends towards zero the mesh size must approach zero and the stress increase towards infinity. An alternative approach to the simulation of fracture proposed by Silling is that of peridynamics [61].

Peridynamics is a formulation of non-local solid mechanics theory that uses displacements, rather than spatial derivatives, to define the movement of nodes relative to one another [37]. By calculating the displacements of points connected within a defined cut-off distance known as the horizon, the peridynamics approach uses an integral formulation of a constitutive model [5]. As such peridynamics does not lead to the formation of singularities, and shows much less mesh dependence than FEM, in the presence of defects such as cracks and voids. It also means the stress fields are, provided the mesh is adequately refined, both finite and convergent. However, in peridynamics the definition of material properties is dependent on a specific network of truss elements. As each node is connected to every other node within a defined horizon, there is a natural reduction in the number of connections constraining the nodes at the edge of a simulation. This reduction in constraint of the edge nodes effectively reduces the stiffness of this part of the network. This is typically corrected for by the appropriate application of boundary conditions and material properties.

The present work combines the peridynamics approach with finite element analysis to assess the tetragonal to monoclinic phase transformation in zirconium oxides. This includes factors affecting destabilisation, and prediction of the how the phase transformation can induce crack formation.

2. Model construction

2.1. Peridynamics and material properties

The peridynamics method was implemented into the commercial FE code Abaqus as describe in detail in [5]. The explicit version was used to model the dynamics of the transformation and cracking. In peridynamics the material is represented by a series of material points (nodes in Abaqus). Mass elements were tied to each node and the material volume is dependent on the distance between material points, calculated with the bulk material density. In these simulations the nodes are connected by a network of truss elements which carry the force. This is done over a circular (2D) or spherical (3D) horizon (h). The horizon has been shown to give good results for reasonable computation time for a horizon of 3 lattice or material point spaces and this is what was used here [5]. The force carrying truss elements need to be tuned to give the correct bulk material elastic response. A sensitivity study has been carried out for the elastic modulus that was applied to the individual truss elements in order to generate a mesh that has an elastic modulus equivalent to that of zirconia (253 GPa) [51]. As this is a bond based 2D peridynamics simulation, equivalent to a pair potential method in the atomic scale method, the Poisson ratio is fixed as 1/3 [5].

In this work a square FE mesh was tied to the peridynamics mesh so that ε_{11}, ε_{22}, and ε_{12} strain components could be determined for the peridynamic truss network. The continuum elements to which the truss elements have been tied do not contribute towards the stress in the simulation. As such, negligible values have been assigned for the elastic modulus ($E = 1 \times 10^{-6}$ MPa) of the continuum elements. Peridynamics distributes material mass only to the material points/nodes, as such the density of all of the elements has also been defined as a negligible value of 5×10^{-10} g/cm^3. The point masses applied to the nodes in the simulations generate an overall material density equivalent to that of zirconia (5.68 g/cm^3).

In order to incorporate damage into the model, a history dependent critical mechanical strain was applied to the truss element in the surrounding oxide region. Beyond this strain the bond will lose all stiffness for the remainder of the simulation. This critical strain is correlated with the strain energy release rate using Eq. (1), derived from the Griffith criteria for creating two new surfaces over the area of one whole horizon [62].

$$S_0 = \sqrt{\frac{5\pi G_0}{9hE}}$$

where h is the horizon distance and G_0 is the total energy per unit crack surface necessary to totally separate two halves of a material [38]. S_0 is one of the primary factors under investigation. This study tested four critical fracture strains defined as 0.00711, 0.00553, 0.00395 and 0.00237, which gives fracture stresses of 1.8 GPa, 1.4 GPa, 1 GPa and 600 MPa. These values are based on the fracture stresses and strains defined for manufactured stabilised zirconia [17,18,46], and values obtained for zirconia formed as an oxide layer on ZIRLO™ [53]. After a truss element has reached S_0, and failed, the elastic modulus of the truss becomes negligible ($E = 1 \times 10^{-6}$ MPa). Here we used a zero order model of fracture, i.e. once S_0 is reached the truss reduces in stiffness without further strain.