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Nanoindentation study of zirconia with non-transormable tetragonal phase: experiments and simulation of elastic and plastic behavior

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Abstract – Zirconia based materials with a t´-phase are typically used as thermal barrier coatings due to good fracture toughness at high temperatures, due in part to its low thermal conductivity [1,[2]. It is well known that ferroelastic domain switching can have a direct impact on the mechanical properties of such materials [3,[4]. Several reports have shown indirect evidence of domain switching in zirconia based ceramics that might be the source of its high toughness [5]. However, most of the reported phenomena remain to be understood.

Nanoindentation tests with single load indentation cycles, using diamond tips with Berkovich and cono-spherical geometries were carried out on dense polycrystalline zirconia ceramics with t´- and cubic phases ($66.8ZrO_2$-$16.6YO_{1.5}$-$16.6TaO_{2.5}$ and $69.8ZrO_2$-$22.5YO_{1.5}$-$7.7TaO_{2.5}$, respectively), to study the elastic – plastic indentation behavior and these were represented by 3D finite element modeling (3D-FEM). From the experimental behavior reported by Baither et.al. [4] a constitutive model that describes the experimental stress – strain curve was extracted and implemented in the FEM simulated curve. This ferroelastic-plastic 3D-FEM model seems to be key to reproduce the elastic-plastic deformation in zirconia with the t´-phase and elastic recovery during the nanoindentation process. The *P-h* curves of both materials obtained with both indenter geometries showed clear differences at loads above the elastic limit. The load-displacement (*P-h*) curves were transformed to indentation stress-strain curves (P_m-a/R; P_m= mean contact pressure, a, R= contact and tip radii, respectively) following a methodology based on the Hertzian theory and considering equivalent spherical tip. For instance, the results obtained with a Berkovich indenter will be discussed as follows (Figs.1a,b, 2a,b). The material with cubic-phase shows a typical transition of P_m above the purely elastic regime where the indentation contact area increases at a rate that practically gives no increase in the mean contact pressure for further increases in indenter load. For the t´-phase the elastic behavior reached a higher mean contact pressure than the cubic phase. Special attention was paid to the slope of the P_m-a/R curve of the t´-phase in the purely elastic regime and its behavior after the appearance of a so called pop-in (extra penetration at constant load in the loading curve). This pop-in in the 3D FEM simulated curve was found to correlate with the coercive stress as observed in previously reported compression tests [4]. Above the pop-in, a linear behavior was still observed, but with a change in the elastic modulus from 209 to 132 GPa. All these differences and the higher hardness obtained from the sample with t´-phase are probably correlated to ferroelastic switching phenomena. Moreover, topography changes were observed on zirconia with non transformable tetragonal phase around indentation imprints with the Berkovich indenter (Fig.2b) that cannot be directly correlated with the typical plastic deformation of the indentation imprint. These, also represent encouraging results giving further support to the hypothesis of ferroelastic switching of domains as a toughening mechanism.

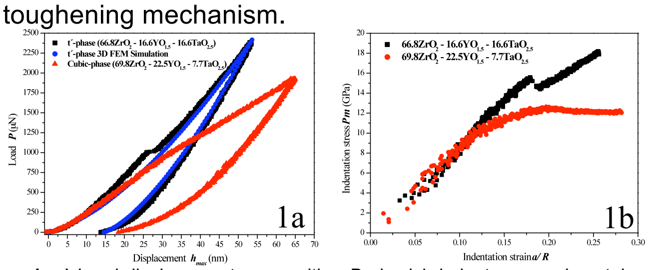

Figure 1: a) Load-displacement curve with a Berkovich indenter, experimental and FEM simulation. **b)** transformation to indentation stress-strain experimental curves.

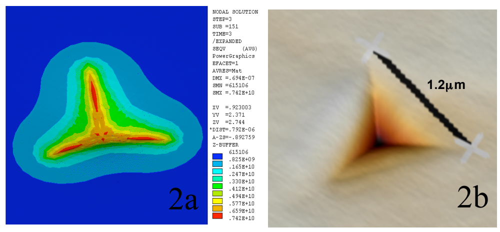

Figure 2: indentation imprints of polycrystalline t´-zirconia. **a)** experiment and **b)** 3D-FEM simulation.

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