

## Lattice and grain boundary diffusion of cations in tetragonal zirconia

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### 1. Introduction

Zirconia is a widely used oxide ceramic in various high performance applications due to its attractive mechanical, electrical and thermal properties. In particular, the material 3 mol% yttria stabilized tetragonal zirconia (3YTZ) has been shown to undergo superplastic deformation [1]. One crucial step in the understanding of processes like superplasticity involves the knowledge of appropriate cation lattice and grain boundary diffusion coefficients. However, there are no diffusion data available on 3YTZ. The present study was carried out with the objective of obtaining lattice and grain boundary cation diffusivities of Y and Zr in high purity 3YTZ, using stable tracers and secondary ion mass spectrometry (SIMS) for analyzing the resulting depth profiles.

### 2. Experimental Details and Results

High purity 3YTZ (alumina+silica < 0.1 wt%) powder was cold compacted at 40 MPa and sintered in air at 1723 K for 3 hours at a heating and cooling rate of 3 K min<sup>-1</sup>. The compacts were further annealed at 1873 K for 10 hours to obtain an initial grain size of 0.8 μm. For the diffusion experiments two different cations were used, Hf<sup>4+</sup> and Yb<sup>3+</sup>. Thin films of hafnium oxide and ytterbium oxide were deposited on the surface of 3YTZ with a pulsed excimer laser. The samples were diffusion annealed at temperatures from 1673 to 1873 K for various times by suppressing grain growth. Cameca IMS 3F and 5F SIMS machines were used to measure the variation of concentration of the diffusing species with time. An example of the depth profile for the determination of lattice and grain boundary diffusivities of hafnium in 3YTZ at 1673 K is shown in Fig. 1. Fig. 2 shows an Arrhenius plot of the diffusion coefficients.

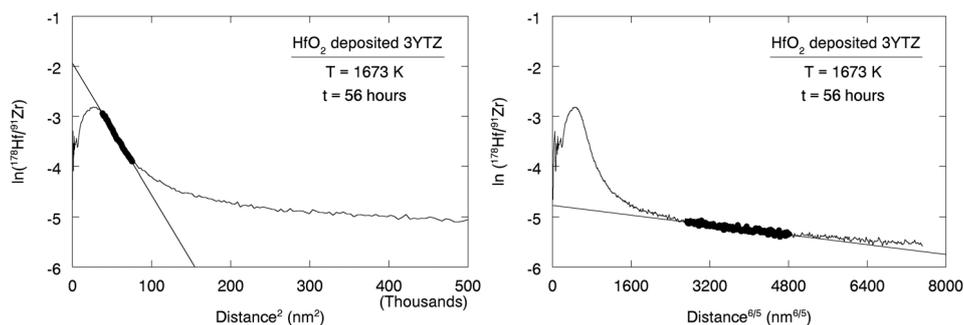


Fig. 1 Calculation of lattice (left) and grain boundary (right) diffusivity of Hf in 3YTZ.

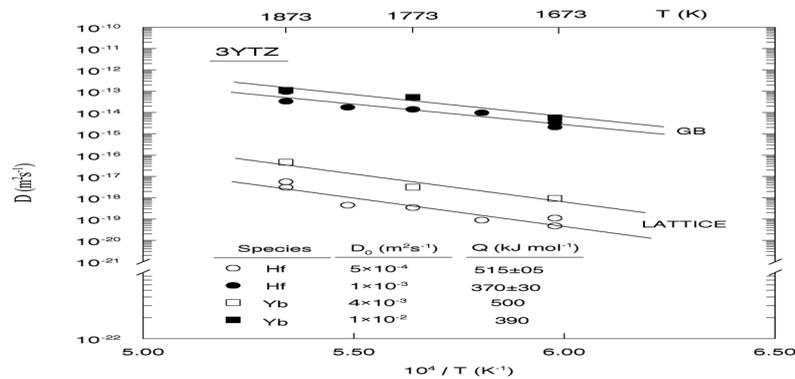


Fig. 2 Arrhenius plot of Hf and Yb diffusion in 3YTZ along lattice and the grain boundary.

### 3. Discussion and conclusion

From the analysis of the diffusion data and comparison of the present data with previous studies on cubic zirconia it was found that the diffusivities did not have significant dependencies on the mass of the diffusing species, crystal structure and yttria content of the material. Thus,  $Hf^{4+}$  and  $Yb^{3+}$  diffusivities along lattice and grain boundaries were not significantly different from the self diffusivities of  $Zr^{4+}$  and  $Y^{3+}$  ions respectively in cubic zirconia. In addition, the lattice diffusivity of  $^{96}Zr$  in 2.8YTZ in an earlier study [2] was found to match with the results of the present study. Further, it was shown previously that ytterbium could be used as a tracer for yttrium, when Jimenez-Melendo *et al.* [3] investigated the grain boundary diffusion in yttrium aluminium garnate. This was confirmed in the present study for the investigation of the yttrium diffusion in 3YTZ. Therefore it was concluded that  $Hf^{4+}$  and  $Yb^{3+}$  acted as tracers for  $Zr^{4+}$  and  $Y^{3+}$  respectively. Similar to the results on cubic YSZ, zirconium diffusion is slower than yttrium diffusion. Surprisingly, the difference is more pronounced for bulk diffusion than for grain boundary diffusion. The differences in the lattice diffusivities of cations could be rationalized based on charge densities [4], the diffusivity decreasing with the increase in charge density of the species. The  $Hf^{4+}$  (or equivalently  $Zr^{4+}$ ) diffusion along lattice and grain boundary was found to be the slowest and hence rate controlling the high temperature processes such as superplasticity.

### References

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