

# EFFECT OF POROSITY ON THE MECHANICAL PROPERTIES OF YSZ/NiO COMPOSITE ANODE MATERIALS

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## Introduction

Porous Ni/YSZ composite has been used widely as anode for solid oxide fuel cells. Ni/YSZ anodes are usually made by co-sintering NiO and YSZ [1]. Various types of experiments have been utilized to analyze the mechanical properties of NiO/YSZ composite [1-3]. Miladin and Edgar [2] measured the Young's modulus of the fully reduced Ni/YSZ and the unreduced NiO/YSZ. They found that the decrease in Young's modulus was caused mainly by the increase of the porosity through NiO reduction. Wang et.al.[3] investigated the effects of powder sizes and reduction process on the strength of NiO(Ni)/YSZ. They demonstrated that specimens with higher initial porosity had lower mechanical strength. Evaluating the mechanical properties and performance of composites requires large amount of experiments and is prohibitively costly. In addition, it is difficult to measure the effect of variable macropores and micropores on properties and behavior. In this paper, we present mechanics-based mathematical models to predict the effect of macropores and micropores on the mechanical strength, Young's modulus and Poisson's ratio. We investigated the morphology of the material system experimentally as model inputs.

## Experimental and Modeling

### 1.1 Material properties

Table 1 Measured elastic properties.

Material	Porosity	E (GPa)	$\nu$
NiO	0%	171.8±1.3	0.384±0.006
	5%	171.8±3.2	0.413±0.006
	25%	171.8±3.2	0.360±0.013
YSZ	0%	198.6±1.0	0.312±0.007
	5%	198.6±1.0	0.325±0.005
	25%	198.6±1.0	0.313±0.009

Table 1 shows the Young's modulus  $E$  and Poisson's ratio  $\nu$  of NiO and YSZ at different porosity levels. They were measured by using in-situ neutron diffraction at the Oak Ridge National Laboratory. The specimens were made of NiO and

YSZ, with volume ratio of 1:1. The total porosities of the YSZ/NiO composite ranged from 0%, 5% to 25%. In average, the  $E$  of NiO is 171.8 GPa, and the  $E$  of the YSZ is 198.6 GPa. The  $\nu$  of both the NiO and YSZ varies at different total porosity levels.

### 1.2 Modeling of Young's modulus

Several models have been developed to consider the effect of porosity on Young's modulus [4, 5, 6, 7]. For our YSZ/NiO composite material, the  $E$  is calculated based on Eqs. 1 and 2 [6, 7]:

$$E = E_0 \cdot [(1 - p_{micro}) - (N_c - 1) \cdot (1 - p_{micro})^{2/3}] \cdot (1 - p_{macro})^m \quad (1)$$

$$E = E_s (1 - \Phi/\Phi_0)^n \quad (2)$$

where  $N_c$  is the mean coordinate number derived from the SEM pictures.  $N_c=0.58$  for 5% porosity YSZ/NiO,  $N_c=0.32$  for 25% porosity YSZ/NiO.  $m$  depends on the tortuosity of the porosity, but is usually close to 2 for ceramic materials [6].  $n$  and  $\Phi_0$  are empirical correlation parameters [7]. Sensitivity checking of  $n$  and  $\Phi_0$  was performed to investigate how much they affect Young's modulus of YSZ/NiO. The results showed that  $E$  was more sensitive to the change of  $\Phi_0$  than that of  $n$ . The macroporosity ( $p_{macro}$ ) and microporosity ( $p_{micro}$ ) were determined based on the calculation of macropore areas (pore with area over  $100\mu\text{m}^2$ ) and micropore areas (pore with area less than  $100\mu\text{m}^2$ ) over the cross-section area from SEM pictures, as shown in Fig. 1.

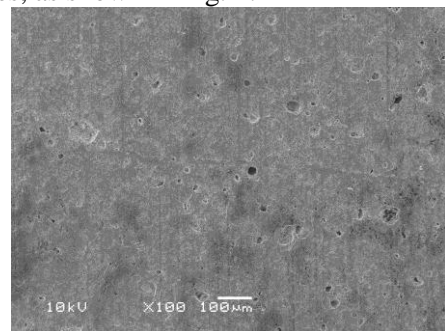


Fig. 1 SEM picture of 5% porosity YSZ/NiO. The  $E$  of the YSZ/NiO composite was determined as 173.81GPa for 5% porosity and 129.63GPa for 25% porosity. For 5% porosity and 25% porosity

YSZ/NiO composite, the  $E$  decreases linearly with the increase of microporosity, as shown in Fig. 2 and Fig. 3. It was found that the volume ratio of macropore and micropore is near to 1:1 for either 5% porosity or 25% porosity.

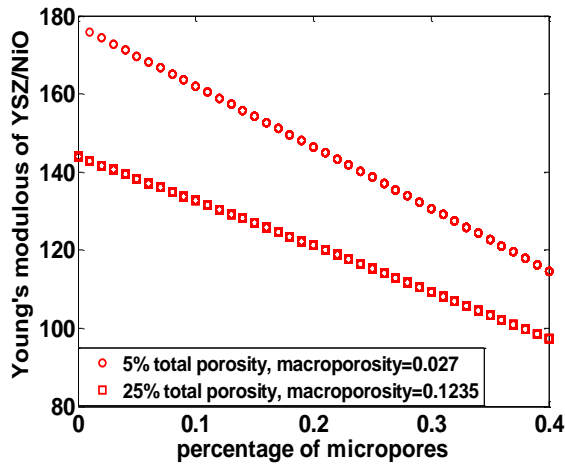


Fig. 2 Microporosity vs. Young's modulus NiO/YSZ .

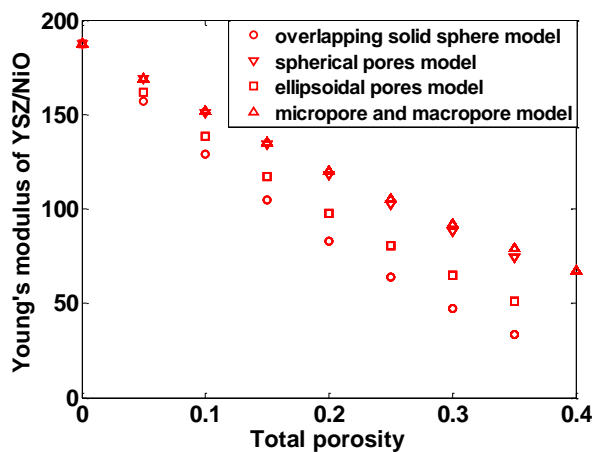


Fig. 3 Total porosity vs. Young's modulus of NiO/YSZ .

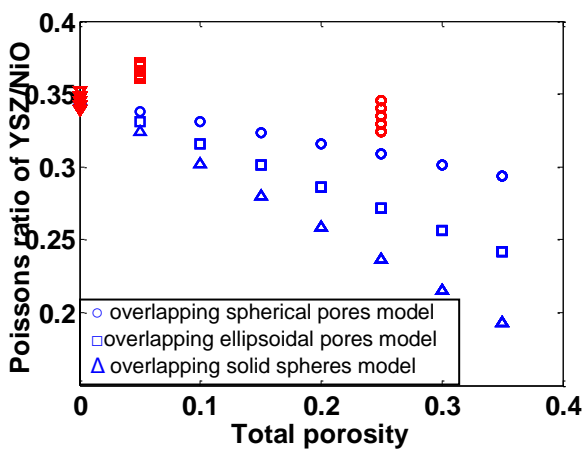


Fig. 4 Total porosity vs. Poisson's ratio of YSZ/NiO (red points are experimental data).

### 1.3 Modeling of Poisson's ratio

Fig. 4 shows that the models underestimated the Poisson's ratio of the YSZ/NiO composite. The Poisson's ratio changes nonlinearly with the increasing total porosity. Results of the overlapping spherical pores model are the most closely to the experimental data among the three Poisson's ratio models. The  $\nu$  models verified the statement that the effective Young's modulus of a two-dimensional media with holes does not depend on the Poisson's ratio of the matrix material [8].

### Conclusions

The Young's modulus of the YSZ/NiO composite decreases linearly with the increase of microporosity and total porosity. The Poisson's ratio changes nonlinearly with increasing total porosity. The Poisson's ratio is independent on the Young's modulus. Future research is needed to improve the Poisson's ratio modeling. When the models for estimating mechanical properties are verified, it is possible to predict phase stress and strain in the YSZ/NiO composite.

### Reference

1. An, K., B. Clausen, et al. In-situ neutron diffraction study of phase stress evolutions in a Ni-based porous anode solid oxide fuel cells under uniaxial load. *Appl. Phys.*, **A 99** (2010) 579–584.
2. Radovic, M. and E. L. Curzio. Elastic Properties of Nickel-Based Anodes for Solid Oxide Fuel Cells as a Function of the Fraction of Reduced NiO. *J. Am. Ceram. Soc.*, **87** (2004) 2242-2246.
3. Wang, Y., M. E. Walter, et al. Effects of Powder sizes and reduction parameters on the strength of Ni-YSZ anodes. *Solid State Ionics*, **177** (2006) 1517-1527.
4. Wong, D., J. Koplik, et al. Conductivity and permeability of rocks. *Phys. Rev. B* **30** (1984) 6606-6614.
5. Wagh, A. S., R. B. Poepfel, et al. Open pore description of mechanical properties of ceramics. *J. Mater. Sci.*, **26** (1991) 3862-3868.
6. Tancret, F., et al. Modelling the mechanical properties of microporous and macroporous biphasic calcium phosphate bioceramics. *J. the European Ceramic Society* **26** (2006) 3647-3656.
7. Roberts, A. P., Garboczi, E. J. Elastic properties of model porous ceramics. *J. Am. Ceram. Soc.*, **83** (2000) 3041-3057.
8. Cherkaev, A. V., et al. Invariant properties of the stress in plane elasticity and equivalence classes of composites. *Proc. R. Soc. Lond. A*, **438** (1992) 519-520.