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Numerical Analysis of Strong Buckling Behavior of Square Thin Membranes Using ABAQUS

1. Motivation, and Project Goal

Understanding stress and deflection states of square thin membranes is critical to design thermomechanically stable thin membranes, because such membrane structure was employed to improve efficiency of Yttria-stabilized Zirconia (YSZ) based micro solid oxide fuel cell (μSOFC) in an inter-departmental project at MIT. As shown in Figure 1, a μSOFC consists of three layers: anode (Platinum-YSZ), electrolyte (YSZ), and cathode (Pt-YSZ). The power is generated by decomposing gases (oxygen and fuel), requiring that the electrolyte conducts oxygen ions selectively. Although μSOFCs and fuel cells in general have an improved efficiency (~60-80%) when compared with other fossil-fuel plants (~35-40%) [1], the efficiency still needs to improve because the power production is still limited by the low voltage output determined by the electrolyte material. The solution investigated in the project was to decrease the thickness of tri-layer membranes, and thus shortening the physical length that the oxygen needs to go through. Square thin membranes were employed as the preliminary design of the μSOFC structure. However, this thin structure could experience high stress that might cause structural failure. Thin films come with residual stress as deposited. In addition, solid oxide fuel cells operate only at high temperature (~500-1000 C). When thin membranes are heated up to such high temperature with their four side boundaries fixed, membranes could experience high stress, and thus a variety of failure modes were observed as shown in Figure 2. Thus, clever design (geometry, material properties, and residual stresses) of thin membrane is critical to achieve thermomechanically structure at high operation temperature. Various methods can be taken to achieve the design or aid the designing process, including analytical prediction and experimental fabrication. However, analytical prediction is relatively difficult due to the solutions' non-linearity, and the trial-and-error method with experiments takes significant efforts in microfabrication process. Meanwhile, with a simple finite element model (FEM), it is effectively easy to characterize the effect of various parameters on the stress/deflection states, regardless of the solutions' non-linearity. Naturally, the goal of this project is to model square thin membranes under in-plane stresses with finite element method, and predict their buckling behaviors including stress and deflection states over varying parameters.
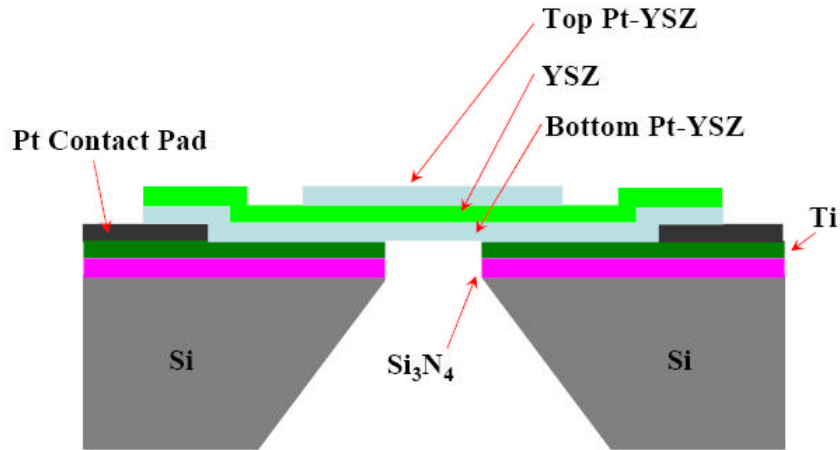
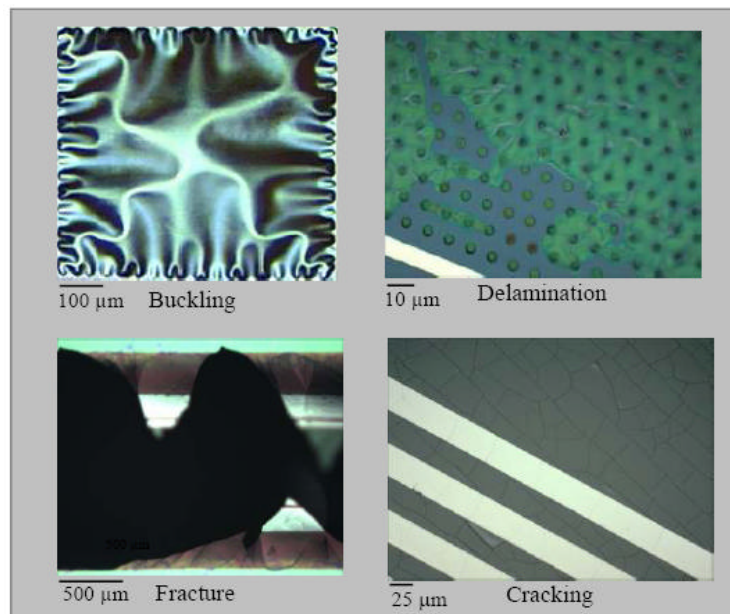Figure 1. Cross-sectional view of the tri-layer structure of the solid oxide fuel cell [2].

Figure 2. Failures of μSOFC thin films experimentally observed due to high stresses [3].

2. Method

This section will explain how buckling behaviors were simulated using a FEM software. The difficulty was to model buckling behavior that will involve with system instability in solving eigenvalue problems. This difficulty was cleverly avoided using pressure application, as suggested by Ziebart [4], which will be explained in the following.

ABAQUS/CAE version 6.6 was used. Thin square membranes were modeled as 3-dimensional deformable shell plate. Their sidelength was varied from 5 to 1000 μm

(the largest membrane size achievable experimentally), and the thickness was varied from ~300 to 600 nm (thin enough for significant efficiency improvement). Isotropy and no plastic deformation were assumed for simplicity. Since the Pt-YSZ anode/cathode layers have porous structure for better catalyst reaction, their structural significance was ignored, and only the single layer of YSZ was modeled in the FEM. Material properties of the YSZ are shown in Table 1. Young's modulus and the coefficient of thermal expansion (CTE) were experimental obtained from the relationship between the buckled center deflection and the residual stresses, with Poisson's ratio assumed to be the same as the bulk YSZ, 0.2. Experimentally, the material properties and residual stresses were confirmed to vary much depending on fabrication and geometrical conditions. The four side boundaries were modeled as fixed, since the thicknesses of the films are much smaller than the thickness of the substrate. The thin membrane structures were meshed by ~10x10.

Buckling behavior was simulated by using thermal loading and pressure loading as shown in Figure 3. Instead of solving eigenvalue problems that might cause instability, buckling simulation was broken in to three steps. First, pressure was applied to the thin membrane to deflect it. Any amount of pressure works as long as the membranes experience the out-of-plane deflection. Second, the membrane was thermally loaded to simulate the residual stress. Using the biaxial stress assumption, the amount of the temperature rise (ΔT) that gives the same in-plane stress as the residual stress was calculated.

$$\boldsymbol{s}_0 = -(\Delta T)E\boldsymbol{a}/(1-v) \tag{1}$$

where

$\boldsymbol{s}_0$: residual stress

ΔT : temperature rise

Finally, the pressure with the same amount as the first step was applied to the opposite direction to cancel out. In this way, only the residual stress, simulated by thermal loading, remains in the model. In addition, no eigenvalue solving is necessary since the membrane experiences out-of-plane deflections before the residual stress loading.

Young's modulus, E	64 [GPa]
Poisson's ratio, v	0.2
CTE, α	11.4 [10^{-6}/K]

Table 1. Material properties used in the FEM calculation.

Temperature Field
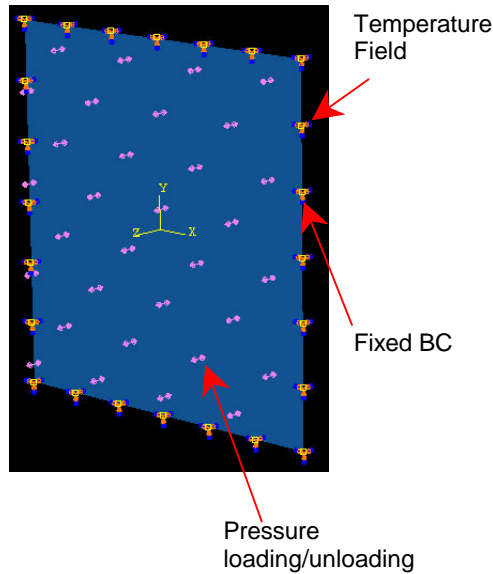
Fixed BC

Pressure loading/unloading

Figure 3. ABAQUS capture picture of the three loading steps (pressure loading, thermal loading to simulate residual stress, and pressure unloading) and boundary conditions.

4. Results
4.1. FEM validation

Before investigating stress/deflection evolution with parameter changes, first FEM results were compared with available experimental data to confirm the validity of this FEM calculation. As will be illustrated below, the numerical deflection values and the pattern evolution tendency were confirmed to be satisfactorily similar to the experimental results.

The center deflection of the YSZ membrane with the residual stress of -66 MPa was calculated. The deflection profiles after the three steps of loading are expressed in Figure 4. The center deflection obtained from the FEM was 3.07 μm, and this was comparable with the experimentally obtained deflection 2.46 μm. Thus, this FEM calculation can be said to properly working in the right range.

The pattern evolution with sidelength change was also calculated by FEM. Experimentally, the pattern evolution and its symmetry evolution were observed as shown in Figure 5. With smaller sidelength just after the first critical buckling, the deflection profile has folding-symmetry about two perpendicular axes in the membrane plane, and rotation-symmetry about the out-of-plane axis. With the larger sidelength, after the second critical buckling, the profile loses the symmetry about the two axes, but keeps the rotation symmetry. The pattern evolutions calculated by FEM is shown in Figure 6. Since the geometrical parameters and the material properties are different from the experimental ones, the two results are not directly comparable. Nevertheless, the buckled profiles showed the similar tendency as the experimental results: two-axis and rotation symmetry with smaller sidelength, and only rotation symmetry with larger sidelength.
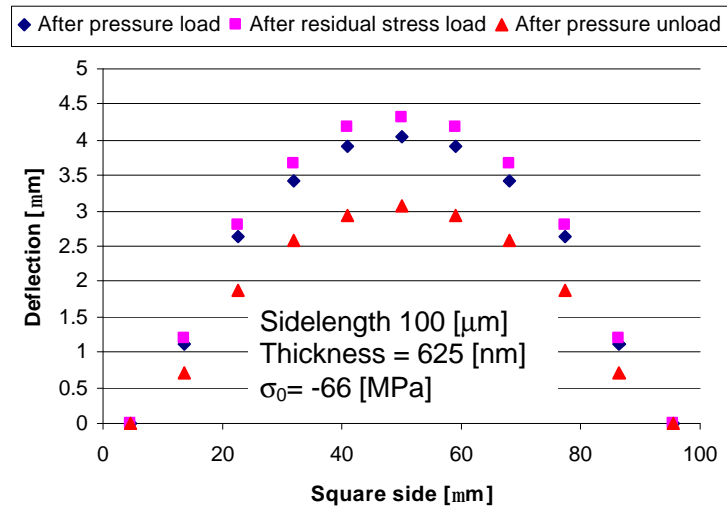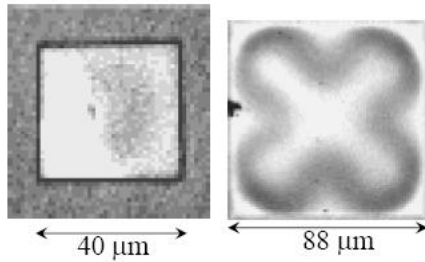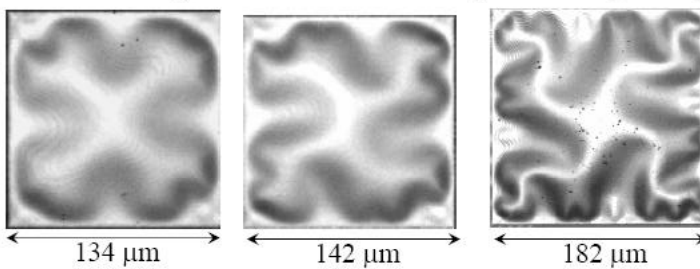
Figure 4. Deflection profiles of the YSZ membranes after each loading step.

First Buckling Mode Evolution with 2-Axis and Rotation Symmetry

40 μm
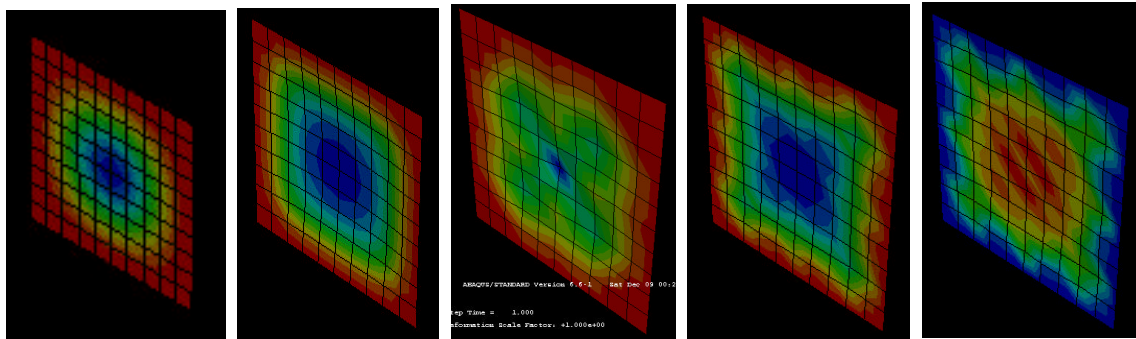
88 μm

Second Buckling Mode Evolution with only Rotation Symmetry

134 μm

142 μm

182 μm

E=24 [GPa], v=0.2,
CTE=9.74 [10^{-6}/K]
σ_0= -38 [MPa]
thickness= 368 [μm]

Figure 5. Buckling pattern evolution with increasing sidelength [2].

σ_0= -66 [MPa], thickness=625 [nm]

Sidelength: [not in scale]

| 20µm | 100µm | 300µm | 500µm | 1000µm |

Figure 6. Deflection profiles of buckled thin membranes with increasing sidelength calculated by FEM.

4.2. Stress evolution with sidelength

Now that the FEM calculated was confirmed to be valid, stress states were calculated for varying sidelengths, and were compared with the extreme stresses calculated analytically.

Previously, extreme stresses were estimated using energy minimization method (EMM). Based on deflection pattern observation as above, the deflection profiles were modeled as a sum of symmetric deflection functions, but only with the first buckling mode. The strain energy was calculated with von Karman non-linear pate theory, and minimized to obtain coefficient of the symmetry functions. Extreme stresses were calculated from the deflection. As shown in Figure 7, the calculated extreme stresses can be roughly broken into the three regions. With smaller sidelength, the aspect ratio of the film thickness over the sidelength is small, and thus the membrane stays flat. Once the sidelength increases and reaches the first buckling mode, the stress increases significantly. With even larger sidelength, the out-of-plane defection is large enough to release the stress, and thus the extreme stress decreases and converges. FEM calculation results are superposed over the EMM results as shown in Figure 8. The FEM results expressed the three regions as mentioned above. The extreme stress values coincided well with the EMM values, except for the tensile stress in the region right after the buckling.
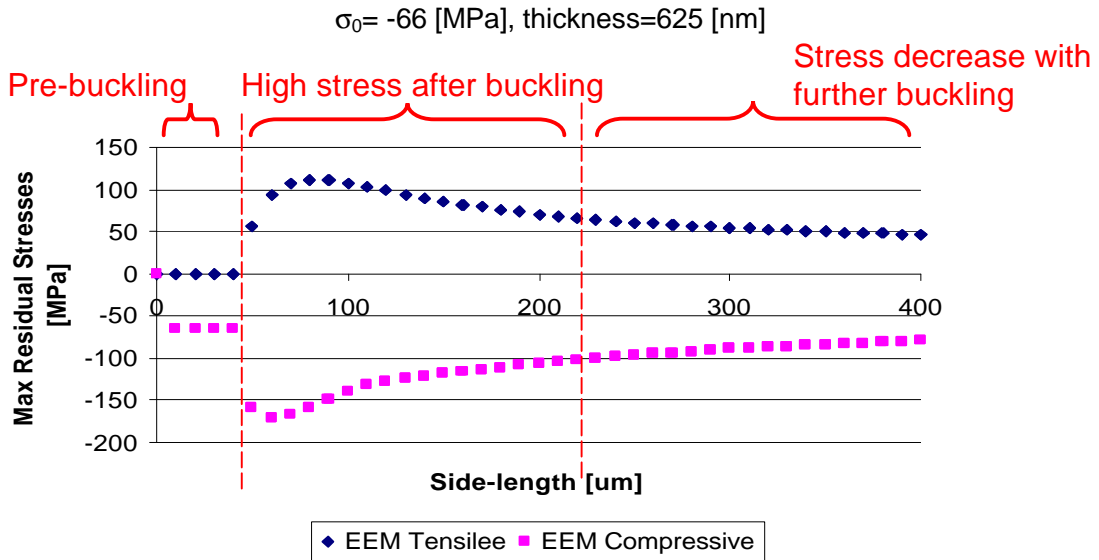
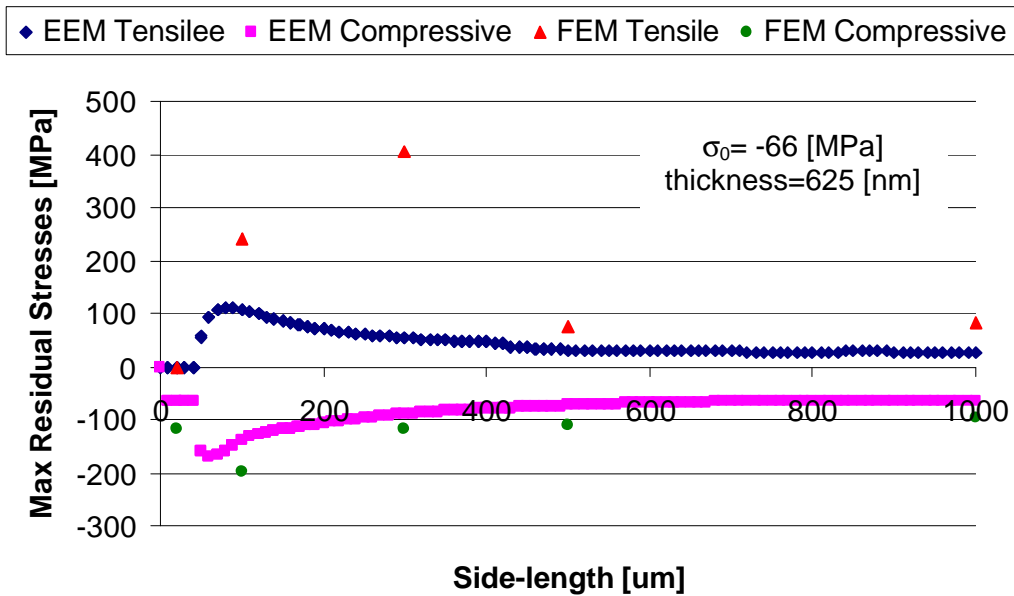Figure 7. Extreme stress evolution with sidelength calculated by EMM [2].

Figure 8. Extreme stress evolution with sidelength calculated by EMM and by FEM

4.3. Effect of Poisson's ratio

In this analysis, Poisson's ratio has been assumed to be 0.2, the bulk YSZ Poisson's ratio. Setting Poisson's ratio was important because only the in-plane modulus $E/(1-\nu)$ is obtainable experimentally. This assumption is relatively valid, considering that Ziebart [2] has confirmed that the effect of Poisson's ratio on the deflection and thus stresses is weak. However, the effect of Poisson's ratio was once again here examined.

Poisson's ratio was varied from 0.15 to 0.25, and the center deflection of the buckled membrane was calculated as shown in Table 2. The center deflection did not vary much, and thus again the effect of Poisson's ratio was confirmed to be weak.

Poisson's ratio	Center deflection [μm]
0.15	3.11
0.2	3.06
0.25	3.01

σ_0= -66 [MPa], thickness=625 [nm]

Table 2. Center deflections calculated by FEM with varied Poisson's ratio.

4.4. Stress evolution with temperature change

Deflection and thus stress distributions across the square membranes under thermal loading were calculated. This analysis is critical to design thermomechanically stable μSOFC membranes at high operation temperature. As shown in Figure 9, the deflection profiles were still under the scheme of the first and second buckling patterns.
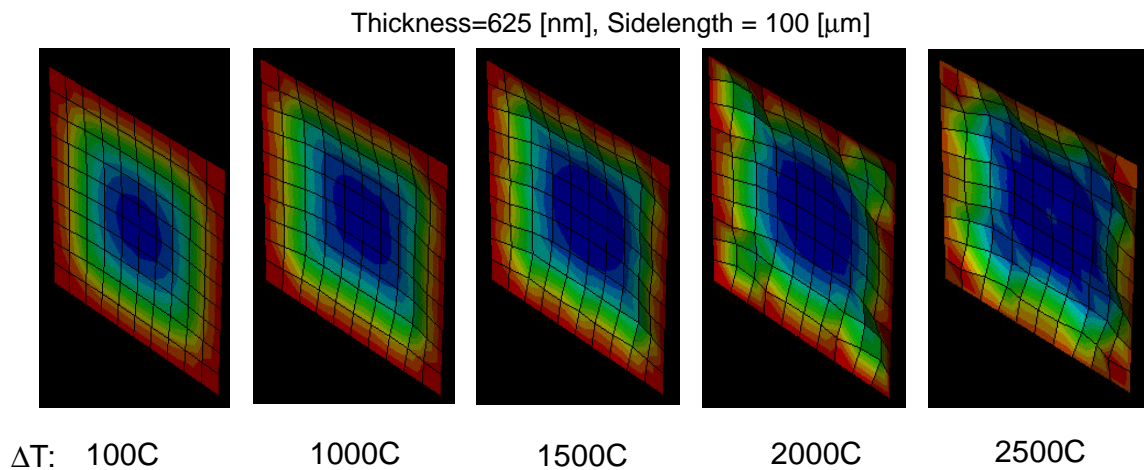
Thickness=625 [nm], Sidelength = 100 [μm]

ΔT: 100C   1000C   1500C   2000C   2500C

Figure 9. Deflection pattern evolution with increasing temperature

5. Discussion

Deviation of FEM results from experimental and analytical results was observed above. This difference most likely comes from the following factors. First, the finite element model used in this project does not exactly model the actual YSZ membrane. Experimentally, plastic deformation was observed, and the YSZ thickness slightly varied across the membrane, while no plastic deformation and uniformity was assumed in the FEM model. In addition, the silicon substrate, which expands after heating, was not modeled in FEM either. More mesh number with smaller element might have produced more accurate results. Besides, experimental values might contain some errors. The EMM analysis also has its limitation because only the first buckling mode was considered.

6. Conclusion

Major achievements in this project are listed in the following.

- Buckling behaviors due to residual stresses were successfully modeled with thermal loading.
- Pattern evolutions (1st and 2nd modes) with increasing sidelength were predicted.
- Stress evolutions with increasing sidelength, including three regions, were predicted.
- Effect of Poisson's ratio on center deflections of buckled membranes was confirmed to be weak.
- Stress/deflection evolutions with increasing temperature were predicted.

Thus, it can be concluded that this simple FEM analysis can produce preliminary prediction of buckling behavior (stress and deflection) of thin membranes under residual stress or thermal loading.

As for future work, modeling can be improved in terms of mesh size, material property (plasticity), or modeling of substrates. FEM analysis of the tri-layer structure (Pt-YSZ/YSZ/Pt-YSZ) of μSOFC will also be feasible with tri-section element.

References
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[2] N. Yamamoto. Thermomechanical Properties and Performance of Microfabricated Solid Oxide Fuel Cell (μSOFC) Structures. Master's thesis, Department Aeronaturics and Astronautics, Massachusetts Institute of Technology, 2006.
[3] D. J. Quinn. Microstructure, Residual Stress, and Mechnical Properties of Thin Film Materials for a Microfabricated Solid Oxide Fuel Cell. Master's thesis, Department of Mechanical Engineering, Massachusetts Institute of Technology, 2006.
[4] V. Ziebart, O. Paul, and H. Baltes. Strongly buckled square micromachined membranes. Journal of Microelectromechanical Systems, 8:423–432, 1999.