Finite Element Modeling for the Mechanical Behavior of Silicon Diaphragms Using Comsol Multiphysics 3.5

J. Ren, M.Ward  University of Birmingham
Peter Kinnell, Russell Cradock, GE Druck Limited
jxr551@bham.ac.uk
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• Constitutive equations
• Use of COMSOL Multiphysics
• Results and discussion
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  – Diaphragm displacement
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1. Introduction

The key components of a micromachined pressure sensor

- **Pressure**
  - Sensing element
    - A micromachined silicon diaphragm
  - Physical movement
- **Transduction mechanisms**
  - 1. Piezoresistivity
  - 2. Capacitance
  - 3. Optical tech
  - 4. Resonant tech
  - 5. Piezoelectricity
- **Electrical signal**
1. Introduction

Objective: simulate the load-deflection behaviour of silicon diaphragms at elevated temperatures (>600°C) using constitutive equations proposed by Alexander and Hassen.

The plastic deformation results from the crystallographic slip of the dislocation. Initial stage: dislocation density governs plastic shear strain rate (Alexander and Hassen’s model) Later stage: slip resistance governs the plastic shear strain rate
2. Experiment procedure

Process flow

(a) A prime silicon wafer was first etched by deep reactive ion etching (DRIE) in order to form the cavity.

(b) The prime silicon wafer was bonded with a BESOI wafer using silicon fusion bonding.

(c) The handle layer and the silicon dioxide layer of the BESOI wafer were removed using KOH and HF wet etching separately.
2. Experiment procedure

Before annealing → Annealing → After annealing

Measure surface profiles of the test samples under atmospheric pressure at room temperature.

Measure surface profiles of the test samples again under atmospheric pressure at room temperature.
3. Constitutive equations

Alexander and Hassen’s model

1. The plastic shear strain rate:
   \[ \dot{\epsilon}_{ij} = \dot{\epsilon}_{ij}^{el} + \dot{\epsilon}_{ij}^{vp} + \dot{\epsilon}_{ij}^{th} \]

2. The effective stress:
   \[ \tau_{eff} = \tau - \alpha \mu b \sqrt{\rho} \]

3. The evolution equation for dislocation density
   \[ \dot{\rho} = \left( \frac{K}{b} \right) \dot{\gamma}^p \tau_{eff} \]

4. The viscoplastic strain rate tensor:
   \[ \dot{\epsilon}_{ij}^{vp} = \frac{3}{2} \dot{\gamma}^p \frac{S_{ij}}{\sigma_e} \]

5. The strain rate tensor:
   \[ \dot{\epsilon}_{ij} = \dot{\epsilon}_{ij}^{el} + \dot{\epsilon}_{ij}^{vp} + \dot{\epsilon}_{ij}^{th} \]

6. The total strain rate:
   \[ \dot{\gamma}^p = \rho b v_0 \exp(-Q / kT) \left( \frac{\tau_{eff}}{\tau_0} \right)^{1/m} \text{sign}(\tau_{eff}) \]
4. Use of COMSOL Multiphysics

FEA model

- PDE general form mode 1 (Dislocation density)
- PDE general form Mode 2 (Viscoplastic strain)
- Stress-Strain application mode (Total displacement)
4. Use of COMSOL Multiphysics

**Isotropic elastic properties**

<table>
<thead>
<tr>
<th>Property</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Young’s modulus</td>
<td>E</td>
<td>151.3e9[Pa]</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
<td>ν</td>
<td>0.1615</td>
</tr>
<tr>
<td>Density</td>
<td>ρ</td>
<td>2329[kg/m^3]</td>
</tr>
</tbody>
</table>

**Viscoplastic properties**

<table>
<thead>
<tr>
<th>Property</th>
<th>Symbol</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Boltzmann’s constant</td>
<td>k</td>
<td>1.38e-23[J/K]</td>
</tr>
<tr>
<td>Burgers vector magnitude</td>
<td>b</td>
<td>3.83e-10[m]</td>
</tr>
<tr>
<td>Initial dislocation density</td>
<td>ρ₀</td>
<td>2e7[1/m²]</td>
</tr>
<tr>
<td>reference dislocation velocity</td>
<td>ν₀</td>
<td>6.5e3[m/s]</td>
</tr>
<tr>
<td>activation energy</td>
<td>Q</td>
<td>3.47e-19[J]</td>
</tr>
<tr>
<td>strain rate sensitivity parameter</td>
<td>m</td>
<td>0.9</td>
</tr>
<tr>
<td>shear modulus</td>
<td>μ</td>
<td>64e9[Pa]</td>
</tr>
</tbody>
</table>
5. Results and discussion

The dislocation density distribution after annealing (radius=1.75mm)

- The dislocation multiplication rate is very low at the region close to the middle plane of the diaphragm.
- The maximum dislocation densities results from the stress concentration at the round corner.

Von Mises effective stress of the diaphragm under the atmospheric pressure before annealing (radius=1.75mm)
5. Results and discussion

The dislocation density distribution after annealing at the region near the diaphragm edge (deformed geometry)

- The larger the diaphragm radius, the larger the maximum dislocation density is.
- For the diaphragm with a radius of 2.5mm, the dislocation density becomes negative at the region close to the middle plane (indicated by the blue colour). The convergence problem is caused by the highly non-linear material properties. Since the stress near the middle plane is very low, the dislocation density at the blue region should be very close to the initial value.
5. Results and discussion

The maximum displacement with annealing time (Radius=1.75mm)

• The initial displacement is induced by the atmospheric pressure.
• The creep process is much faster at 1173K (900°C) than that at the temperature ramp.
• The simulated maximum displacements are close to the measured values.

The surface profile shows the maximum displacement is 10.45µm before annealing

The surface profile shows the maximum displacement is 18.29 µm after annealing
5. Results and discussion

The comparisons of experimental data and model prediction for the diaphragm displacement

(a) before annealing
(b) after annealing

- The simulated deformations before annealing are close to the measured data for all the diaphragm radius.
- The simulated deformations after annealing are close to the measured data for the diaphragms with a radius of 1.5mm, 1.75mm and 2mm.
- Because the effect of the dislocations interaction on the plastic deformation is not included in the model, the predicted maximum displacement of 318.19µm is much larger than the measure data of 110 µm for the diaphragm with a radius of 2.5mm.
6. Conclusions and future work

Conclusions

• The mechanical behavior of micromachined silicon diaphragms at 900°C in the initial deformation stage was simulated using AH model.
• The model assumes that the material properties are homogenous.
• The dislocation density distribution and the diaphragm displacement are obtained.
• The results show that the predicted displacements are in agreement with the measured data for the diaphragms with a radius of 1.5mm, 1.75mm and 2mm.
• The model neglects the slip resistance caused by the interaction of the dislocations. So it is not valid for the diaphragm with a radius of 2.5mm.

Future work

• Compare the predicted dislocation density with the measured data.
• Apply AH model to each slip system of single crystal silicon.
7. Reference

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