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

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Introduction

Silicon diaphragms are one of the most common structures in micro-electro-mechanical systems (MEMS). For micromachined pressure sensors, silicon diaphragm is widely used as sensing element to detect the magnitude of the external pressure. Since high temperature pressure sensors are highly demanded for industrial, automotive and aerospace sensing applications, the load-deflection behavior of silicon diaphragms at elevated temperature is studied by experiment and is modeled using Comsol Multiphysics.

Single crystal silicon is brittle at low temperatures. But at temperatures higher than 550°C, the dislocation motion under an applied stress is thermally activated, therefore, silicon becomes ductile. As a result, the silicon diaphragms which are intended to work above 600°C may suffer from plastic deformation. Wherever applied stress exceeds the critical resolved shear stress (CRSS), the crystallographic slip of the dislocations occurs. The plastic deformation is dependent on the operating temperature, the applied stress, the dislocation multiplication, and the time.

A set of test samples with different radius was made using MEMS technology. As shown in figure 1, the pressure is applied on the top of the silicon diaphragm, and the boundaries of the silicon substrate can be considered as fixed boundaries. The surface profiles of the test samples were measured before the thermal treatment and after the thermal treatment using white interferometer. These measured data are then used to validate the finite element models.

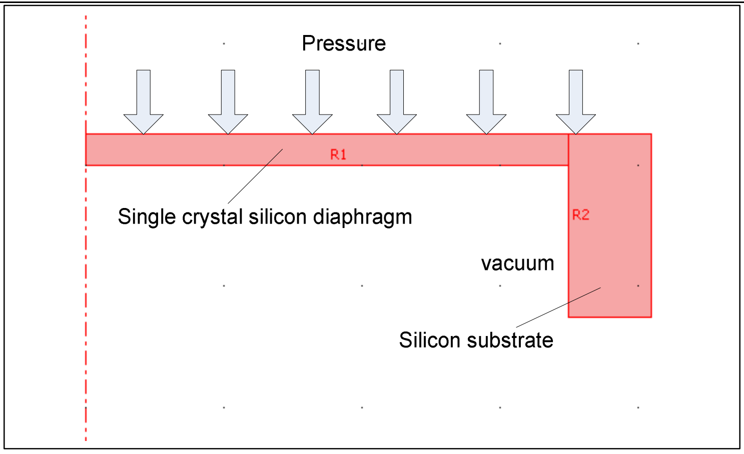

Figure 1: A schematic of the silicon diaphragm with fixed edge *(2D axial symmetrical view)*

Use of COMSOL Multiphysics

The deformation of single crystal silicon at elevated temperature is usually simulated using the constitutive model proposed by Alexander and Hassen. It is assumed that the deformation is uniform in the whole sample. The plastic shear strain rate, which is related to the motion of the mobile dislocations, can be expressed as:

$$\dot{\gamma}^p = \rho b v_0 \exp(-Q/kT)\left(\frac{\tau_{eff}}{\tau_0}\right)^{1/m} sign(\tau_{eff}) \qquad \text{(Equation 1)}$$

where ρ is the dislocation density, b is the Burgers vector magnitude, v_0 is a reference value for dislocation velocity, Q is the an activation energy, k is the Boltzmann constant, T is the absolute temperature in Kelvin, τ_0 is a reference stress, m is a strain rate hardening exponent, and τ_{eff} is the effective stress given by:

$$\tau_{eff} = \tau - \alpha \mu b \sqrt{\rho} \qquad \text{(Equation 2)}$$

where τ is the equivalent shear stress, α is a constant and μ is a shear modulus. The second term at the right hand side of equation 2 represents the internal stress produced by the interaction of the dislocations. The evolution equation for the dislocation density is given by:

$$\dot{\rho} = \left(\frac{K}{b}\right)\dot{\gamma}^p \tau_{eff} \qquad \text{(Equation 3)}$$

where K is a multiplication rate constant.

The diaphragm behavior was modeled using two PDE general form modes coupled with the stress-strain application mode. A PDE mode calculates the evolution of the dislocation density ρ with time. The plastic shear strain rate is defined in the scalar expressions, and is valid only when the effective stress is larger than zero. Another PDE mode calculates the plastic strain tensor which is related to the plastic shear strain rate. The axial symmetry, stress-strain application mode in Structure Mechanics Module is used to calculate the displacement field of the silicon diaphragm. The plastic strains obtained from the second PDE mode were deduced from the expressions for the elastic stresses because the stress-strain relation is based on Hooke's law.

For single crystal silicon, the initial dislocation density is on the order of 10^6 to 10^7 /m^2. The Burger's vector is 3.83×10^{-10} m. The activation energy is 3.47×10^{-19}J. Therefore, the value of the reference dislocation velocity and the reference stress should be selected carefully in order that the plastic shear strain rate is estimated properly. At the same time, the evolution of the dislocation density is mainly controlled by the multiplication rate constant K.

Expected Results

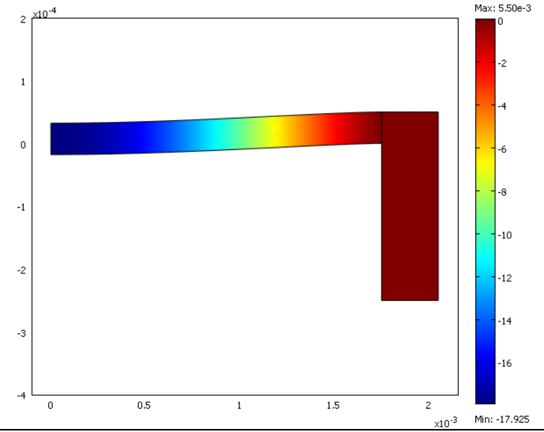 	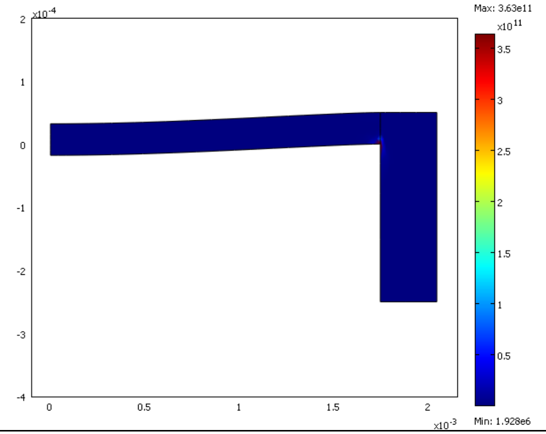
Figure 2. The deformation of a silicon diaphragm after thermal treat at 900°C for 1 hour	Figure 3. The dislocation density distribution of a silicon diaphragm after thermal treat at 900°C for 1 hour

The deformation of a silicon diaphragm after the thermal treatment at 900°C for 1 hour is shown in figure 2. The maximum displacement is 17.925 µm at the diaphragm center. The measured maximum displacement is 17.971 µm. Therefore, the simulated data is very close to the experimental data. Figure 3 predicts the distribution of the dislocation density in the silicon diaphragm. It can be seen that most dislocations are distributed near the edge of the diaphragm.

Conclusion

A finite element model is presented in this paper to predict the mechanical behavior of silicon diaphragm at elevated temperature. The model is based on the constitutive equations proposed by Alexander and Hassen. The model uses two PDE general form modes coupled with the stress-strain application mode. The plastic deformation is determined by the plastic shear strain rate, which is related to the evolution of the dislocation density. The simulated maximum displacement is very close to the measured data. However, this model assumed that the material is homogenous and the deformation is uniform. Therefore, the model could be improved if the plastic deformation on each slip system is concerned.