

Supplementary information

Nanolithography using thermal stresses

Gangadhar Purohit,^{a,b} Deepak,^{a,b} Monica Katiyar,^{*,a,b}

^aMaterials Science & Engineering

^bNational Centre for Flexible Electronics,

Indian Institute of Technology Kanpur, UP-208016, India

Corresponding author

*E-mail: mk@iitk.ac.in

We have used a finite element based software package, ABAQUS/CAE (version 6.11-2) for thermal stress calculation. The finite element analysis is carried in three stages, namely, pre-processing, simulation and post-processing. The pre-processing ABAQUS environment is divided into several modules; where each module defines a logical aspect during computation process. Here we define the geometry of the structure, assigning material properties and then generating mesh with the prescribed condition and constraints. After completing all modeling process, the running of simulation is carried out and at last, the post processing functions are executed by visualization module. The in-built code inside ABAQUS's preprocessor is like to construct and solve a set of linear or non-linear algebraic equations. For thermal generated computation, a displacement based finite element method is formulated with assuming equilibrium equations of stress-strain analysis.

Nature of simulation A general static analysis procedure was considered for this theoretical study, assuming multilayer stacking of thin films on a thick substrate.

Geometry taken for simulation Only one-fourth of the geometry was chosen for modeling because of the symmetry of structure in all x, y and z- directions. Dimensions of each thin layer were defined, in units of micrometer (μm). The schematic view of assumed thin film is shown in the Fig.S.1 and the borosilicate glass as thick substrate is shown in Fig. S.2.

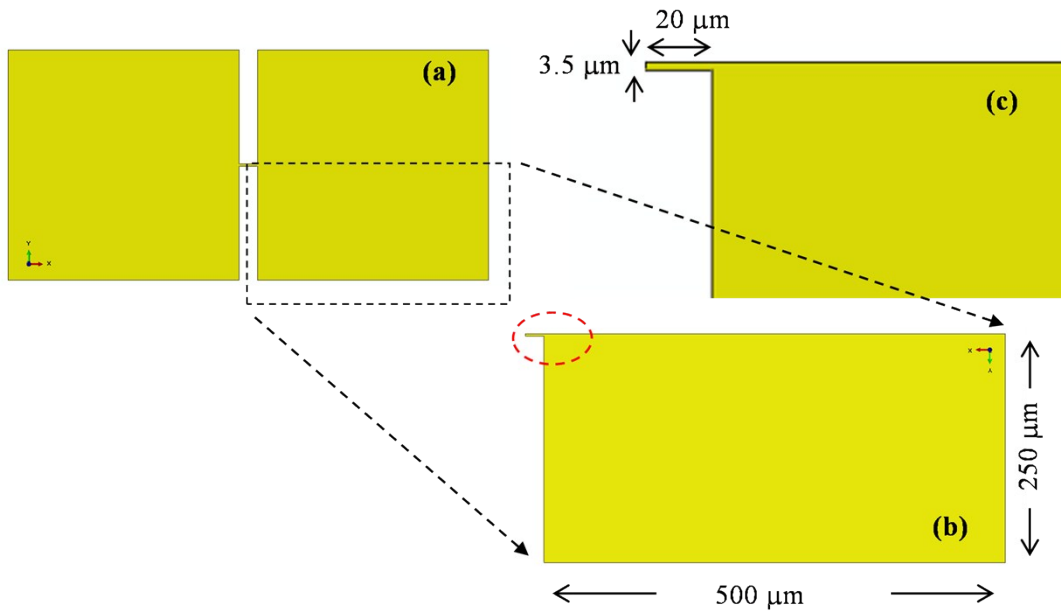


Fig. S.1 Schematic view of Au thin film on glass substrate seen from top surface in (a), and one-fourth of the geometry was considered for simulation in (b) due to its symmetry shape. The enlarged section of electrode bridge shown in (c) from red dotted oval of (b), which is the area of interest in whole theoretical calculation. The dimensions are also defined in unit of μm .

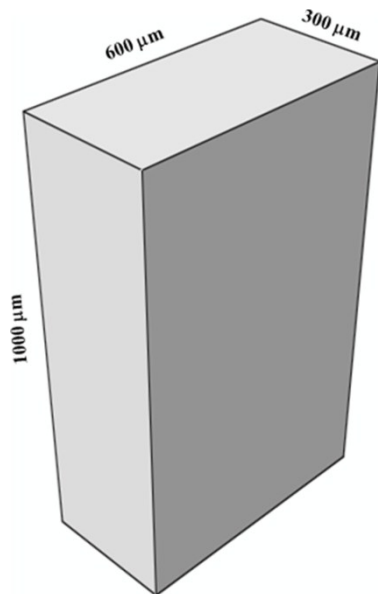


Fig. S.2 The structure and dimension of borosilicate glass assumed in defining the model

Defining material properties We assumed the materials are linearly elastic, isotropic and homogeneous and they remain elastic during analysis. We assigned material properties taken from literature to each part of model geometry using ABAQUS's property module.

Boundary conditions and thermal load

For simulation, the boundary conditions are chosen as follows

$U_1=0$ (at the wall to notched electrode bridge, i.e. across the bridge length)

$U_3=0$ (at the side wall of glass/Ti/Au/SiO₂ interface)

$U_2=0$ (at the bottom part of the glass substrate)

Where U_1 = displacement in x-direction, U_2 = displacement in y-direction and U_3 = displacement in z-direction.

The temperature is imposed as field in the numerical model in various steps for heating/cooling analysis.

Assembling and mesh generation Here the individual parts such as SiO_x, Au, Ti and glass have their own co-ordinate systems. By using assembly module, part instances are created to position the instances relative to each other in a global co-ordinate system.

We meshed the model using isoparametric hexahedral elements (C3D8R, 8-noded with reduced integration), where the simulation entails the calculations of the results at each node. In meshing module, we follow two basic operations such as, first seeding the edges of the part instance, and then mesh the part instance. The numbers of seeds are chosen based on the desired element size or the number of elements we want along an edge. The size of the mesh determines the accuracy of the result on the one hand and the computation time on the other hand. Smaller elements result in a higher accuracy of the calculations, but increases the computation time. Hence, a sufficient mesh has to be defined in order to do accurate calculations.

Finite element meshing By doing fine meshing at the notch tip, we want more accurate result. In other way, we can say this is a mesh convergent test for observing same stress value even if we increase the number of mesh elements after a certain number. Here we are using around 439400 numbers of elements to the whole model (Fig. S.3). And more numbers of elements with smaller shape and size are used at the notched bridge location. We have used hexahedral elements in entire model while doing simulation by ABAQUS finite element package.

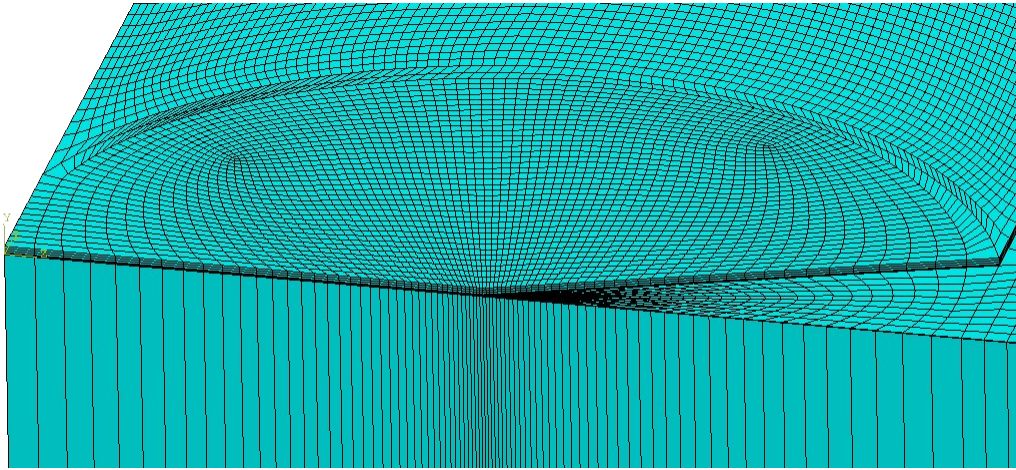


Fig. S.3 The meshing of all layers Au/Ti/Glass by applying local seeding in each components and then meshing throughout the whole model having elements of hexahedral shape.

A hemicircle region at the notch tip location of electrode bridge was considered for meshing using very small mesh elements. So we obtain a decreasing size of elements towards notch tip and thus more elements at the notch feature area. This process of modeling gives more accurate results, as most of the stress concentrate at the notch tip which is tensile in nature and gradually decreases towards inner side from notch edge.

Here we have taken sweep technique to do mesh over whole model, and in algorithm option, medial axis was selected which help in minimize the mesh transition.

Stress analysis Finally, the magnitude and the distribution of stresses formed on thin film were measured from visualization module.

We have observed here the tensile and compressive stresses (as represented by the color bar) at the left top corner when opened in the visualization module of ABAQUS. The sign convention for tensile and compressive stresses are +ve and -ve, respectively. We have selected the node points on top surface of SiO_x layer at the edge going across the electrode bridge starting from the notched point. The normal stresses σ_{11} and σ_{33} were noted at these selected node points as a function of temperature (either cooling or heating) and the computed stress was then compared with the critical stress of fracture. Finally, the thermal stress at which temperature the SiO_x film fractures was noticed from computational data. The value shows a reasonable match with experiment.