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Failure characterization of nodular defects in multi-layer dielectric coatings

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ABSTRACT

Nodular defects in multi-layer dielectric coatings have been computer modeled to characterize the electro-mechanical responses to laser pulses with wavelengths of $1.06\text{ }\mu\text{m}$ and pulse lengths between 1 and 20 ns. The simulation begins with an axisymmetric electric field model using AMOS^[1,2], a full-wave Maxwell solver with lossy (dispersive) electric and magnetic material models. Electric fields calculated by this code determine the spatial distribution of absorbed laser energy in the vicinity of the nodule. This data is linked to a thermal/stress model and mechanical calculations are executed using the general purpose finite element code COSMOS/M.^[3] The simulation estimates the transient temperature response of the nodule and the surrounding medium and predicts the dynamic stresses caused by the thermal impulse. This integrated computer process has been exercised to characterize failure of nodules as a function of defect characteristics, including seed size and depth.

1. INTRODUCTION

Nodular defects in $\text{SiO}_2/\text{HfO}_2$ multi-layer, high-reflectivity coatings have been identified as critical elements in determining laser damage thresholds. Scanning electron micrographs made by Tench et al.^[4] have indicated that micron-sized seeds of HfO_2 can be spattered onto the mirror surface during the electron beam vaporization process. This forms a discontinuity in the coating stack that disrupts the electric field distribution, resulting in localized electric field enhancements in the vicinity of the nodule.^[5] For laser pulses between 1 and 20 ns this results in significant joule heating of the localized region. Since the materials involved are dielectric the heat absorption is not primarily at the surface of the defect seed as it would be for a metal inclusion. Instead more complex distributions develop which can cause multiple intensity peaks both in and around the seed. Since we seek to understand failure of the coating we must calculate the stresses that are developed by the rapid expansion of material caused by the thermal impulse. This requires coupling the time dependent temperature profile with a structural model capable of simulating the dynamic displacements and stresses. In this paper we report on initial results of computer modeling that simulate this complex interaction of electric field, temperature and stress responses of idealized nodular defects. The overall goal is to develop a tool that will enable us to better understand coating failure mechanisms and extrapolate results to other coating designs and laser exposure conditions.

MASTER

2. MODELING TECHNIQUE

The nodule geometry that was used in all of the analyses is shown in Fig. 1. The coating is assumed to be a 23-layer, quarter-wave stack of HfO_2 and SiO_2 and contains a seed that is idealized as an HfO_2 sphere located below the surface of the coating stack. The size of the seed and depth below the surface were treated as variables with values ranging from 0.25 - 1.5 μm and 1.0 - 3.0 μm , respectively. The shape of the nodule is defined as the shape of the discontinuity in the coating caused by the seed and follows the relationship $D = (8 \cdot T \cdot d)^{0.5}$, where D = diameter of the nodule caused by a seed of diameter d located at a depth T below the surface of the coating.^[6]

Figure 1. Idealized model of a nodular defect.

We have employed two computer codes, AMOS and COSMOS/M, to simulate the coupled electro-mechanical responses. AMOS is a full-wave Maxwell solver with lossy (dispersive) electric and magnetic material models which will calculate the electric field distribution in a coating with arbitrary geometry and material properties. COSMOS/M is a general purpose finite element code capable of simulating the mechanical response of two-dimensional axisymmetric or full 3-dimensional structures. For our problem, the COSMOS/M model calculates both the temperatures and stresses caused by a temporally varying heat deposition that is spatially non-uniform. Inertial effects caused by the rapid expansion of material and the relative densities and stiffness of the seed and coating layers are simulated.

The complete AMOS computer model, shown in Fig. 2, simulates the nodular defect and the coating layers over an area much larger than just the nodule. This was done to prevent spurious boundary effects from contaminating the data in the region around the defect. The simulation is axisymmetric (cylindrical

coordinates) and uses a regular grid of 200,000 cells which is used to represent the geometry in Fig. 2. All 23 dielectric layers are modeled as well as the vacuum above the outermost silica layer. The partial differential equation solver used to analyze the electro-magnetic field structure employs a finite integration approach which is second order accurate in time and space. Essentially, in this approach the Maxwell equations (integral form) are directly integrated yielding a full wave solution. Improvements to this technique are embodied in discrete surface integration techniques^[7] which work both on arbitrary as well as regular meshes.

Figure 2. AMOS computer model.

The COSMOS/M computer model is shown in Fig. 3. It is also an axisymmetric simulation consisting of 1680 elements and 1767 nodes. Each of the 23 dielectric layers are modeled as well as part, but not all, of the BK7 substrate. The volume of material modeled is much greater than the size of the nodule so as to minimize the spurious effects of pressure waves reflecting off of the artificial boundaries of the model and distorting the stresses in the vicinity of the seed. The density of nodes and elements in the region of the seed is much higher than the surrounding area to improve accuracy in the area of interest.

Figure 3. COSMOS/M computer model.

The analysis technique that we employed is a four step process shown in Fig. 4. The AMOS model is first executed to determine the spatial distribution of electric field within the nodule. This result is then transformed into the heat generation terms required by COSMOS/M. To do this a transformation code has been written which receives the element description and electric field information from AMOS, squares the electric field values and then multiplies these values by the loss tangent of the appropriate material to obtain the energy loss for each element in the model. It then takes model geometry information from COSMOS/M and transforms the AMOS energy loss data to heat generation values for each COSMOS/M element. With these heat generation terms the COSMOS/M model is run to determine the transient temperature profile. Subsequently, temperatures are transferred to the COSMOS/M structural model where the transient stresses are finally calculated.

Figure 4. Integration of AMOS and COSMOS/M computer models.

Within COSMOS/M the heat generation terms are multiplied by a time-dependent function to simulate the temporal profile of the laser pulse. Square pulses were considered with three different pulse lengths, 1, 5 and 10 ns. In addition, we also considered a temporally varying pulse, Fig. 5, to exercise the capability of the technique to simulate a more complex input function. In all cases the amplitude of each time curve was adjusted so that the total energy deposited was the same. This enables a valid relative comparison of the temperatures and stresses between laser pulses with different pulse lengths.

3. RESULTS

Figure 6 shows a gray scale contour plot of the electric field for a nodule with a seed diameter of $0.73 \mu\text{m}$ and a seed depth of $1.97 \mu\text{m}$. Multiple, high-intensity peaks caused by the superposition of the reflected electric field waves in the vicinity of the seed are generated along the axis of the model for the normal incidence models studied. For this particular geometry four peaks are generated, one near the center of the seed and three others located both above and below the seed. This data is highlighted in the lineout of the electric field data passing through the central axis of the nodule, Fig. 6. The E-field has been squared and

multiplied by the loss tangent to obtain a plot proportional to the energy absorption. Each peak has a width of about $0.4 \mu\text{m}$ or less. The degree to which thermal diffusion will effect the peak temperature is dependent on the width of these spikes; diffusion will be more important at smaller widths.

Figure 5. Temporally varying laser pulse.

Figure 6. Electric field enhancement around a HfO_2 nodular defect:
seed diameter = $0.73 \mu\text{m}$, seed depth = $1.97 \mu\text{m}$

The temperature profile corresponding to this electric field distribution at time 5 ns after the start of the pulse is shown in Fig. 7. Four discrete peaks are still dominant although diffusion has smeared the profile and eliminated each of the closely spaced double peaks. To quantitatively see the effects of diffusion we plot the temporal response of several nodes in the model in Fig. 7. The results have been normalized so that the temperature rise at the center of the seed is equal to 1. If there is no diffusion then the seed's adiabatic temperature rise is easily calculated knowing the heat absorption and the heat capacitance of the seed. We calculate that the peak temperature rise would be about 20% greater if this were the case. The effect of diffusion is depicted in the graph as the linear temperature rise peaking at a value of 1.2.

Figure 7. Spatial and temporal temperature profiles of a HfO_2 nodular defect: seed diameter = $0.73 \mu\text{m}$, seed depth = $1.97 \mu\text{m}$, time = 5 ns.

Figure 8. Dependency on maximum temperature rise of seed depth and diameter.

Figure 9. Exaggerated deformations in the nodule 5 ns after start of the laser pulse.

Figure 10. Thermally induced stresses in the region of the nodular defect.

Figure 11. Dependence of maximum temperature rise and maximum tensile stress on pulse length.

The localized hot spots will cause affected regions to expand rapidly resulting in areas of high compressive stress surrounded by thin layers of tensile stress. Failure will occur when these tensile stresses exceed the fracture strength of the material. In the deformed shape plot of Fig. 9 we see in exaggerated detail the expanded areas corresponding to the four temperature peaks of Fig. 7. This expansion, however, is complicated by the fact that HfO_2 has a thermal expansion coefficient and a modulus of elasticity which is much greater than SiO_2 . As a result, we see the HfO_2 coating layers expanding and pinching the SiO_2 layers which are located in between. The resulting stress contours, Fig. 10, depict the complex stress distribution that results. The highest tensile stresses are located around the seed and at the surface of the nodule along the model centerline. Fracture of the nodule would be initiated at either of these two locations.

The dependency of both maximum temperature rise and maximum tensile stress on pulse length has also been quantified, Fig. 11. Temperature rise, as expected, is larger for shorter laser pulse lengths because heat does not have as much time to dissipate during energy deposition. This sensitivity, however, does not vary significantly for all of the seed size and depth cases considered. The dependence can be approximated by $t^{-0.2}$, where t = pulse length. Maximum stress follows a much stronger dependence, about $t^{-0.4}$. Dynamic inertial effects and relative stiffness of the materials involved account for this significant difference.

Also shown in Fig. 11 is the maximum temperature rise and tensile stress calculated for the time varying laser pulse defined in Fig. 5. Seed diameter and depth for this calculation were 0.73 and 1.97 μm , respectively. For this particular geometry the nodule responds to the pulse as if the pulse was temporally flat with the same total energy and a pulse length of about 8 ns.

4. CONCLUSIONS

An integrated analytical technique has been established that simulates the combined electro-mechanical response of a nodular defect in a multi-layer dielectric coating stack. Analyses have been performed for

square laser pulses of 1, 3, 5 and 10 ns and for a laser pulse that varies as a function of time. Preliminary results which are based on specific geometries with varying seed diameters and seed depths support the following conclusions:

- 1) An axisymmetric nodular defect causes significant electric field enhancements along its centerline. Peak field intensities may or may not occur in the seed depending upon the size of the seed and the distance of the seed from the surface of the coating. The width of the peaks and their location are important factors in determining the temperature rise of the heated material.
- 2) The maximum temperature rise and maximum tensile stress in a nodule exposed to a square laser pulse have a different dependence on pulse length, t :
maximum temperature rise is proportional to $t^{0.2}$
maximum tensile stress is proportional to $t^{0.4}$.
- 3) Nodules that are shallow and have a seed size of about 1 μm will develop the highest temperatures and stresses. Seed sizes less than 0.25 μm have reduced electric field enhancements and lower temperatures. Eliminating seeds in nodules greater than this size would significantly improve the capability of the defect to resist laser damage.
- 4) The analytical technique that has been assembled is proving to be a powerful method for studying the electro/mechanical behavior of nodular defects. Future analyses will be directed towards studying the sensitivity of the results to material properties and other system variables.

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