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Utilizing OOF2 Software to simulate Silicon Nitride Thermal Residual Stress

Abstract

In this simulated experiment, OOF2 Finite Element Analysis software will be used to assess residual thermal stress from a micrograph of Silicon Nitride (Si3N4). This will further enable the understanding of the microstructural behavior of this compound. Si3N4 is known for having a high strength and fracture toughness at high temperatures. As a result, it is a material often used for structural components in hot temperature environments like automotive engines [1]. Today, this type of experimentation would require Si3N4 samples to have a means for a controlled high temperature to be applied on it. In this approach, there is much time and resources that have to go into making the overall experiment. By using this simulated approach, we will be able to eliminate much of these requirements and enable the establishment of conclusions without the use of heavy-duty experimentation. Industry research product developers would be interested in this simulated approach because it allows them to drastically cut down the time and resources that would be needed to choose materials for a product. Thus, success in the planned experiment would promote the usage of OOF2 to simulate microstructures of all materials under question in the development of products. The risk in this, however, is that OOF2 can only give a relative measurement between the micrographs due to the lack of units generated by OOF2 simulation. While simulation using this software can cut down research time by narrowing materials that should further be tested, OOF2 simulation does not completely eliminate the need for experimental assessment. I believe that the total simulation time should take 3-4 hours while data analysis should take around 5 hours. Success in this documented experiment will be defined by produced data that correctly explains why silicon nitride is a material well suited for high temperature environments.

Introduction

The assessment of the effects of thermal residual stress of materials is important especially when the material is subject to large temperatures. Thermal residual stress occurs when the application of heat energy on a material causes expansion at different rates further producing stress within the microstructure of the material due to varying thermal expansion coefficients as well as the geometry during a period of heating. For materials that are repeatedly subject to large amounts of heat energy and required to maintain some kind of structural integrity, it is common to see a specimen that experiences little expansion that will corresponded to large amount of residual stress inside the system. In addition, the software that will be utilized is OOF2 which uses the method of finite element analysis to break down the separate problems in the system that is simulated. Utilizing boundary conditional differential equations, the overall system of a sample of Si3N4 being heated on one side can be assessed for its produced thermal residual stresses.

Methods

In order to perform this experiment, an OOF2 simulation has to be set up. First off, a micrograph is required for the sample of Si_3N_4 which was obtained through a study done by Andrew C.E. Reid [2] and is given in the figure 1 below:

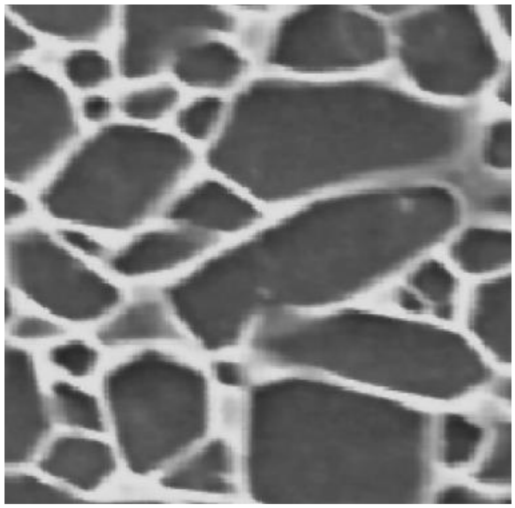

Figure 1. Initial Image of Si_3N_4 micrograph. The black boundaries indicate the crystalline structure of Si_3N_4 while the white boundaries indicate amorphous structure.

From this initial figure, in order to help with the pixel differentiation that is required for the simulation a Material Map was made creating a more color contrasted image between the two regions of amorphous and crystalline. This was done by utilizing texture maps and isolating the different regions to a specific color of pixel to avoid ambiguity. Fortunately, this step was also refined by Andrew C.E Reid [2] and so that image is utilized to minimize error in the running of the experiment. The modified image is given in Figure 2 below:

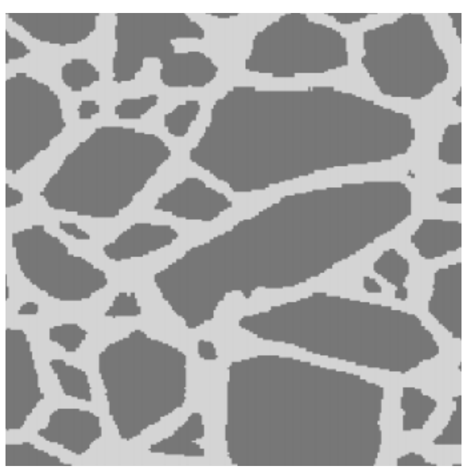

Figure 2. Modified and pixelated image given by Andrew C.E Reid.

While this configuration was beneficial in helping the software determine boundaries, it is important to note that the pixelization of the phase boundaries acquire an error due to the unnatural jagged edges shown in figure 3 below.

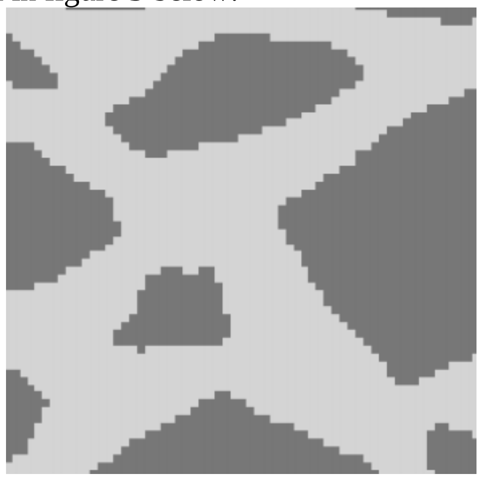

Figure 3. Zoomed in image of modified micrograph indicating jagged edges.

Uploading this image into the OOF2 software, the pixel groups were first established in the software to separate the two phases of amorphous and crystal. Next, the material properties were specified for Si3N4 and applied throughout the body. The material properties used are indicated in Table 1 below.

Table 1. Built material properties specified in the OOF2 software [3]

Young's Modulus (GPa)	297
Poisson's Ratio, v	0.28
Thermal Conductivity, κ (W/m°C)	43
Thermal Expansion Coeff., α @ T0=25°C (C-1)	3.7*10-6

Next a skeleton is formed over the micrograph. The number of x-elements is specified as 50 while the number of y-elements are specified as 11. Next a series of procedures are done given by "annealment", "swap edges", and "smooth". This is done in order to help the phase boundaries given in the skeleton lie within the different phase boundaries. In addition to this, a mesh needs to be generated and specified in the software prior to specifying the equations as well as boundary conditions. Through the use of the boundary conditions, we set a direct source of heat energy to come from the right side of the sample in order to test it for formed residual stress after heating period. The heat source will have a temperature of 500 °C which is done by setting that as that value as the right boundary condition.

Results

The produced images below show the created contour plots from the OOF2 software for temperature gradient, displacement and thermal residual stress along with their corresponding color key.

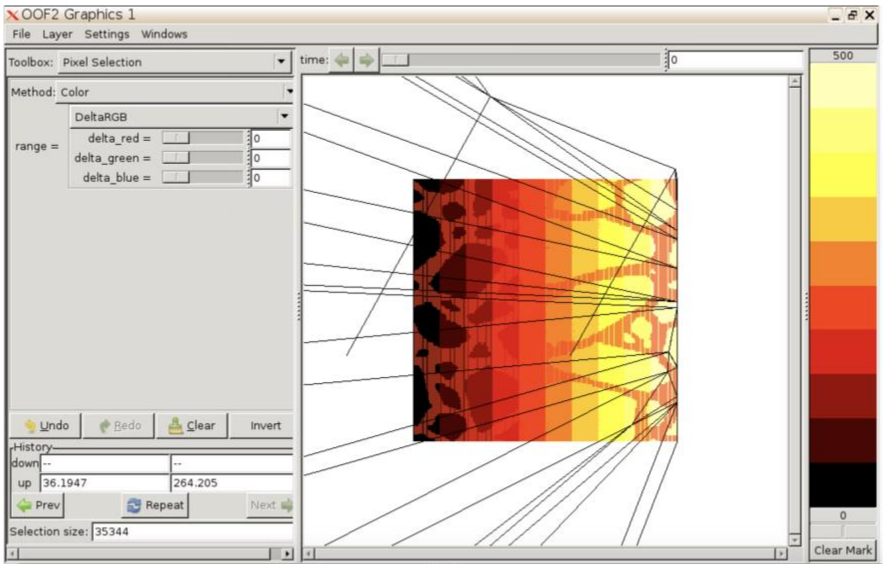

Figure 4. Contour plot for Temperature. This image looks rather uniform since the material properties were extended throughout the entire body.

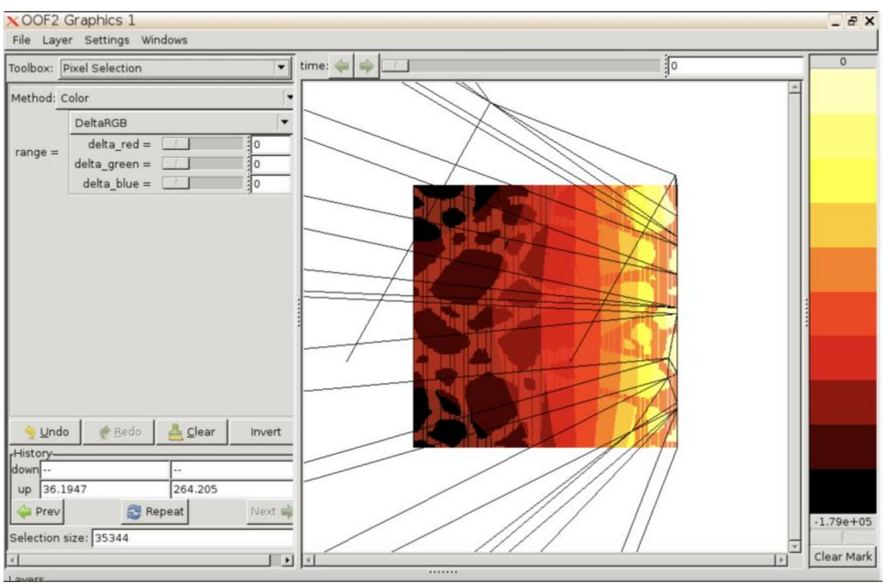

Figure 5. Contour plot for displacement. There does not seem to have large amounts of displacement due to the scale (-1.79E05, 0). Note that the negative is due to the heat being applied onto the right side

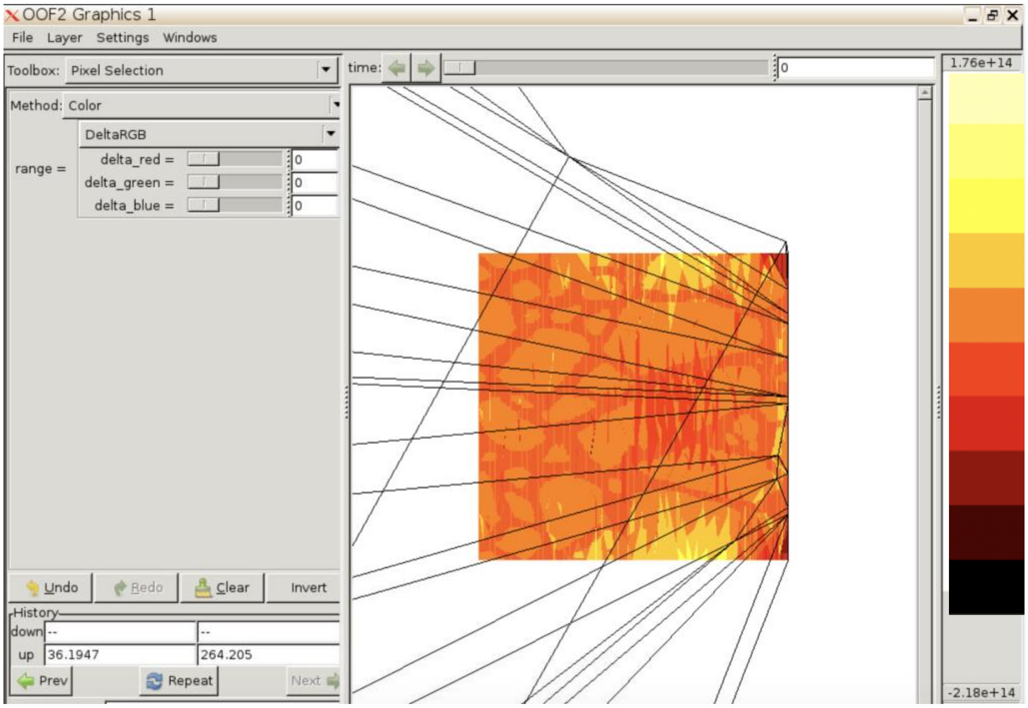

Figure 6. Contour plot of thermal residual stress plot. The plot looks jagged and the most stress seems to be in the top and bottom corner indicated by the yellow.

After assessing all three of these plots it looks as though the run simulation was not as effective as was thought. Although the minimal movement in displacement supported the use of Silicon Nitride in high temperature environments since we expect the Si3N4 to have little movement as it is a ceramic, the residual stress plot makes little sense. This would further indicate an unsuccessful experiment and emphasizes the reason why experimental testing is still important.

Conclusion

Based on the produced displacement contour plot of the specimen with a right boundary condition of 500°C the data seemed to validate the reason why Silicon Nitride has high fracture toughness and strength. However, in the production of the thermal residual plot the noise in the plot would indicate an error in parameter initialization. One of these can be attributed to the overall assignment of material properties to the system. This short coming came from the inability to find ground truth metrics for the specific microstructure (amorphous, crystalline) material specifications – only the material. As such a uniform assignment of these material properties – further highlighted by the uniform temperature plot – caused a massive error in the initialization of the experiment. In addition to this, more time could be used trying to fit the skeletons within the phase boundaries. After dedicating time trying different skeletal initializations one that fit within the phase boundaries of the amorphous and crystalline regions was hard to achieve. As a result, the experiment was not necessarily successful, but highlighted some of the important factors to pay attention to when trying to build an effective simulation.

Bibliography

[1]- "Silicon Nitride: Fine Ceramics (Advanced Ceramics): KYOCERA," *KYOCERA GROUP GLOBAL SITE*. [Online]. Available: https://global.kyocera.com/prdct/fc/list/material/silicon_nitride/silicon_nitride.html. [Accessed: 17-Dec-2020].

[2]- A. C. E. Reid, "Modelling Microstructures with OOF2," *Research Gate*. [Online]. Available: https://tsapps.nist.gov/publication/get_pdf.cfm?pub_id=51176. [Accessed: 16-Dec-2020].

[3]- F. Y. F. I. Technologies, F. ZwickRoell, F. M. Panalytical, F. Ducom, F. B. W. Tek, F. S.-G. Seals, and F. M. K. Technology, "Properties: Silicon Nitride (Si3N4) Properties and Applications," *AZoM.com*, 02-Dec-2020. [Online]. Available: https://www.azom.com/properties.aspx?ArticleID=53. [Accessed: 17-Dec-2020].