COMSOL® Simulation of Flash Lamp Annealed Multilayers for Solid State Electrolyte Fabrication

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INTRODUCTION: Flash lamp annealing (FLA) is a modern annealing technique in the range of milliseconds, which is predestinated for roll-to-roll fabrication of battery electrodes. However, the existing methods for a direct temperature measurement, like pyrometry for FLA, are unable to detect background radiation of the intense flash light, emissivity and the shadow effect. COMSOL Multiphysics® is used in order to model thermal cycling of FLA and the temperature distribution through $Si/SiO_2/Al_2O_3$ layers. Furthermore, since on a time scale of only a few milliseconds heat dissipation is dominated by heat conduction towards the substrate, two sample holder of FLA of both steel and quartz are investigated.

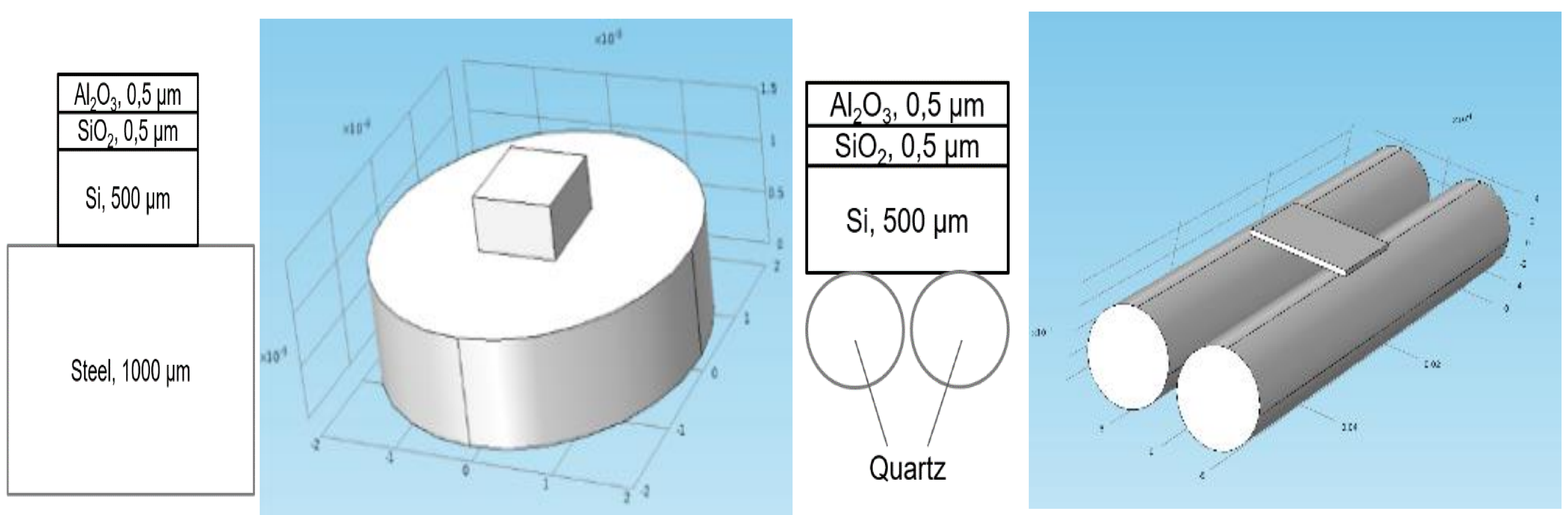

Figure 1. Two configurations of FLA sample holder using steel and quartz rods

COMPUTATIONAL METHODS: Computational Methods: FEM was utilized using the COMSOL Multiphysics® code. The Heat Transfer with Surface-To-Surface Radiation interface contains the heat transfer in solid (eq.1) and irradiative flux of the external source (eq.2) as well as a diffuse surface boundary including on the radiation process (eq.3):

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p u \cdot \nabla T + \nabla(-\kappa \nabla T) = Q \quad (1)$$

$$G_{ext} = F_{ext}(x_s) \cdot P_s \quad x_s = (0,0,d_z = 10cm) \quad (2)$$

$$e_b(T) = n^2 \cdot \sigma \cdot T^4 \quad (3)$$

Mesh: For the modeling physics-controlled meshing and adaptive mesh refinement were used. The top thin layer was finer meshed by sweeping perpendicular to the sweep direction.

RESULTS: FLA lamps are capable to generate pulse durations between 0.5 and 20 ms. The spectral energy of the lamps is ranged between 400 – 800 nm. Both the 1.27 ms pulse and spectrum of Xe-lamps were experimental measured and implemented in the model.

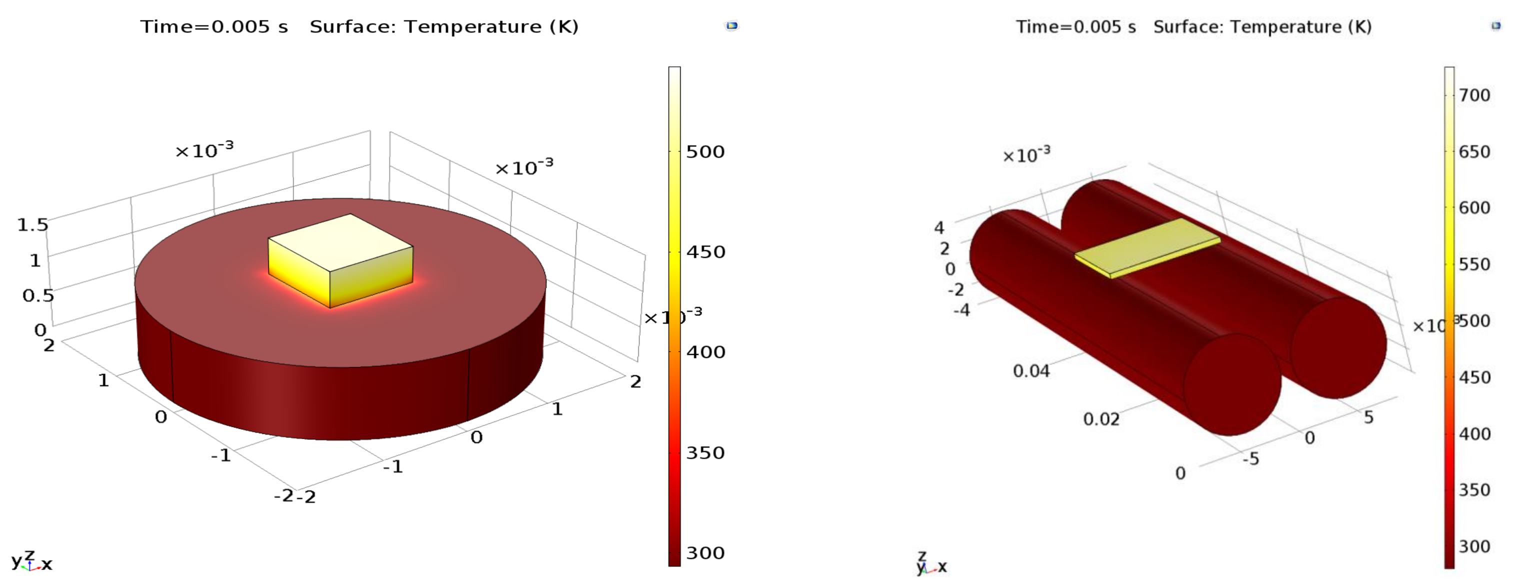

Figure 2. Temperature distribution of the surface using steel and quartz holder at 0.005s flash pulse. The emissivity ε of Al_2O_3 is set to 0.2

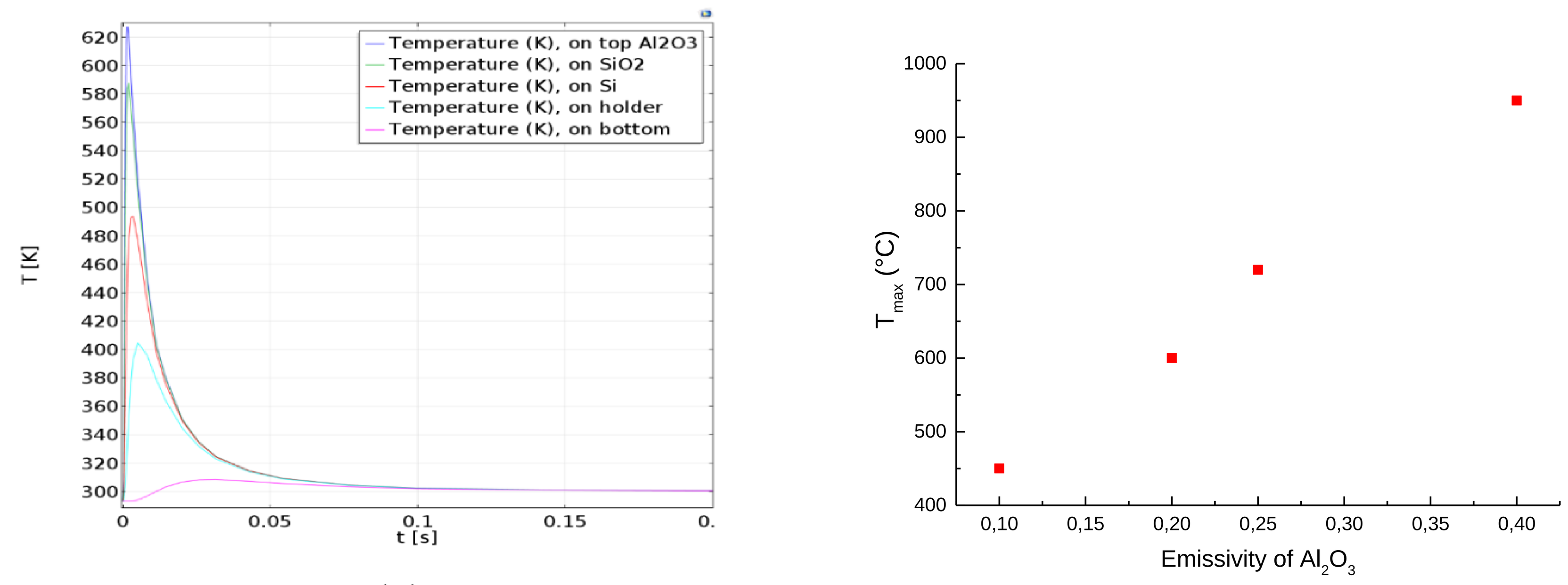

Figure 3. (left) $T(t)$ simulation on layer stacks after FLA treatment using a steel holder and (right) maximum temperature on the top of Al_2O_3 as function of the emissivity ε

- No accurate data for emissivity of Al_2O_3 in literature. The found values vary between 0.1 and 0.4
- The value of ε implemented influences strongly the maximum temperature on the top of Al_2O_3 layer.
- T maxima are comparable for both FLA setup using steel and quartz holder
- $T(t)$ decreases very slowly using quartz holder

CONCLUSIONS: COMSOL® was used to simulate temperature distribution on $Si/SiO_2/Al_2O_3$ using FLA treatment. It was shown how different parameter, e.g. the surfaces emissivity or the both geometries influence the heat distribution. However, the strongest effect which causes the shifting towards lower or higher temperatures is the surface emissivity.

Acknowledgments

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