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Reducing the Thermal Effects during Coating of SRF Cavities: A Case Study for Atomic Layer Deposition of Alumina with a Combined Numerical and Experimental Approach

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Coating the inner surface of superconducting radio frequency (SRF) cavities is one of the approaches to push ultimate limits in next generation accelerators. One of the potential coating techniques for such intricate and large volume structures is atomic layer deposition (ALD), as it offers full and uniform layer coverage. In order to predict the process parameters for coating SRF cavities on the large substrates with ALD, we simulate the ALD of alumina (Al_2O_3) using the ANSYS Fluent 19.1 commercial package by solving vapor transport and chemistry equations. The computational domain in the numerical model is based on the homemade ALD setup for thin film sample chamber and a 1.3 GHz Tesla-shaped niobium cavity. Trimethylaluminum (TMA) and water (H_2O) were used as precursors. In the simulation process for the cavity, two steps were carried out: first, the simulation of precursor distribution, followed by the simulation of surface reactions. The simulations show that saturation is achieved with precursor pulses of only 50 ms after 1.05 s for TMA and 750 ms for H_2O , obviating the necessity for prolonged exposure times. Furthermore, the resulting predicted growth per cycle of these process times of $\approx 1.22 \text{ \AA}$ for Al_2O_3 was experimentally validated, affirming the credibility of our simulations. Experimental findings also showcased a remarkable 66.2% reduction in process time while upholding film homogeneity and quality. Our approach presented here carries profound importance, particularly for coating intricate and large volume structures, like SRF cavities, and provides another approach to minimize time- and resource-intensive parameter scans. The methodology is also transferable to other coating materials and volumes.

Presenter: DEYU, Getnet Kacha

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