# Plasma-Assisted Molecular Beam Epitaxy and Electronic Transports in a SrTiO<sub>3</sub>-Based Heterostructure

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## **Abstract:**

*In-situ* electrical measurements were performed for an oxide heterojunction unstable to the atmosphere. The molecular beam epitaxy (MBE) method was utilized and assisted with oxygen plasma to deposit barium oxide (BaO) films on an atomically smooth strontium titanate (STO) single-crystal substrates. XRD analysis confirmed the formation of epitaxial barium oxide films on the STO. After the depositions, the samples were stored in a glovebox connected to the MBE chamber and fixed in a compact microprobe system. This allowed the electrical measurements to be conducted without exposure to air, and metallic conduction was observed at the BaO/STO interface, indicating an STO-based 2-dimensional electron gas.

## **Summary of Research:**

**Background.** Two-Dimensional Electron Gas (2DEG) in oxide heterojunctions have been triggered by discoveries of strontium titanate (STO)-based 2DEGs. Examples of STO-based 2DEGs include lanthanum aluminate, gamma-alumina, and LSAT, all of which are formed using pulsed laser deposition (PLD) [1]. Recently, barium oxide (BaO) on STO junction was reported as a new 2DEG. One advantage of that this system has a very low lattice mismatch of -0.3%, which can be expected to make a highly crystalline interface, that can exhibit strong electrical properties [2].

Molecular beam epitaxy (MBE) is a method conducted in an ultra-high vacuum environment, keeping the samples clean and contaminant-free. MBE also enables atomic-level control in layer-by-layer growth with compositional control with better than  $\sim 1\%$  accuracy. Therefore, MBE was selected for our experiments to grow BaO films.

**Goals of Project.** The main goal of this project is to observe intrinsic electron transports in the BaO/STO junctions. A challenge though is that BaO is reactive to water vapor in the

atmosphere and therefore must be protected, either in a glove box or with a capping layer. The glove box allowed us to observe metallic conductive properties, while semiconducting properties were observed with a capping layer.

**Experimental Conditions.** The selected substrate used in all experiments was the STO <100> crystal with a selected growth temperature of 600°C. The oxygen partial pressure was kept at  $2.5 \times 10^{-3}$  Pa and beam equivalent pressure (BEP) measurements were used to select the barium temperature of 570°C. We also did post-deposition annealing in vacuum for 1-2 hours.

Characterization methods used include X-ray diffraction (XRD), atomic force microscope (AFM), profilometry (thickness measurements), and resistivity and Hall effect measurements.

# **Results and Discussion:**

The first step was to treat the STO substrates so they were ready for thin-film deposition. As seen in Figure 1, AFM scans showed that as supplied, STO was a rough surface. After annealing in a furnace at 1050°C, AFM scans showed that the terracing straightened out, resulting in a much flatter surface, which is more suitable for a film to form.

Next, we deposited the barium and oxygen on the substrate, which only takes minutes, or even seconds if you want a 3 nm thin film. After deposition, the film is annealed in vacuum, without oxygen. Annealing in this environment causes an oxygen deficiency in the barium oxide layer, creating the basis for an electron transfer by the oxygen movement from the STO to the BaO, creating electrical conductivity, as seen in Figure 2. Figure 3 shows an XRD scan obtained from the BaO film on the STO substrate, where it is clearly seen that the BaO is c-axis oriented without any side products.



*Figure 1: AFMs of the STO substrates before and after annealing in a furnace, the terracing straightened out, resulting in an atomically flat surface.* 



Figure 3: The XRD analysis showing the elements in STO (peaks labeled with \*), and the peaks showing the formation of BaO. No side products were discovered in the film.



*Figure 2: A schematic that shows how conductivity and electron transfer are possible.* 



Figure 4: Resistivity measurements of the BaO/ STO interface with and without a capping layer. As seen, without the capping layer, there is conductivity consistent with metallic conducting despite both STO and BaO being insulating materials on their own.

Lastly, we conducted electrical measurements. Without the capping layer, we were able to prove that conductivity exists at the interface as the resistivity pattern is consistent with metallic conductors. However, with a  $\text{TiO}_2$  capping layer, the resistivity was consistent with insulating materials, as seen in Figure 4. This shows the validity of our measurement system to observe electrical properties without interference.

#### **Conclusions and Future Steps:**

While barium oxide films were successfully deposited on atomically flat  $SrTiO_3 < 100>$  substrates at 600°C using molecular beam epitaxy, the electrical properties observed were not constant. Resistivity displays a clear temperature-dependent pattern, but the capping layer interfered with the conducting. Future steps include improving the stability of the conductive qualities, as well as experimenting to find a capping layer that does not interfere with the electrical properties of the BaO/STO interface.

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