## Institute for Plasma Research

Title:	Study of Plasma Oxidation of Copper Substrates
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Venue:	Committee 4, IPR

## Abstract

The rising population and increasing energy demands are pressing issues that require urgent action. Currently, we rely heavily on carbon-based fuels to meet our basic energy needs. However, these fuels generate substantial amounts of CO<sub>2</sub>, contributing significantly to environmental challenges. Capturing and converting excess CO<sub>2</sub> into useful fuels has therefore become a key research focus. To make this transformation feasible, catalysts are essential to overcome thermal and kinetic barriers. A variety of catalytic materials, including Fe<sub>2</sub>O<sub>3</sub>, NiO, CeO<sub>2</sub>, MgO, CuO, zeolites, and activated carbon doped with Zn<sup>2+</sup>, Fe<sup>2+</sup>, and MgO, have been explored for this purpose<sub>1</sub>. Among these, CuO has demonstrated the highest efficiency in capturing CO<sub>2</sub> compared to other absorbent materials<sub>1</sub>. CuO can be synthesized through several methods, with thermal oxidation being a commonly used and well-studied approach. However, producing a single-phase CuO via thermal oxidation typically requires high temperatures (~500 K) and therefore consumes more energy. Plasma oxidation offers a promising alternative, enabling CuO formation at room temperatures (required in thermal oxidation) and chemically reactive environments (as in electrooxidation)<sup>2</sup>. Additionally, plasma treatment can enhance catalytic activity by increasing surface-to-volume ratios, inducing defects, promoting grain boundary formation, and exposing active crystal planes<sub>3</sub> etc.

This study focuses on the oxidation of copper (Cu) using cold plasma at room temperature in air and oxygen environments under sub-atmospheric pressure. Raman spectroscopy confirms the formation of the CuO phase while the presence of Cu<sub>2</sub>O phase can't be neglected. Surface morphology analysis via SEM corroborates the formation of mixed copper oxides. To further understand the oxidation process, we conducted simulations using density functional theory. The results suggest that the Cu (111) surface is the most stable; however, the (100) surface oxidizes more readily at low temperatures<sup>4</sup>. Therefore, we examined the oxidation behaviour of both the (100) and (111) surfaces through simulations. Additional findings show that oxygen atoms have a stronger bonding affinity to the Cu surface than oxygen molecules. In summary, this research primarily targets the formation of CuO at room temperatures using cold plasma. Future work will focus on achieving a pure CuO phase at low temperatures and simulating the interaction between the Cu surface and plasma. This may include high end XPS analysis and other advanced characterization techniques to corroborate the results.

## References:

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