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PLASMA PROCESSING UPDATE

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<u>RESEARCH ARTICLE</u>

Antibacterial copper oxide coating on polypropylene fabric using magnetron sputtering



Team members

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Polypropylene (PP) is widely utilized in the textile industry for various applications, including single-use fabric bags, biomedical gloves and tapes, sanitary products, melt-blown fabrics, and masks, owing to its lightweight nature, durability, and recyclability. Many biomedical applications of PP necessitate the presence of antibacterial properties on its surface. Previous research indicates that copper and its oxides (CuO) exhibit enhanced antibacterial activity when applied to surfaces. In this work, coatings of copper and its oxides have been deposited on polypropylene (PP) fabrics through magnetron sputtering, with variations in oxygen partial pressures to facilitate the formation of copper oxides. The presence of these oxides has been verified through surface morphology analysis using Scanning Electron Microscopy (SEM) and X-Ray Diffraction (XRD). Additionally, the antibacterial efficacy of the coated fabrics has been investigated. The antibacterial results shows that both copper and copper oxides perform well with 4 log reduction of gram-positive bacteria.



Figure 1: Images of coated and un-coated fabric

UC- PP: Uncoated polypropylene, **CPP**: Copper coated polypropylene. **COPP5**: Copper oxide at 5 % oxygen partial pressure, **COPP20**: Copper oxide at 20 % oxygen partial pressure, **COPP30**: copper oxide at 30 % oxygen partial pressure

The images of coated fabrics at different oxygen partial pressure are presented in Figure 1, along with their corresponding terminologies for identification. The appearance of the coating surfaces is influenced by the partial pressure of oxygen, which may result from the varying amounts of oxide formation. Figure 2 illustrates the X-ray diffraction (XRD) and scanning electron microscopy (SEM) results for polypropylene (PP) coated with copper and copper oxide. The copper-coated polypropylene (CPP) fabric exhibits prominent peaks corresponding to copper, alongside minor peaks for Cu₂O, CuO, and Cu₄O₃. High-magnification SEM images of CPP and copper oxide, obtained under different oxygen partial pressures (COPP5, COPP20, and COPP30), reveal that variations in oxygen incorporation affect the morphology of the coatings. In contrast to the coated fabrics, the uncoated fabric appears very smooth. The CPP fabric displays uniform clusters of copper crystallites, resembling the structure of the COPP5 fabric.



Figure 2: (A) XRD peaks and (B) SEM Images of coated and un-coated fabric

Three types of fabrics—uncoated, copper-coated, and copper oxide-coated (COPP20)—have been chosen for the AATCC-100 test, which assesses the contact killing mechanism and provides quantitative data. Among these fabrics, COPP20, which consists solely of oxide phases, has been compared to CPP and UC-PP in terms of antibacterial effectiveness. The number of colonies formed on each fabric type for both gram-positive bacteria (Staphylococcus aureus) and gram-negative bacteria (Klebsiella pneumoniae) is illustrated in Figure 3. The quantified CFU results indicate that the uncoated fabric (UC-PP) supports a higher growth of bacterial colonies after 24 hours of contact. In contrast, the coated fabrics (CPP and COPP20) demonstrate a significant reduction in colony formation.



Figure 3: Antibacterial efficacy by AATCC-100 method for (a) CPP (b) COPP20 and (c) UC-PP

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<u>RESEARCH ARTICLE</u>

Reactive Molecular Dynamics simulation of the carbendazim degradation induced by reactive oxygen plasma species



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Many In contemporary agriculture, pesticides are extensively utilized to boost the productivity, leaving residues in water, soil, and food items. These residues pose health hazards as they accumulate in organisms, prompting concerns regarding food safety. Carbendazim (CBZ), a systemic benzimidazole carbamate fungicide, used in agriculture, forestry, and veterinary practices to combat fungal diseases, is notably classified as a hazardous chemical by the World Health Organization. Cold Atmospheric Plasmas (CAPs) have demonstrated successful pesticide degradation with notable removal rates, energy efficiency, and eco-friendly attributes. Limited by experimental parameters and equipment availability, scientists are hypothesizing about reaction pathways, which remain elusive. However, through Reactive Molecular Dynamics (RMD) simulations [1], researchers can now predict breaking and formation of chemical bonds that occur during interactions. In this article, we employed RMD simulations to investigate how reactive oxygen species (ROS) such as O atom, OH radical, and O₃ molecule

induce degradation pathways in CBZ. CBZ is classified within the Benz imidazole family, specifically as 2-aminobenzimidazole, where the primary amino group is replaced by a methoxycarbonyl group and the chemical structure of Carbendazim is shown in figure 1.



Figure 1: Chemical structure of Carbendazim

After simulation, the primary reaction pathways were identified. During the reaction process of ROS with the methoxycarbonyl group, four potential interaction mechanisms (labeled as R₁, R₂, R₃, and R₄) have been identified, as depicted in **Fig. 2**. Due to the presence of electron rich methyl group, the first reaction is H-abstraction reaction from the $-CH_3$ which results in unstable



Figure 2: Different reaction pathways obtained at the methoxycarbonyl group of CBZ

structure that triggers four different reaction pathways.

The reaction R_1 can be observed with OH radicals and O₃ molecules, while R_2 , R_3 and R_4 can occur with O atoms and O₃ molecules. The disruption of the methoxycarbonyl group always leads to a reduction in toxicity. Several experiments on CBZ degradation [2-4] and simulation by density functional theory [5] have demonstrated this conclusion.

The dose effect was explored by varying the number of ROS within the simulation box,

representing different dosages used in practical applications. As a result, the likelihood of chemical bond formation and breakage will fluctuate with the quantity of ROS delivered, necessitating careful consideration. The primary focus of the reactions is on the dissociation of C-H bonds and the formation of C-O and C=O bonds. The changes in bond breakage and formation for CBZ during the oxidation processes are presented and compared under identical conditions. Our simulation results indicate that as the concentration of ROS increases, there is a corresponding rise in Habstraction and C-O bond formation. Furthermore, we observe that different types of ROS exhibit varying efficiencies at the same density level.

Our simulation results show that OH, O, O₃ lead to the destruction of the toxic methoxycarbonyl group through processes like hydrogen abstraction/dehydrogenation, oxidation, decarbonization, and decarboxylation reactions, resulting in the formation of small molecules such as CO₂. The destruction of this key structure suggests a reduction in CBZ activity. The elucidated chemical pathways and statistical data provide insights into the atomic-scale degradation mechanism of CBZ, offering a



Figure 3: Dose Effect

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<u>VIP VISITS</u>

Visit by Chairman, AEC

Secretary of the Department of Atomic Energy (DAE), Chairman of the Atomic Energy Commission (AEC), and Chairman of IPR Governing Council **Dr. Ajit Kumar Mohanty**, visited IPR on 24/02/2025. On the same day, it was also scheduled to visit FCIPT campus of the institute. At FCIPT, he took stock of progress of the 5 TPD Plasma Pyrolysis system which would be ultimately installed at Varanasi. He has interacted with the pyrolysis and team and also with the FCIPT staff. A few pictures of his visit are presented below. He was accompanied by Director, IPR; Project Director, ITER-India; Dean (Administration); and Dean(R&D) of IPR.



VIP VISITS

IPR Director's Visit

Dr. Dinesh Kumar Aswal, the new officiating Director of Institute for Plasma Research, joined the institute on 1st January 2025. Apart from this additional responsibility, he is a senior member of Trombay Council (TC) - the APEX decision making body at Bhabha Atomic Research Center (BARC), and also holds other several key positions. On the same day of assuming office at Institute for Plasma Research, the Director has visited the FCIPT campus of the Institute and interacted with the staff there. A few pictures of his visit are presented below.



<u>ONE DAY SEMINAR</u>

One day seminar on Surface Modification using Plasma Technologies (SMPT-2025)

As a part of ongoing efforts for commercialising plasma based technologies, Institute for Plasma Research and 'AIC-IPR Plasmatech Innovation Foundation', in association with Gujarat Chamber of Commerce & Industries (GCCI) have organised one day seminar titled "Surface Modification using Plasma Technologies (SMPT-2025)" on 4th February,2025 at FCIPT campus of IPR, Gandhinagar. Objective of the seminar was to give a platform to researchers and industries for showcasing their activities & results in the field of surface modification using plasma based technologies. Various interesting topics were covered in this seminar including Plasma nitriding, Plasma carburizing, Plasma assisted physical & chemical vapour deposition, Nano textured surfaces for super hydrophobicity, Plasma surface modification of textiles & polymers, and Plasma surface modification for agricultural applications etc.

The seminar was inaugurated by the Chief Guest Shri. R. D. Barhatt, Joint Commissioner of Industries, Government of Gujarat, and the guest of honour was Shri. Rajeshbhai Gandhi, Senior Vice-President, GCCI. In the inaugural session, the guests were felicitated by Dr. S. Mukherjee, Dean Admin, IPR and Dr. Paritosh Chaudhuri, Dean R&D, IPR. In the seminar, two sessions focussed on plasma surface modification for various applications, while an additional session has covered the funding opportunities for startups, AIC-IPR and Incubation at AIC-IPR etc.

There were around 60 participants from industries, universities, research institutes etc. took part in this event. There were total twelve invited talks presented during the seminar. After the technical sessions, a panel discussion was organised during which delegates representing industries, academic institutes, start ups had actively interacted with the audience and gave valuable feedback and suggestions.

Lab visit was also organised for all the delegates after the panel discussion.

A few pictures of the event are shown below.



Inaugural Session



Panel Discussion & Lab Visit



<u>STUDENTS"/PDF NEWS</u>

THESIS DEFENCE

Mr. Sagar Agrawal gave his Ph.D. thesis defence talk on 06/01/2025, titled "Study of Process Parameters affecting Secondary Phase Formation and Grain Size in Cu₂ZnSnS₄ Thin Film for Solar Cell Application". Congratulations Dr. Sagar.



Participation in International Conference

Ms. Tarundeep Kaur gave an oral presentation title "Sequential deposition of Ag NPs on rippled Si pattern for SERS application" in the *13th International Conference on Photonics, Optics and Laser Technology, at Portugal*, from 22-24 February 2025.



STUDENTS"/PDF NEWS

BEST POSTER AWARD

IPR postdoc, **Dr. Sebine Augustine**, working with Dr. Mukesh Ranjan got the first prize in poster presentation titled "Self-organized ordered nanoparticles for SERS application" in the workshop on "Photonics for Energy, Sensing, and Education"; organised by IIT Gandhinagar, during 16-17 January 2025. Dr. Sebine earlier completed his Ph.D. from IPR as DGFS fellow.



<u>OTHER NEWS</u>

DAE PLATINUM JUBILEE NATIONAL SCIENCE DAY AT IPR

DAE platinum Jubilee National Science Day was celebrated in Institute for Plasma Research (Institute for Plasma Research), during 15-16 February 2025. On this occasion, many events were organised by IPR. Around fifty schools from various parts of Gujarat have presented scientific models prepared by them. This year, the primary focus of the models was on Smarts cities, Agrotech, pollution control, woman safety, AI, Robotics etc.



A TALK ON CSR FUNDS FOR RESEARCH

Mr. Manuj Tripathi (Principal Scientist at CSIR- IMTECH) gave a talk on "Advancing R&D through Corporate Social Responsibility (CSR)", at FCIPT on 05/02/25. Talk was organised by Dr. Mukesh Ranjan (Nodal Officer CSR funds, IPR) and Dr. Nirav Jamnapara (Head, AIC PlasmaTech Innovation Foundation). Talk was focused on the underutilisation of CSR funds in India's research & development (R&D) ecosystem. The talk enhanced the knowledge of CSR landscape in context of R&D, CSR project proposals, funding cycle, and carve out a path to learn from some of the best practices across the organisations.



OTHER NEWS

SWACHATA PAKHWADA

Under Swachhata Pakhwada 2025, a 'swachhata pledge' ceremony has been organized on 17.02.2025 at FCIPT campus also. It was followed by a Plog-a-thon (cleanliness walkathon with plogging) was also organised.



OTHER NEWS

SAFETY WEEK - Demonstration of 'Using fire extinguishers'

As a part of 54th National Safety Week campaign, demonstration of using fire extinguishers was organised at FCIPT campus also on 07.03.2025. A few pictures are shown below.



OTHER NEWS

WOMEN'S DAY CELEBRATIONS

As a part of week long women's day celebrations, women staff of house-keeping personnel were felicitated, at FCIPT campus also on 07.03.2025. Their efforts were appreciated by presenting them with small gifts.



TALKS DELIVERED / POSTER PRESENTATIONS

TALKS DELIVERED

- 1. Dr. Mukesh Ranjan gave an invited talk on "Detection of Hazardous Molecules with Dense nanoparticles arrays" at the *Indo-UK Workshop on Photonics for Energy, Sensing, and Education* organised by IIT-Gandhinagar during 16-17 January 2025.
- 2. Dr. Mukesh Ranjan gave an invited talk on "Plasma surface engineering for sensing and wettability applications" at *One day seminar on Surface modification using Plasma Technologies (SMPT-2025)* on 04/02/2025 at FCIPT, IPR, Gandhinagar, India.
- 3. Dr. Ramkrishna Rane gave an invited talk on "Surface modification using plasma enhanced PVD/CVD coatings" at *One day seminar on Surface modification using Plasma Technologies* (*SMPT-2025*) on 04/02/2025 at FCIPT, IPR, Gandhinagar, India.
- Dr. Mukesh Ranjan gave an invited talk on "Ar plasma Nanostructuring on PTFE surfaces for the self-cleaning and sensing application in Food, Agriculture and Medical Science" at the *International workshop on Cold Plasma Technology and Applications (CPTA-2025)* at BIT MESHRA campus, Jaipur during 6-8 February 2025.
- 5. Dr. Ramkrishna Rane gave an invited talk on "Dielectric Barrier Discharge Plasma and its Biomedical Applications" at the International Workshop on Cold Plasma Technology and Applications (CPTA-2025) at BIT MESHRA campus, Jaipur during 6-8 February 2025.
- As a part of National Science Day celebrations, Dr. Mukesh Ranjan delivered invited talks on "Harnessing Plasma for Societal Applications" and "Surface Enhanced Raman Scattering for health and medical science" at IIIT-Vadodara, Gandhinagar campus; and Gandhinagar Science college respectively.



PUBLICATIONS

RESEARCH / TECHNICAL REPORTS

- Electrochemical Corrosion Investigation of Plasma Nitrided Ti-6Al-4VAlloy in Different Simulated Solution Pravin Dwivedi, Ramkrishna Rane, Ghanshyam Jhala, Chinmay Ghoroi, Alphonsa Joseph IPR/RR-1716/2025
- Microstructure and Thickness Dependent Steam Oxidation of TiN Coating Developed on Zircaloy-4 using Cylindrical Magnetron Sputtering Kunal Trivedi, Ramkrishna Rane, M. Kiran Kumar, Tarundeep Kaur Lamba, Alphonsa Joseph, Supratik Roychowdhury IPR/RR-1719/2025

JOURNAL PAPERS

- Viliya, Kundan, Uttam Sharma, Manisha Thakur, Kadur Narayan Guruprasad, Jayshree Sharma, Ramkrishna Rane, Amulya Sanyasi, and Joydeep Ghosh. "Enhancement of Maize (Zea mays var: GS-2) Plant Growth and Yield: Seed Treatment with Non-thermal Plasma using Different Gases."
- Viliya, K., U. Sharma, Manisha Thakur, Kn Guruprasad, Jayshree Sharma, R. Rane, A. Sanyasi, And J. Ghosh. "Enhancement Of Soybean (Glycine Max Var. Js-9560) Growth And Yield After Pre-Sowing Treatment Of Seeds Using Non-Thermal Plasma Of Different Gases." *Romanian Journal of Biophysics* 34, no. 4 (2024).
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- Kaur, Gagandeep, Puneet Negi, Ruhit Jyoti Konwar, Hemaunt Kumar, Nisha Devi, M. Ranjan, K. P. Sooraj et al. "Exploring the role of nitrogen doping in tuning the band gap and electrical properties of sol–gel synthesized anatase titanium dioxide nanoparticles." *Optical Materials* 162 (2025): 116851.
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