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Atmospheric pressure plasma surface functionalization of polystyrene[1] JORDYN POLITO, Univ. of Michigan, MARK DENNING, RICHARD STEWART, DAVID FROST, Agilent Technologies, MARK J. KUSHNER, Univ. of Michigan — Atmospheric pressure plasmas (APPs) sustained in air are used to functionalize commodity polymers for packaging and printing. Functionalizing polymers such as polystyrene (PS) for higher value applications in biotechnology often instead use rare-gas plasma jets seeded with oxygen. Plasma treatment creates alkyl radicals by abstraction of H from the polymer by O or OH (from impurities or air-mixing). O or O_2 then fixes to the polymer to form alkoxy and peroxy sites, increasing hydrophilicity and wettability. Subsequent reactions produce a mix of hydroperoxy, alcohol and acid groups. Correlating plasma conditions with desired functionality would help in process design. We report on results from a computational investigation of surface functionalization of PS using APP jets sustained in Ar/O_2 and He/O_2 flowing into ambient air. GlobalKin, a global-plasma chemistry model, simulated RF excited plasmas exiting into room air onto PS a few mm from the jet nozzle, and then exposing the PS to ambient air. A surface site balance model addresses plasma-surface and surface-surface reactions leading to functionalization. Results for coverage of O-containing groups on the PS as a function of power, gas flow rate, distance of the PS from the nozzle and post-plasma air exposure will be discussed. Results from the model will be compared to experimental trends for water contact angle as a measure of oxygen content.

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Mark Kushner
Univ of Michigan - Ann Arbor

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