

ABSTRACT

Marrafino, Francesco, *Application of Artificial Neural Networks to the design and optimization of superhydrophobic coatings*, Ph.D. program in Drug Discovery and Development, 2021, University of Salerno.

Recently, considerable attention has been devoted to developing superhydrophobic surfaces due to their advantageous antimicrobial and self-cleaning properties. While significant effort has been devoted to their fabrication, very few polymeric superhydrophobic surfaces can be considered durable against externally imposed stresses. This work focuses on developing a coating with strong superhydrophobic properties and abrasion resistance, using a simple and scalable preparation process. Pyrogenic hydrophobic silica nanoparticles were used to confer superhydrophobic properties to the coatings. 450 samples were prepared using a layer-by-layer approach, depositing an epoxy resin or PDMS layer as adhesive on a substrate (PC/ABS), followed by one or more layers of silica nanoparticles or silica-resin mixed layers. The coating with the best properties shows a contact angle of 157° and a tape peeling grade resistance. The developed preparation method involves the spray deposition of a multilayer coating composed of four layers. Layers 1-3 are 1) silica nanoparticles, 2) epoxy resin, and 3) silica nanoparticles, followed by partial curing of the coating (15 minutes, 70°C); another silica layer is then sprayed on the surface and is cured for 10 minutes. In the second part of the work, the focus shifts to optimizing the coating and preparation process using Artificial Neural Networks. Given the high number of parameters involved, process optimization is a complex operation. Artificial Neural Networks are the best tool to deal with multivariate analysis problems. For this reason, data from all the prepared samples were collected into a dataset used to train a neural network capable of predicting the degree of hydrophobicity and abrasion resistance of a silica nanoparticles-based coating. The algorithms were used to prepare an optimized coating with a contact angle $>160^\circ$ and a high degree of abrasion resistance, currently under patent evaluation for potential application in antibacterial surfaces.

Finally, the application of Artificial Neural Networks to develop two bioinformatics predictive tools will be very briefly discussed.

KEYWORDS: Superhydrophobic, Artificial Neural Network, Antimicrobial, Antifouling, Self-cleaning, Surfaces.