Synthesis, computational studies and characterization of polydiphenylamine nanocomposite with embedded silver nanoparticles

I. V. Brazhnyk[1], Yu. P. Vyshnevska[2], S. A. Kudrya[1], D V. Rumiantsev[2]
[1]Institute for Renewable Energy, Kiev, Ukraine, e-mail: vishnevsk@mail.ru
[2]National Technical University of Ukraine "Kiev Polytechnic Institute", Kiev, Ukraine

A promising research area is the development of methods for obtaining hybrid materials and nanocomposites which are based on the introduction of the nanoscale objects into the polymeric matrix. Of particular interest are thin films of conducting polymers with incorporated palladium or silver nanoparticles, as well as bimetallic core–shell objects. At the same time obtaining of such materials with desired functional properties requires the precise control over the polymers conductivity and the coating morphology. In present study, hybrid polymeric PDPA–Ag coatings were obtained via *in situ* oxidizing polymerization of diphenylamine involving Fe^{3+} cations as catalyst in stationary conditions directly on substrate. Synthesis of silver nanoparticles was performed as given in [1] and adapted by Steve Ng and Chris Johnson:

$$Ag^{+} + BH_4^{-} + 3\ H_2O \rightarrow Ag^{0} + B(OH)_3 + 3.5\ H_2$$

PDPA and PDPA–Ag coatings characterization was carried out using SEM, AFM and FTIR methods. Quantum-chemical calculations were performed on MP2 level of theory with the cc-pVTZ basis set using the NWChem 6.5 computational chemistry package [2].

It was found, that the introduction of silver nanoparticles suspension during formation of polydiphenylamine film leads to a marked decrease in polymerization rate that can be caused by the suppression of the iron catalyst redox system. Morphology of PDPA–Ag coating (Figure *b)* has irregular domain structure compared to pure PDPA. It should also be noted that the presence of silver NPs has a significant influence on the PDPA–Ag nanocomposite conductivity due to electron delocalization during the redistribution of electron density or the interfacial electronic interaction. According to the performed simulations, obtained materials can show better stability and improved electrocatalytic performance. *In situ* synthesis of hybrid polymeric materials provides rich capabilities to control the deposition process and provides fine tuning the characteristics of functional coatings that is essential for fuel cell applications.

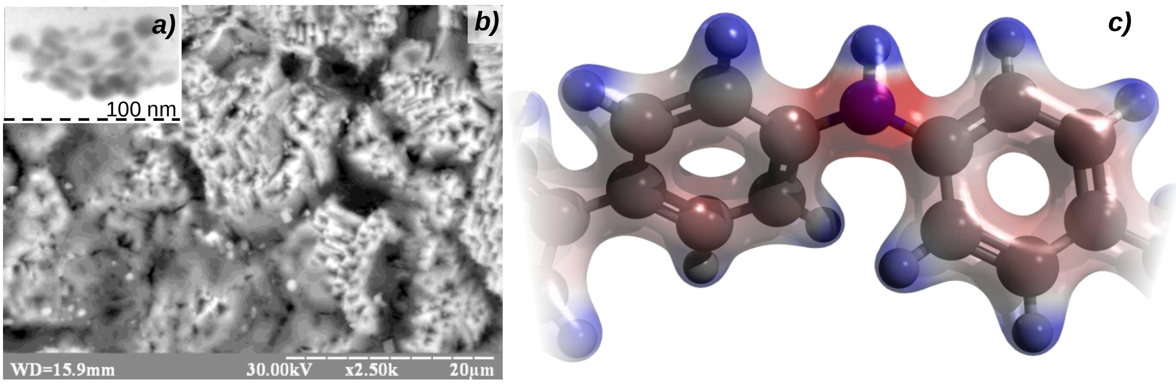

Fig. TEM image of silver NPs (*a*), SEM image of PDPA–Ag coating (*b*) and PDPA electron density distribution (*c*)

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References

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