MODELLING OF ELECTROPHORETIC DEPOSITION (EPD) OF SOFT PARTICLES AND EXPERIMENTAL VERIFICATION.

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Evaluating the EPD process by model predictions is a key factor in the development and optimization of this colloidal technique to reduce costs and production time. Among every theoretical models, in 2017, B. Giera et al. developed a molecular dynamics method in which the particles interactions are simulated, to provide previously inaccessible information about colloidal packing within empirically relevant EPD systems. In this work, a new parameter was included to make the model fit the use of stabilizers and predict their effect during deposition. We consider the nanoparticles surface modifications by the adsorption of additives, which it is well know that influences the electrophoretic mobility and nanoparticles assembly at the deposit.

The use of organic additives (such as surfactants or polyelectrolytes) is a regular strategy to preserve suspension stability in colloidal processing. In particular, in EPD, the employment of polyethyleneimine (PEI) with different molecular weights (MW) affects colloidal motion within the suspension and particle packing degree at the electrode, since an electro-steric barrier occurs.

This soft layer of PEI could overlap when nanoparticles approach, and depending of the length (MW) and conformation of the electrolyte, the suspension acquires different stabilization levels. The new potential included into the theoretical model assumes an applied force that is pushing apart the particles due to the steric interaction of the polymer brush. Thus, “soft” pairwise interaction potentials, varying from neutral to entirely repulsive forces, were simulated to study the polymer brush interactions between the PEI layers attached onto suspended particles.
We have estimated EPD-model predictions of deposition, morphology and microstructure of the deposit using a series of simulations in which electric field and the soft pairwise interaction energy was systematically varied. Finally, the theoretical simulations were compared with experimental analysis in order to verify the theoretical results, where experimental analyses were developed with nanoparticles of different nature.