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Multiscale modelling of the sintering process of printed nano-ink

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In recent years plastronic technologies have expressed needs for new economical, more-accessible and innovative ways to integrate electronic components in injection-molded plastic parts. The present work is dedicated to one particular technology called printed electronics; it is based on the selective laser sintering of printed metallic nanoparticle ink.

Numerical modelling is a must in order to investigate the adhesion of the metallic circuit on the plastic substrate while maintaining its integrity during the selective laser sintering process. Herein, multiscale thermal modelling is proposed to predict temperature evolution and distribution through both the deposit and the plastic substrate.

The multiscale approach combines two uncoupled models. First, a local model (Figure 1a) is used to characterize the effective thermal properties of nanoparticle charged ink by means of homogenisation. A finite element model of a representative volume element is used to model a number of silver particles embedded in ink. A thermal gradient is imposed to the domain through periodic boundary conditions and the effective thermal conductivity of the medium is computed. The level-set and the X-FEM methods enable solving the heat conduction equation without explicitly representing the particle-ink interface. A mesh adaptation step is performed beforehand in order to optimize the mesh size and hence increase the computational efficiency. Multiple runs with varying material properties and particle volume fraction help establish a new analytical mixture rule to predict effective thermal conductivity of nanoparticle ink.

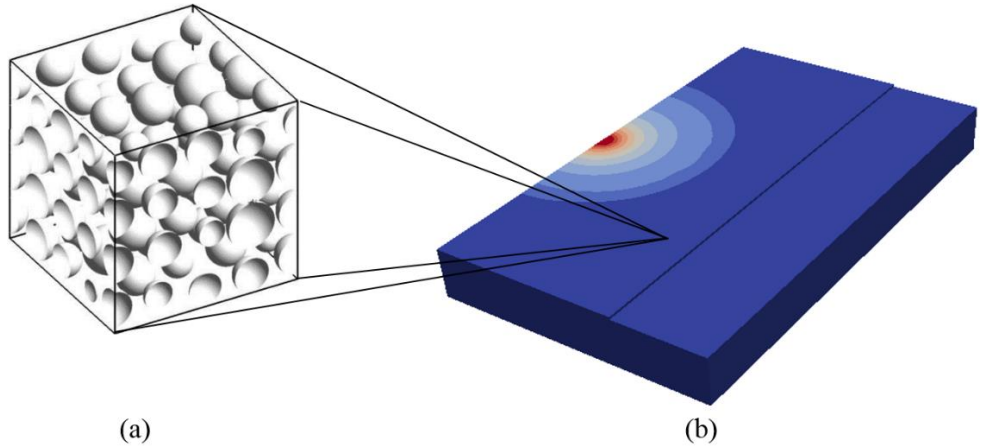

Figure 1 : (a) local model for the prediction of the effective properties of the nano-ink; (b) global model for the sintering simulation

Then this mixture rule is utilized within the so-called “global model” (Figure 1b), which simulates the sintering of the printed material. In this model, the metallic track is represented as a homogeneous material whose properties depend on the nanoparticle volume fraction. The vaporisation of the ink is also accounted for, which results in an evolution of the material properties during the process. The laser is modelled owing to a Beer-Lambert heat source, for which the optical properties of the nano-ink are measured experimentally. The purpose of the simulation is to determine the operational parameters, such as laser power and speed, which optimize the cost efficiency of the process, while ensuring an adequate electrical conduction of the sintered material and preserving the integrity of the flexible plastic substrate. Sensitivity analyses highlight the material parameters which have a prominent effect on the predictions, as well as the process parameters which can be tuned to optimize the process.