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Laser pyrolysis : a method of interest for the controlled synthesis of amorphous or crystalline Si@C nanoparticles - application as anode materials in Li-Ion batteries

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In Lithium Ion Batteries, the replacement of graphite (372 mAh.g^{-1}) as anode active materials by higher specific capacity materials is a strategy to answer the continuous demand for increased energy storage. Silicon appears as an attractive material thanks to its high theoretical specific capacity (3579 mAh.g^{-1}). Use of silicon based anodes has not yet been realized because performances degrade rapidly. Silicon nanostructuration together with association of carbon enhances performances. In particular, core-shell silicon-carbon Si@C nanoparticles are attractive candidates to increase the capacity of Li-ion batteries while mitigating the detrimental effects of volume expansion upon lithiation processes.

Such nanoparticles were synthesized in a single step by a continuous gas phase method, the laser pyrolysis, interesting for industrial production. We report here how flow simulations helped in the design of a reactor where decomposition of silane and ethylene are conducted in two successive reaction zones. This reactor could work in stable conditions for several hours leading to the single-step synthesis of amorphous or crystalline silicon nanoparticles coated with a carbon shell (a-Si@C). The advantages of the a-Si@C material is emphasized by comparison with c-Si@C material. In particular, cyclic voltammetry demonstrates that a-Si@C composite reaches maximal lithiation during the first sweep, which is attributed to the amorphous core. After 500 charge/discharge cycles, it retains a capacity of 1250 mAh.g^{-1} (C/5 rate) and 800 mAh.g^{-1} (2C), with a 99.95% coulombic efficiency Moreover, post-mortem observations show an electrode expansion of less than 20% in volume with preserved nanostructuration.