

# Carbon encapsulation of elemental particles for energy storage

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Carbon coating of metallic particles are of considerable interest in a number of contexts. One is related to the high reactivity of nanoparticles below the size of 100 nm. It is, therefore, necessary to protect or passivate them so as to prevent their reaction with air[1]. Due to this high reactivity, nanoparticles also tend to agglomerate and, in the process, tend to lose the functionality arising from their small size. For this and other similar purposes, carbon is an ideal material for encapsulation due to its high stability even at extreme conditions. The high stability of carbon both in acidic and alkaline environments, together with their high electrical conductivity, add further functionality to the carbon coating. This is particularly useful in some of the active materials used in electrochemical energy storage as they often have low electrical conductivity. Silicon anodes in Lithium-ion batteries is a well-known example where carbon encapsulation help improve the conductivity. Perhaps the most critical need for encapsulation in electrochemical energy storage is related to large volume changes that often occur during cycling[2]. This leads to particle fragmentation and to the loss of active material resulting in the capacity decay. Carbon encapsulation is not only useful to constrain this volume change, but by keeping the fragmented particles together and conductive help provide a solution to the capacity decay.

Particles can be carbon coated with a variety of methods. Although recently solution based methods became quite common, traditionally this has been achieved via gas-phase synthesis. These include such methods as carbon arc discharge, spark discharge, chemical vapor deposition and thermal plasma. Magnetic nanoparticles Fe, Ni, Co were successfully synthesized using thermal plasma where the particles were typically between 20 to 50 nm in size wrapped with several layers of graphite. Similar encapsulations were achieved for these metals using arc discharge or spark discharge processes. Since encapsulation, regardless of the method used, brings C and the element in contact with each other at high temperature, many of the elements are converted into carbides. A detailed account of the possible routes leading to encapsulation was given by Seraphin et al.[3] and Elliot et al.[4]. They mainly center on two distinct possibilities in the formation of carbon shell. One is the expulsion of carbon trapped within the metal or carbide to the surface during crystallization of the core; this is the so called inside-out growth model. The other is direct deposition of carbon shell onto the particle from external carbon source.

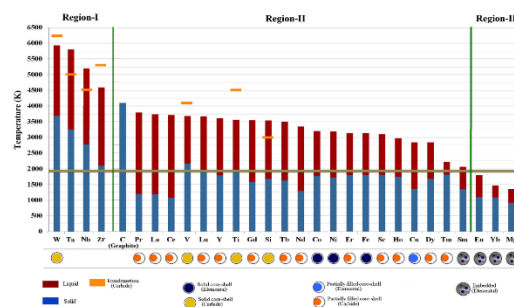


Figure 1. Three categories in the encapsulation of elemental particles [5].

The current study makes use of two methods; spark discharge and thermal plasma in obtaining carbon encapsulated nanoparticles. The study showed that elements W, V, Ti, and Si formed carbides which were encapsulated successfully by graphitic layers forming a sound core-shell structure. Copper formed a partially filled core-shell structure, attributed to its relatively low condensation temperature, where considerable shrinkage seemed to have occurred after the encapsulation. Mg could not be encapsulated in a core-shell form but rather yielded an embedded structure where Mg is condensed onto already condensed carbonaceous material. Analysis of current observations coupled with those already reported data imply a simple mechanism for encapsulation. Metals/compounds that are solid above the condensation temperature of carbon give rise to a sound core-shell structure. Elements whose condensation temperature is less than that of carbon could still produce core-shell particles but they may be partially filled. It is estimated that the process of graphitic encapsulation may be complete around 1900 K and partially filled core-shell structure might develop depending on the volume shrinkage upon cooling to room temperature. Elements/compounds whose condensation temperature is below the encapsulation temperature fail to develop core-shell structure. Instead they form embedded composite structure.

During the presentation we will concentrate on two anode materials; one is silicon within the context of Li-ion batteries and the other is Mg within the context of for NiMH batteries

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