Modelling the diffusive growth of fullerenes and carbon nanotubes

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Abstract: It has been observed that carbon atoms and clusters can be continuously incorporated into a closed fullerene cage at high temperatures, leading to an increase in the fullerene diameter and consequently leading to the formation of giant fullerenes. The metal catalyzed enlargement of fullerenes can be demonstrated by in situ high-resolution transmission electron microscopy, and the video of the growing fullerene within a carbon nanotube, initiated by a tungsten catalyst, provides a dramatic realization of a complex nanoscale process. While there may be many detailed mathematical models that may account for this growth, we first propose one of the simplest possible models that is consistent with the major observed features of the growth process. In particular, we assume that the fullerene is immersed in a carbon vapor environment, and that the growth occurs as a consequence of the diffusion of the carbon vapor into the fullerene. Moreover, we assume that the classical diffusion equation applies in the region exterior to the fullerene and that a standard Stefan condition applies at the moving fullerene surface. We assume that the gaseous medium through which the carbon atoms diffuse is represented through the value of the diffusion coefficient $D$ appearing in the classical diffusion equation. We also assume that the influence of the catalyst is felt through the value of the Stefan constant appearing in the Stefan condition. Based on these assumptions, we derive simple similarity solutions for both spherical and ellipsoidal fullerenes that are entirely consistent with the observations. An extension of the model is proposed, which also admits a simple similarity solution, involves an arbitrary power-law parameter $m$. A third approach is proposed based on the assumption that the fullerene grows in such a way that the surface density of atoms remains constant throughout the growth process, and again a similarity solution is presented, which turns out to arise from the case $m=1$. A brief analysis is noted for the longitudinal growth of a carbon nanotube.

