Theoretical Model of CNT Aerogel Formation

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The aggregation of particles in (dense) particulate systems is well studied. It has been shown that for certain conditions an aerosol can gel. To understand the gelation phenomenon it is useful to look at the kinetics of cluster aggregation which in its simplest form can be described by using the Smoluchowski Equation

$$\frac{dn_c}{dt} = -K(t)dt.$$

In this paper we present our results on adopting existing aggregation and gelation theories and modifying and changing them to describe the aggregation in CNT aerosols which eventually leads to an aerogel formed of CNTs. These findings can then for example be related to the continuous gas phase process for the bulk production of CNTs (Figure 1) that we are using in our lab, to identify important process parameters.

We will describe the aggregation in a CNT aerosol by assuming that the CNT growth takes longer than the CNT agglomeration and that agglomeration is therefore the dominant mechanism:

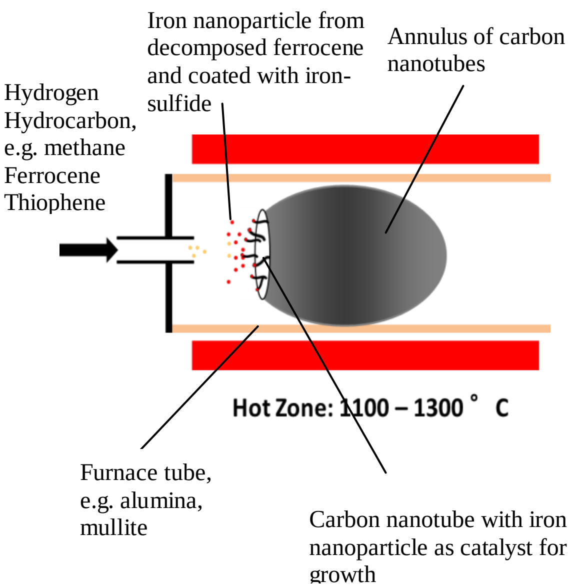

Figure 2: Very small quantities of ferrocene and thiophene are dissolved, mixed with hydrogen and then injected into a tube furnace, in which an aerogel of nanotubes forms.

$$\tau_{CNT growth} \gg \tau_{agglomeration}.$$

Parameters like a CNT diffusion coefficient, a rotational diffusion coefficient of CNTs and a CNT collision kernel will be defined. A characteristic CNT rotation time as a function of CNT length and diameter can be derived as (also see Figure 3):

$$\tau_r = \frac{\pi^3 L_{CNT}{}^4 \mu \left[\left(\frac{1}{6}+\frac{1}{8\beta^3}\right) + f\left(\frac{\pi-2}{48}+\frac{1}{8\beta}+\frac{1}{8\beta^2}+\frac{\pi-4}{8}\frac{1}{8\beta^3}\right)\right]}{kT\lambda\beta}$$

A characteristic time is defined upon which the CNTs start to form clusters and the CNT cluster – cluster aggregation becomes the dominant mechanism of growth. The cluster – cluster agglomeration is modelled until aggregation probability within the aerosol approaches unity, which is defined as the gelation of the CNT aerosol.

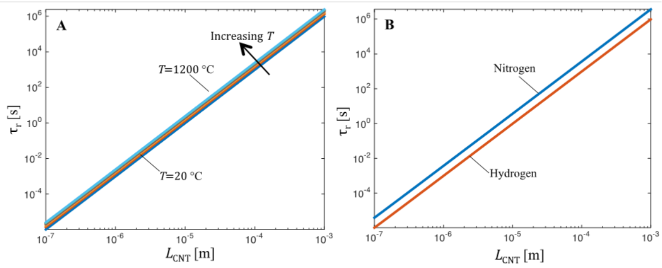

Figure 1: Characteristic CNT rotation time as a function of CNT length for A) various temperatures, with D_{CNT} = 8 nm, in nitrogen; B) nitrogen and hydrogen, with d_{CNT} = 8 nm, T = 20°C;

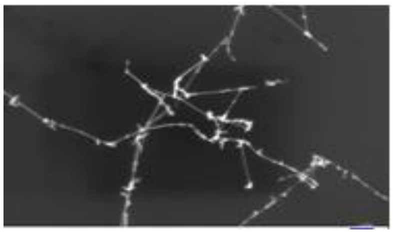

Figure 3: SEM image of a cluster of CNTs sampled from a CNT aerosol.

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