# Technical Abstract No. 4

## Is It Worth the Effort, to Put Carbon Nanotubes Into Polymers?

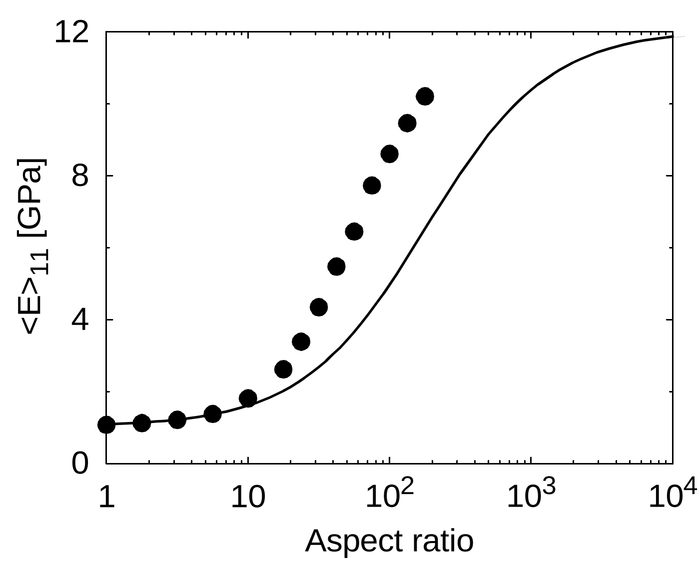
When molded into complex shapes, carbon fibers dispersed in a polymer are usually chopped during processing resulting in a maximal aspect ratio only of about 100. For the longitudinal Young's modulus $\langle E_{11} \rangle$ of short-fiber reinforced composites, the Halpin-Tsai equation states:

$$\frac{\langle E \rangle_{11}}{E_m} = \frac{1 + 2a\eta f}{1 - \eta f} \qquad \text{with} \qquad \eta = \frac{E_f / E_m - 1}{E_f / E_m + 1}$$

where $E_m$ is the matrix Young's modulus, $E_f$ is the longitudinal ($E_{11}$) modulus of the fibers, $f$ is the fiber volume fraction, and $a$ the fiber aspect ratio. For $a = 1$ and $a \rightarrow$ infinity, the Halpin-Tsai equation reproduces, within engineering accuracy, most theoretical results obtained with the "rational" composite and three-phase composite models proposed for composites of spherical inclusions or infinitely long, continuous fibers. The Halpin-Tsai equation predicts that with such chopped fibers one can realize only about a third of the maximal performance. Therefore, **it is commonly believed that one should work with carbon fibers of an aspect ratio of at least 1000 to make significantly stiff materials.** Nanotubes can have aspect ratios of 1000 and more, attracting lately much attention as potential high-aspect-ratio fillers, despite their currently absurd cost of roughly ten times the price of gold.

*Palmyra* allows to accurately assess these claims. Modeling a polymer reinforced by a random dispersion of perfectly aligned fibers (assuming the properties of a typical epoxy resin and H370 carbon fibers), one finds, as illustrated in the Figure, that up to $a = 10$, the Halpin-Tsai equation reproduces numerical results. However, at these small aspect ratios, the reinforcing effect is practically absent. Disappointingly, for moderate aspect ratios between 10 and 1000, the Halpin-Tsai equation does not render any realistic prediction. In practice, this domain of moderate fiber aspect ratios is technologically the most significant one.

Maximal reinforcement can obviously be obtained with continuous fibers ($a \rightarrow$ infinity). But the problem is to understand at which fiber aspect ratio one can realize, say, 80 % of this maximal performance. For the carbon fiber filled polymer studied, the Halpin-Tsai equation predicts this point out at $a = 800$. On the contrary, *Palmyra*'s numerical predictions are much more optimistic, indicating that at $a = 100$ one can already realize 80% of the maximal reinforcement. **It is not necessary to invest in polymer composites with costly nanotubes, if the primary aim is that of mechanical reinforcement – short carbon fibers will do the job.**




Reinforcing effect of carbon fibers in epoxy according to the Halpin-Tsai prediction (solid line) and numerical calculations by *Palmyra* (dots).

Ref: *A. A. Gusev*, Macromolecules **34**(9), 3081 (2001).