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Thermodynamic instabilities in nano-catalysts and their effects on the diameter of grown nanotubes[1]

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Fe and Fe:Mo nanoclusters are becoming the standard catalysts for growing single-walled carbon nanotubes (SWCNTs) via chemical vapor decomposition (CVD). Contrary to the Gibbs-Thomson formalism, experimental results show that reducing the size of the catalyst beyond a certain limit requires increasing the (minimum) growth temperature. This apparent paradox is addressed in terms of solubility of C in Fe nanoclusters. By using first principles calculations, an innovative thermodynamic model is constructed to determine the behavior of the phases competing for stability. As a function of particle size, there are three scenarios: steady state-, limited-, or no-growth of SWCNTs, corresponding to unaffected, reduced, and zero solubility of C in the clusters. The results are extended to Fe-Mo binary catalysts. The 15+ year long-standing question about the effects of Mo concentration on the growth capability is finally answered. Phys. Rev. Lett. **100**, 195502 (2008), Phys. Rev. B, **77**, 115450 (2008), Phys. Rev. B **75**, 205426 (2007).

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