Structural change of single-walled carbon nanotubes caused by curvature

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Electronic property of single-walled carbon nanotubes (SWNTs) has been studied using tight-binding (TB) method and local density approximation (LDA) in the framework of density-functional theory. Though we can guess the geometry of an SWNT by rolling-up a graphene sheet, it has been reported that relaxed structure of SWNTs are slightly different from that of ideal rolled graphene sheet because of the curvature effect [1]. And, the slight structural difference causes significant deviation in electronic properties [2]. Therefore, structural relaxations are essential to calculate the detailed electronical properties of SWNT.

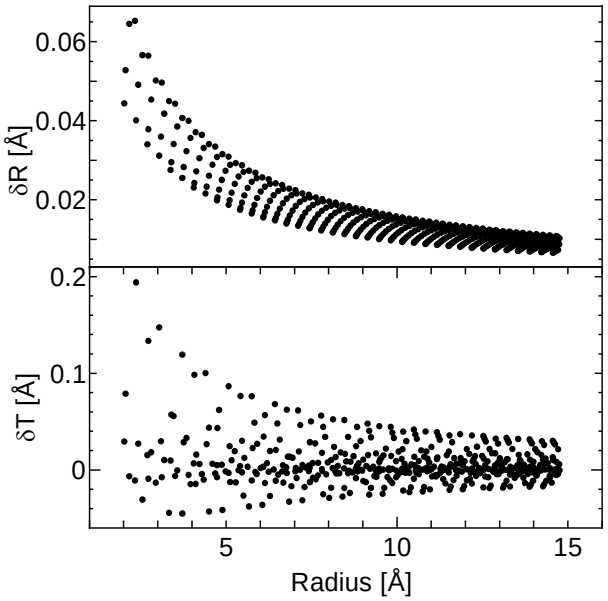

Fig 1. Structural change of the radius (R) and translation vector (T) of SWNTs as a function of R calculated with Tersoff-Brenner potential. Both are displacement from the ideally rolled-up graphene.

Structural properties of limited types of SWNTs have studied by using LDA [2-3]. Dependency of bond lengths and bond angles of some SWNTs on nanotube diameter is described [3]. However, in order to describe the structure of each (n, m) nanotube in general, 5 structural parameters must be determined for each (n, m). Here, a systematic study of structural properties, especially the dependence on chiral angle is reported.

The optimized structure for every nanotubes within diameter range of 4Å-30Å were obtained from Tersoff-Brenner potential and Hamada-TB method [4]. Furthermore, convenient correlation equations which can be used to calculate structural displacements from the ideally rolled graphene sheet are also shown.

References:

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