Growth mechanism and classification of Y-junction carbon nanotubes

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Device miniaturization in semiconductor technology is expected to reach its limits due to the inherent quantum effects as one goes toward smaller size. In such a scenario, an alternative would be nanoelecronics based on molecules. The possible use of carbon nanotubes in nanoelectronics has aroused considerable interest. For such applications it is important to be able to connect the nanotubes of different diameters and chirality. Complex three-point nanotube junctions have been proposed as the building blocks of nanoelectronics, in this regard Y- and T-junctions have been considered as prototypes. Y-junction nanotubes have been produced by using Y-shaped nanochannel alumina as templates [1], and by pyrolysis of methane over cobalt supported on magnesium oxide [2].

Molecular dynamics methods have been used for simulations of different ways of Y-junction growth. Partially, we have considered nucleation process of Y-structures with equal and unequal branches. For these purposes we have classified Y-junctions using different localization of heptagonal and octagonal defects in the graphite net of these structures with zigzag (z) or/and armchair (a) nanotube stem and branches. Thus, (aaa)-, (aza)-, (azz)-,(zzz)-,(zza)-,(zaa) – combination with different angles between branches are considered.

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[2] W.Z. Li, J.G. Wen and Z.F. Ren. Appl. Phys. Lett., (2001), **19**, 1879