탄소 나노튜브의 변형을 위한 비편재 준연속체 접근

박종연†(KAIST 원) · 김성엽*(KAIST 원) · 이영민*(KAIST 원) · 권성진*(KAIST 원) · 임세영**(KAIST)

Nonlocal quasicontinuum approach for deformations of carbon nanotubes

Jong Youn Park, Sung Youb Kim, Youngmin Lee, Sung-Jin Kwon and Seyoung Im

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Abstract : We present a coarse-graining computation for deformations of CNTs (carbon nanotubes) via nonlocal QC (quasicontinuum), particularly targeting analysis of multi-walled carbon nanotubes. Higher order triangular elements are utilized for proper interpolation of atom positions of the CNT on the basis of QC approach. The computing scheme enables one to differentiate between the fully atomistic zone and the coarse-grained zone in the framework of the multiscale computation. Several numerical examples demonstrate the effectiveness and accuracy of the present methodology.