

## Numerical investigation on the influence of defects on the buckling behavior of single- and multi-walled carbon nanotubes

### Abstract :

The effect of defects on the buckling behavior of single- and multi-walled carbon nanotubes based on the finite element method was analyzed. For this purpose, two fundamental carbon nanotubes (armchair and zigzag) were constructed in their perfect forms. Then, the buckling behavior of carbon nanotubes was evaluated by comparing their critical loads obtained from the simulation and analytical calculations. In the second phase, three most likely atomic defects, i.e., impurities (doping with Si atoms), vacant sites (carbon vacancy) and introduced perturbations of the ideal geometry in different amounts to the perfect models were simulated. Finally, the buckling behavior of imperfect carbon nanotubes was numerically evaluated and compared with the behavior of the perfect ones. In addition, simple relations were developed from the obtained results for prediction of the buckling behavior of imperfect carbon nanotubes as a function of the amount of defects. The results reveal the fact that the existence of any type of defects in the structure of carbon nanotubes leads to a lower critical load and as a result, lower buckling properties. As an outlook, curved and composite single walled carbon nanotubes were exemplarily considered as a deviation from the perfect straight form. Investigating this effect yielded that the existence of any curvature or kink in the structure of nanotubes decreases their buckling strength. This study provides a realistic prediction of buckling properties of carbon nanotubes which is of high importance in nano-industry and the production of nano-composites and reinforced materials.