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Calculating the Mechanical Properties of Carbon Nanotubes by a Modified Molecular Mechanics Approach

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Extended Abstract

Carbon nanotubes are a promising material to be used for instance in lightweight constructions. When considering applications in mechanical engineering, the knowledge of the material properties is vital in order to predict the behavior of the structure. As a result of this, and since the experimental determination of the carbon nanotubes mechanical properties is quite challenging, numerical models have been developed to compute the mechanical parameters of carbon nanotubes.

For modeling carbon nanotubes several approaches have been applied during the past years. In first instance these methods can be divided in quantum mechanics approaches and methods based on classical mechanics. The present research deals with classical mechanics. In this context, the applied approach can be further distinguished into continuum mechanical methods and discrete approaches for instance based on molecular mechanics. An enhanced molecular mechanics approach is the topic of the present research. The proposed method is based on the approach developed by Li and Chou (2003). Their model targets on the calculation of mechanical parameters of carbon nanotubes like for example the Young's modulus and the Poisson ratio. To obtain these values the model transfers the properties of the covalent bonds described by a chemical force field into properties of a mechanical truss-beam element. This is done by a detailed investigation of the possible deformation of the covalent bond followed by a comparison of the corresponding deformation energy. This allows the computation of the mechanical properties of the truss-beam element out of the chemical force constants taken from the chemical force field. A carbon nanotube is then modeled as a framework made out of these truss-beam elements. An advantage of this approach is, that the carbon nanotube is described in a discrete manner, enabling a detailed investigation of the local deformation behavior (Eberhardt and Wallmersperger (2014)), whereas continuum models describe the structure in an average sense. Furthermore, the use of truss-beam elements as representatives for the covalent bonds facilitates the use of commercial Finite-Element tools. This molecular mechanics approach provides results for the Young's modulus which are in good agreement with other numerical as well as experimental results (e.g. Tserpes and Papanikos (2006), Wu et al. (2009)). However, the computed results available in literature for the Poisson ratio vary within a substantial range. As a result of this, the present research analyses these drawbacks in the calculation which we assume to be responsible for the shortcomings of the model. Furthermore modifications are proposed to improve the model with respect to these mentioned drawbacks. To do this, we evaluate the model assumptions used to transfer the chemical force field parameters into mechanical properties of the truss-beam element. During this evaluation we calculate the internal forces and moments in order to establish a modified calculation of the truss-beam element parameters. To be more precise, our approach will account for linear internal moments occurring in the truss-beam elements, whereas the original model proposed by Li and Chou assumes constant internal moments. These considerations lead to changes in the calculation of 237-1 the mechanical parameters of the truss-beam elements. The proposed procedure follows a general strategy for the further development of the model which is also introduced in the present research. This strategy is based on the hypothesis, that the overall deformation energy of the carbon nanotube calculated on basis of the chemical force field - using local deformation quantities such as bond stretching - should be equal to the total elastic strain energy of the deformed trussbeam elements.

Concluding, in the current research a general strategy for the modification of the molecular mechanics model based on the work of Li and Chou (2003) is presented.

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