A cellular automata model for the dynamic behavior of carbon nanotubes

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Abstract

An atomic-based cellular automata algorithm (ACAA) is presented to study the buckling of carbon nanotubes (CNTs). Our ACAA simulation for the energy curve and critical strain for (8, 0) SWNT agree well with the existing molecular dynamic (MD) simulations, which verifies the application of the ACAA to study the mechanical properties of CNTs. The numerical examples shows that the proposed ACAA algorithm is as accurate as MD simulations but much faster as it is an order-N algorithm, and thus can simulate large scale problems that would take unbearable amount of time with MD simulations.

A cellular automaton is a dynamical system in which space and time are discrete. A cellular automaton consists of a regular grid of cells, and the state of a cell is determined by the previous states of a surrounding neighborhood of cells. Consider an initial equilibrium configuration of CNT which consists of a system of *N* atoms. The Tersoff-Brenner's many-body potential stored in the atomic bonds is denoted by $U(\mathbf{x})$, where $\mathbf{x} = (x_1, x_2, \cdots, x_N)^T$ is the positions of *N* atoms. Assume an external load $\overline{\mathbf{F}} = \left(\overline{F}_1, \overline{F}_2, \cdots, \overline{F}_N\right)^T$ is applied to atom *i*, thus the total energy is expressed as

$$\Pi(\mathbf{u}) = U(\mathbf{x}) - \sum_{i=1}^{N} \overline{F}_i \cdot u_i \qquad (1)$$

where $\mathbf{u} = (u_1, u_2, \cdots, u_N)^T = \mathbf{x} - \mathbf{x}^0$ is the displacement vector of all atoms, and $\mathbf{x}^0 = (x_1^0, x_2^0, \cdots, x_N^0)^T$ is the initial equilibrium position of *N* atoms.

The equilibrium configuration of the system requests the total energy is minimal, and thus we have

$$\frac{\partial \Pi(\mathbf{x})}{\partial \mathbf{x}} = 0 \qquad (2)$$

Expressing $\Pi(\mathbf{x})$ around an initial equilibrium configuration $\mathbf{x}^0$ yields

$$\mathbf{K}\,\mathbf{u} = \mathbf{P} \qquad (3)$$

where $\mathbf{K}$ is the stiffness matrix and $\mathbf{P}$ is a non-equilibrium force vector. The cellular automaton approach is adopted to solve Eq. (3). The atomic-based cellular automaton is a discrete system which consists of a hexagonal grid of cells, and each atom is taken as a cell. The cellular space is shown in Fig. 1, in which atoms are taken as cells and the grid is two-dimensional hexagon.

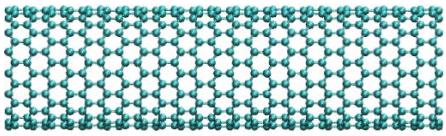

Fig. 1. Cellular space of a carbon nanotube.

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