INTERNATIONAL JOURNAL OF HYDROGEN ENERGY 41 (2016) 15747–15755

Available online at www.sciencedirect.com

ScienceDirect

journal homepage: www.elsevier.com/locate/he

Thermodynamic characteristics and bifurcation of multiwalled carbon nanotubes impacted by hydrogen atoms using Nonlocal continuum theory

Zhiwen Zhu [a], Ce Guo [a], Jia Xu [a,b,*]

[a] Department of Mechanics, Tianjin University, Tianjin 300072, China
[b] Tianjin Key Laboratory of Nonlinear Dynamics and Chaos Control, Tianjin 300072, China

ARTICLE INFO

Article history:
Received 25 March 2016
Accepted 27 April 2016
Available online 27 May 2016

Keywords:
Multiwalled carbon nanotubes
Thermal perturbation
Stochastic Hopf bifurcation
Safe basin

ABSTRACT

In this article, the thermodynamic characteristics and bifurcation of MWCNTs impacted by hydrogen atoms were studied. The impact between MWCNTs and hydrogen atoms was regarded as white noise. Nonlinear differential items were introduced to explain the hysteretic phenomena of MWCNTs stiffness, and a nonlinear dynamic model of MWCNTs impacted by hydrogen atoms was developed where the nonlocal effect is considered. The conditions of stochastic Hopf bifurcation were identified, and the fractal boundary of the safe basin was provided. The reliability function of the system was solved, and the probability density of the first-passage time was determined. Theoretical analysis and numerical simulation show that stochastic Hopf bifurcation occurs in the variation of parameters; the boundary of safe basin has fractal characteristics, the area of safe basin decreases when the intensity of the noise increases; the hysteretic nonlinearity of MWCNTs stiffness can affect the system's stability and safe basin, which decides the actual hydrogen storage capacity of MWCNTs.

Introduction

Hydrogen has been recognized as an ideal energy carrier due to its high efficiency and environmental friendliness [1]. Carbon nanotubes (CNTs) have motivated many theoretical investigations of its fundamental property as hydrogen storage materials [2]. However, the current studies shown that the single-wall carbon nanotubes (SWCNTs) are not the ideal materials for hydrogen storage [3]. Recently, people turn to use multi-walled carbon nanotubes (MWCNTs) to obtain high hydrogen storage capacity [4–10].

Due to the existence of thermal perturbation, the hydrogen atoms will impact the MWCNTs and make it vibrate, which lead to the escape of the adsorbed hydrogen atoms and reduce the MWCNTs' actual hydrogen storage capacity. To obtain the high hydrogen storage capacity, one of the key challenges is how to analyze the thermodynamic characteristics of MWCNTs impacted by hydrogen atoms [11]. In the current years, most of the research in this field focused on molecular simulation based on first-principles [12–19]. Usually, the results based on first-principles are obtained by numerical method, which can not explain the system's response in theory. We regarded the impact of hydrogen atoms on the MWCNTs as Gauss white noise, developed the

* *Corresponding author*. Department of Mechanics, Tianjin University, Tianjin 300072, China. Tel./fax: +86 22 27401981.
E-mail address: xujia@tju.edu.cn (J. Xu).
http://dx.doi.org/10.1016/j.ijhydene.2016.04.186

dynamic model of a MWCNT impacted by hydrogen atoms, and obtained the initial relationship between the motion's stability of a MWCNT and its actual hydrogen storage capacity [20].

MWCNTs have the nonlocal effect, which cause its many special characteristics. Many scholars have studied the dynamic characteristics of CNTs using nonlocal continuum mechanics [21–27]. In this paper, the thermodynamic characteristics and bifurcation of MWCNTs impacted by hydrogen atoms were studied where the nonlocal effect is considered. The impact between MWCNTs and hydrogen atoms was regarded as white noise. Nonlinear differential items were introduced to explain the hysteretic phenomena of MWCNTs stiffness, and a nonlinear dynamic model of MWCNTs impacted by hydrogen atoms was developed. The conditions of stochastic Hopf bifurcation were identified, and the fractal boundary of the safe basin was provided. The reliability function of the system was solved, and the probability density of the first-passage time was determined.

Hysteretic nonlinear model of the MWCNTs

The structure of a multiwalled carbon nanotubes (MWCNTs) is shown in Fig. 1. The presence of voids in MWCNts causes its viscoelastic characteristics, such as hysteresis and stress relaxation. The strain–stress curves of MWCNTs in compressed state are presented in Fig. 2. Evidently, the curves have nonlinear hysteretic characteristics.

In Ref. [20], we proposed a new differential model to describe the hysteretic non-linear characteristics of MWCNTs as follows:

$$\bar{\sigma} = f_1(\varepsilon) + f_2(\varepsilon) = a_1\varepsilon + a_2\varepsilon^2 + a_3\varepsilon^3 + \left(a_4\varepsilon + a_5\varepsilon^2 + a_6\varepsilon^3 + a_7\varepsilon^4\right)\dot{\varepsilon} \tag{1}$$

where $\bar{\sigma}$ is the stress, ε is the strain, $f_1(\varepsilon) = a_1\varepsilon + a_2\varepsilon^2 + a_3\varepsilon^3$ is the skeleton curve of the hysteretic loop; and $f_2(\varepsilon) = (a_4\varepsilon + a_5\varepsilon^2 + a_6\varepsilon^3 + a_7\varepsilon^4)\dot{\varepsilon}$ is the new differential item, which is developed from the deformed Van der Pol item $(ax - bx^2)\dot{x}$; $a_i(i = 1–7)$ are coefficients, which can be obtained in fitting method. The item $f_2(\varepsilon) = (a_4\varepsilon + a_5\varepsilon^2 + a_6\varepsilon^3 + a_7\varepsilon^4)\dot{\varepsilon}$ describes the difference between the skeleton curve and the hysteretic loop.

However, the nonlocal effect of MWCNTs is not considered in the above model. The nonlocal effect of a material is shown in Fig. 3. According to the Nonlocal continuum theory, the stress of nano material has relationship with not only the strain, but also the 2nd order derivative of the strain, which can be shown as follows:

$$\sigma = E\varepsilon + a\ddot{\sigma} \tag{2}$$

Considering Eqs. (1) and (2), we obtain the constitutive model of MWCNTs with the nonlocal effect as follows:

$$\begin{aligned}\sigma &= f_1(\varepsilon) + f_2(\varepsilon)\\ &= a_1\varepsilon + a_2\varepsilon^2 + a_3\varepsilon^3 + \left(a_4\varepsilon + a_5\varepsilon^2 + a_6\varepsilon^3 + a_7\varepsilon^4\right)\dot{\varepsilon} + a_8\ddot{\sigma}\end{aligned} \tag{3}$$

The partial least-square regression software SIMCA-P is used to test the fitting effect of Eq. (3) on the experimental data. The results of the principal component analysis based on the experimental data are shown in Fig. 4, and the values of the coefficients are shown in Fig. 5, where VIP is the variable importance.

The results of DModX and DModY tests are shown in Figs. 6 and 7. DModX and DModY tests can show the residual standard deviations (RSD) of samples in X space and Y space, where X space is the data space of the independent variable and Y space is the data space of the dependent variable. Only little points are singular, which means that most of the forecasted data are effective.

The result of the forecast test to Eq. (3) is shown in Fig. 8, where the black line represents the experimental data and the red (in the web version) line represents the forecast value. Eq. (3) can describe the experimental curves well.

Stochastic stability and bifurcation of a MWCNT-absorbing hydrogen atoms subjected to thermal perturbation

The mechanical model of a MWCNT-absorbing hydrogen atoms subjected to thermal perturbation is shown in Fig. 9. The essence of thermal perturbation is the motion of gas molecules. In this article, the MWCNT is regarded as a simply-supported thin-walled cylinder, and the impact of hydrogen atoms on the MWCNT is regarded as radial Gauss white noise.

The dynamic model of the MWCNT under radial stochastic loads can be shown as follows:

$$\rho hr^2\frac{\partial^2 w}{\partial t^2} = \frac{\partial}{\partial\theta}\left[N_\theta\frac{\partial w}{\partial\theta} + Q_{\theta z}\right] - N_\theta + qr \tag{4}$$

where ρ is the density of the MWCNT, h is the thickness of the MWCNT, r is the radius of the MWCNT, w is the vibration mode, $w = w(t,\theta) = u(t)\sin k\theta$, θ is the torsion angle, $u(t)$ is the radial vibration amplitude, N_θ is the shearing stress, $q = b\varsigma(t)$ is the radial stochastic force of hydrogen atom to the MWCNT,

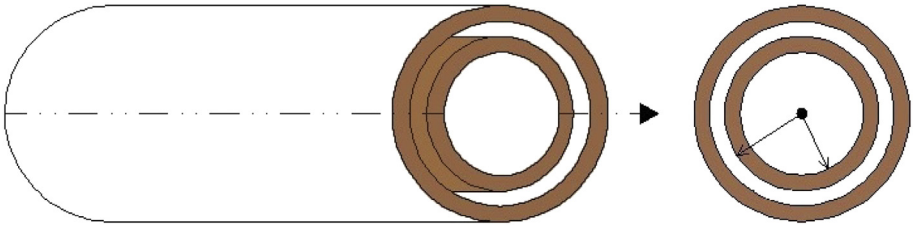

Fig. 1 – Structure of a MWCNT.