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Stochastic stability and bifurcation characteristics of multiwalled carbon nanotubes-absorbing hydrogen atoms subjected to thermal perturbation

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ABSTRACT

In this paper, the stochastic stability and bifurcation characteristics of a multiwalled carbon nanotube (MWCNT)-absorbing hydrogen atoms subjected to the thermal perturbation are studied. A new differential item is introduced to explain the hysteretic phenomena of a MWCNT's stiffness. The constitutive model of a MWCNT is obtained, and its fitting effect on experimental data is proved by the partial least-square regression method. The nonlinear dynamic model of a MWCNT-absorbing hydrogen atoms subjected to thermal perturbation is developed, and the stochastic stability and bifurcation characteristics of the system are analyzed. The system's safe basin and reliability function are obtained, and the probability density of the first-passage time is determined. Theoretical analysis and numerical simulation indicate that the system's stability is effected by the thermal perturbation, and the stochastic Hopf bifurcation will appears, which can reduce the actual hydrogen storage capacity of the MWCNTs; the area of the safe basin is reduced when the thermal perturbation increases, and the system's reliability decreases.

Introduction

Hydrogen is an ideal energy carrier due to its high efficiency and environmental friendliness. For mobile applications, a desirable hydrogen storage system must be compact, lightweight and capable of delivering hydrogen gas to a fuel cell at near room temperature and at a pressure negligible greater than atmospheric pressure [1,2]. One of the key challenges that need to be overcome is how to improve its adsorption and storage capacity using solid-state materials [3,4].

Since the discovery of carbon nanotubes (CNTs) in 1991 by Iijima [5], hydrogen storage in CNTs has shown great promise as a high-energy density absorbent. Single-wall carbon nanotubes (SWCNTs) are chosen as materials for hydrogen storage firstly [6–12]. However, the current studies shown that the pure SWCNTs are not the ideal materials for hydrogen storage [13]. Recently, people turn to use multi-walled carbon nanotubes (MWCNTs) to obtain high hydrogen storage capacity [14–20].

In most of the experimental results about MWCNTs, superior hydrogen absorbing property has been reported under a

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high pressure and often at an extremely low temperature. In this case, the thermal perturbation can not be ignored. The interaction mechanism between carbon and hydrogen has been attributed to physical and chemical adsorption of molecular hydrogen inside the tubes and interstitial sites in tube bundles. The essence of the thermal perturbation is the motion of gas molecules. To a MWCNT absorbing hydrogen atoms, the external hydrogen atoms will impact the MWCNT and cause it vibrate when the thermal perturbation increases. The motion of the MWCNT causes the adsorbed hydrogen atoms to escape, which reduces the MWCNT's actual hydrogen storage capacity. Due to the exist of thermal perturbation, the actual hydrogen storage capacity of MWCNTs remains in a lower level.

This article aims to offer a kind of analysis method to interpret the relationship between the motion's stability of a MWCNT and its actual hydrogen storage capacity. Most of the research results in this field were obtained by experiment or molecular simulation based on first-principles. In this paper, a new differential item is introduced to explain the hysteretic nonlinear phenomena of a MWCNT's stiffness, which make it possible to set up a concise dynamic model of a MWCNT subjected to thermal perturbation. The stochastic stability and the conditions of stochastic Hopf bifurcation of the system are analyzed, and the safe basin and the reliability of the system are 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 hysterestic characteristics.

To a hysteretic loop, most of the models are shown as equations with subsections or double integral functions, which are hard to analyze in theory. In this article, a new differential item, which is developed from Van der Pol hysteretic model, is introduced to describe the hysteretic nonlinear characteristics of MWCNTs.

Van der Pol equation is a kind of nonlinear differential equation. It can be shown as follows:

$$\ddot{x} + x + (1 - x^2)\dot{x} = 0 \tag{1}$$

The item $(1 - x^2)\dot{x}$ is called Van der Pol item. The essences of Van der Pol item $(1 - x^2)\dot{x}$ are two parabolic lines symmetrical about the original point (0,0) when $\dot{x}$ is ±1. It means that the initial Van der Pol model can only be used in some basic parabolic hysteretic loop. To those hysteresis loop whose outset is (0,0), Van der Pol item can be deformed as $(ax - bx^2)\dot{x}$, where a and b are the parameters which determine the width and height of the hysteretic loop.

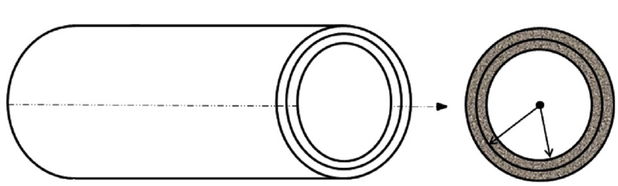

Fig. 1 – Structure of a MWCNT.

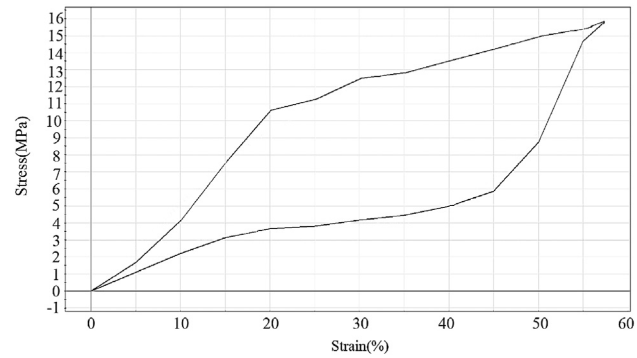

Fig. 2 – Hysteretic loop of the strain-stress curves of MWCNTs in compressed state.

However, the strain–stress curves of the MWCNTs are not parabolic lines. In this paper, a new differential item, which is developed from Van der Pol hysteretic model, is introduced to describe the hysteretic nonlinear characteristics of MWCNTs as follows:

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

where $\overline{\sigma}$ 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 $(ax - bx^2)\dot{x}$; $a_i(i = 1\sim7)$ 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.

The partial least-square regression software SIMCA-P is used to test the fitting effect of Eq. (2) on the experimental data. Partial least-square regression method minimizes the sum of squared errors to find the best match of data, and is usually used for curve fitting. The results of the principal component analysis based on the experimental data are shown in Fig. 3, and the values of the coefficients are shown in Fig. 4, where VIP is the variable importance.

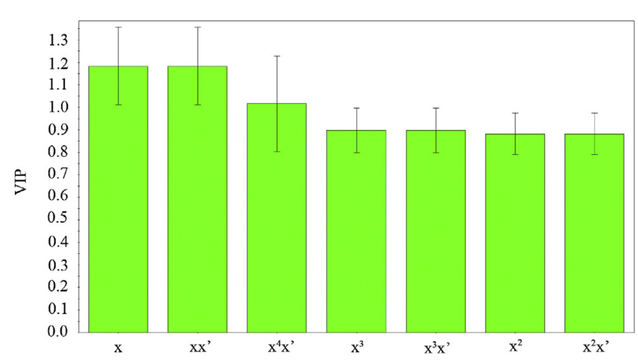

Fig. 3 – Analysis results of principal component.