**Nonlinear vibration of buckled nanowires on a compliant substrate**

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**Abstract**

Buckling of thin nanowires on a pre-strained compliant substrate has been widely used to make nanowire-based stretchable electronics. On nanometer scale, surface effect plays an important role on a buckled nanowire structure. In addition, as the amplitude of the deflection of the buckled nanowire is larger than its thickness, geometrical nonlinearity should be taken into account. Taking the kinetic energy caused by the out-of-plane motion into account, and on the basis of Euler beam theory, a theoretical model for a nanowire-substrate structure is established, combined with the influences of the nano-scale surface effect and geometrical nonlinearity. By means of Lagrange’s equation, the equation of motion is derived and then solved by the Symplectic (Partitioned) Runge–Kutta method (PRK). Several numerical examples are analysed to study the nonlinear vibration of the structure. The analytical expressions of stable and unstable equilibrium points, and the relationship between the vibration amplitude and the natural frequency are obtained. The influences of surface effect and pre-strain on the dynamic behaviour are analysed. Through these numerical results, one can find that when the surface elastic modulus and surface residual stress are considered, the number of unstable equilibrium points would increase to three. The frequency obtained with positive surface elastic modulus is greater than that obtained with negative surface elastic modulus, implying that the positive surface elastic modulus can make the nanowire-substrate structure stiffer. Furthermore, when the pre-strain increases, the locations of stable and unstable equilibrium points move further away from the initial displacement, and the homoclinic orbits become expanded. The results presented in this paper should be useful to guide the design of nanowire-based stretchable electronics.

**Keywords:** Nanowire; Compliant substrate; Stretchable electronics; Nonlinear vibration; Surface effect; Symplectic (Partitioned) Runge–Kutta method

## Introduction

Due to their versatility, tunability and reversibility, the study of surface wrinkling of thin films on a compliant substrate (also known as wavy design) has received considerable attention since they are essential components of stretchable electronic devices [1-8]. As an effective manufacturing strategy, thin films are adhered to a pre-strained elastomeric (compliant) substrate, and they form a wavy (buckled or wrinkling) configuration after the pre-strain is released [9]. Similar concepts can be applied to silicon nanowire [10, 11] and other inorganic nanomaterials to develop high-performance nanowire-based stretchable electronic devices [12-14]. In addition to the stretchability due to their wavy structural configuration, the dynamic behaviour of the buckled-nanowire electronic devices is also very important, because these devices would work in complex environments such as in an electrical field and/or thermal field [15]. Meanwhile, to design a robust stretchable nano-devices avoiding resonance [16], it is essential to have a comprehensive understanding of the nonlinear vibration of a buckled nanowire on a compliant substrate. In addition, due to a large surface-to-volume ratio, the surface effect (also known as size effect or interface effect) is significant for a thin nanowire when its thickness is at nanometer scale [17]. This study aims to accurately predict its mechanical behaviour and to improve the wavy design.

For a better design of the wavy configuration of nanowire-based stretchable electronics, the prediction of the interface effect of nanostructures is a critical issue. In recent years, several researchers [17-22] have studied it. Liang et al. [20] took the residual surface stresses, surface piezoelectricity and surface elasticity into account, and analysed the surface effect on the postbuckling behaviour of piezoelectric nanowire. Accounting for the surface elasticity and residual surface tension, Li et al. [23] developed an energy model for the wrinkles of thin films on a compliant substrate, and they found that their model was more accurate to predict the wrinkling profile at nano scale, compared with the model based on the classic continuum theory. Considering the surface effect, Wang et al. [24] studied the in-plane buckling of nanowire on elastomeric substrates, and they found that the buckling deflection and critical buckling strain were strongly affected by surface elasticity and residual surface tension. With the consideration of surface stress effects, Gao et al. [25] investigated the out-of-surface buckling behaviour of a nanowire on an elastomeric substrate, and they found that the surface properties had a significant influence on the buckling mode.

As mentioned in [15, 16], the dynamic behaviour of buckled thin films is also very important, because stretchable electronics with thin films, would not only work in complicated environments, but also experience dynamic loading [26, 27]. Recently, there are a few studies of the dynamic behaviour of buckled thin films. Wang and Feng [15] studied the dynamic behaviour of buckled thin films, and obtained the analytical expression of the natural frequency. After that work, they [16] investigated the mechanical behaviour of the interconnector. By using Jacobi elliptic functions, Ou et al. [28] analyzed the dynamic response of a wrinkling stiff thin film on a compliant thick substrate subjected to a step load, and they found that the maximum amplitude of dynamic buckling was larger than that of static buckling. Based on von Kármán plate theory, and taking damping into account, Ou et al. [29] investigated dynamic stability of a thin film bonded to a compliant substrate subjected to a uniaxial step load, and they found that at the stage of pre-buckling, the vibration of the film was attenuated, where the maximum response was the initial perturbation. For a thin film-substrate structure, the film’s width is greater than its thickness, thus only the in-surface buckling happens. However, for nanowires-substrate structure, the cross section has a significant influence on the buckling mode [30]. Especially when the thickness to width ratio is smaller than one, the out-of-plane buckling easily takes place [25]. Though nanowires-substrate structure has been widely used in stretchable electronics, to the authors’ best knowledge, there is not reported research on its dynamics, which is the subject of study in this paper.

Based on these previous studies, it can be concluded that there is no study of the out-of-surface dynamic buckling of nanowire-substrate structure with size effect. Hence, the aim of the present study is to investigate the nonlinear vibration of a wavy nanowire on a compliant substrate combined with geometrical nonlinearity and surface effect. This article is organized as follows: In section 2, the detailed formulations of the problem are introduced. Numerical results are given in section 3 to validate the proposed model and method, and the influences of surface effect and pre-strain on the nonlinear vibration of a nanowire-substrate structure are analysed. In section 4, the concluding remarks are given.

## Theoretical formulation

To understand the nonlinear vibration of a buckled nanowire on an elastomeric substrate, the nanowire is modeled as an elastic nonlinear Euler-Bernoulli beam illustrated in Fig. 1 [24]. Because the thickness of the elastomeric substrate (a few millimeters) is much larger than the film thickness (), the thickness of the elastomeric substrate (a few millimeters) is much larger than the buckling wavelength of nanowire, the elastomeric substrate is modelled as a semi-infinite elastic solid, and the surface effect of the substrate is considered negligible [31]. The cross section of the nanowire is rectangular with the thickness and width denoted by and, respectively.

As illustrated in the experiment results of reference [30], out-of-surface buckling is more likely when the thickness to width ratio takes a smaller value. Based on the nanobeam theory, Gao et al. [25] recently reported that when the thickness to width ratio was less than one, the out-of-surface buckling easily took place. In this manuscript, that ratio is set as 0.5, and the out-of-surface buckling mode is assumed to happen in the nanowire-substrate structure.

***2.1 Energy-based mechanics of wrinkling nanowire***

For simplification of the theoretical analysis, the nanowire and elastomeric substrate are assumed to be linear elastic materials. The membrane strain in the nanowire is given by the axial displacement  in the  direction and the out-of-plane displacement in the  direction,

 (1)

where  denotes the longitudinal nanowire direction.

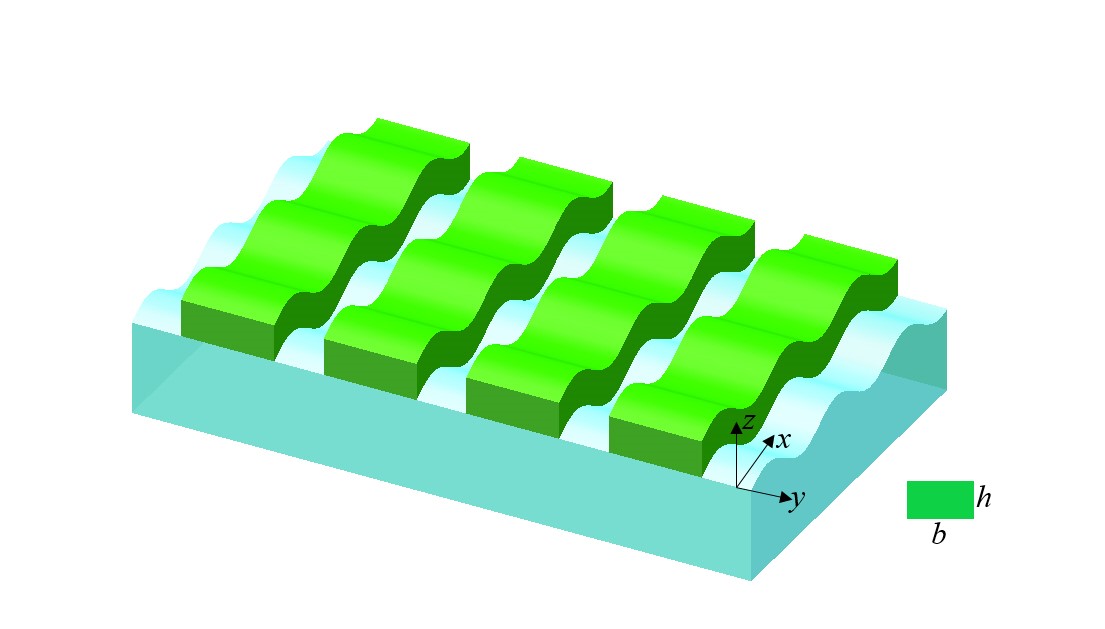


Figure 1. A schematic diagram of out-of-surface buckling of nanowires on a compliant substrate

Since the Young’s modulus of the nanowire (i.e.  for Ag,) is several times greater than that of poly (dimethylsiloxane) substrate ( for PDMS), the shear stress between the nanowire and substrate is negligible [10] . From the FEM simulation results [10], the membrane strain in a nanowire is almost constant and much smaller than the maximum bending strain. Additionally, the shear strain along the axial direction of a nanowire is one order smaller than the interfacial shear strain in the *y* direction. Hence, Eq. (1) can be rewritten as,

 (2)

As shown in the FEM simulation results under the normal stress traction (along thedirection) [30], the out-of-surface deflection of the nanowire is almost sinusoidal, so it can be described as,

, (3)

where  is the ‘modal coordinate’ of the buckled nanowire and  is the buckling wavelength. Here, one needs to point out that when the pre-strain is smaller than , the wavelength is constant and strain independent [32]. Because the membrane strain is constant, submitting Eq.(3) into Eq.(2) and ignoring the rigid body displacement of the nanowire [33] , the axial displacement can be obtained as,

, (4)

where  is the pre-strain.

As only the out-of-surface dynamic buckling is investigated, the kinetic energy caused by the axial displacement is neglected. The kinetic energy due to the out-of-plane motion can be expressed as,

, (5)

where  and  are the density and the length of the nanowire, respectively.

The membrane strain energy of the buckled nanowire can be expressed as [30],

, (6)

where is the effective tensile stiffness. The effective tensile stiffness is written as [25],

, (7)

where  and  are the (bulk) Young’s modulus and surface Young’s modulus of the nanowire.

The strain energy of the buckled nanowire due to bending can be expressed as [30],

, (8)

where  is the effective bending stiffness, and  is the curvature of the buckled nanowire. They can be calculated from [25] [33],

 (9)

For smaller deformation, , the approximate curvature can be expressed as [33],

 (10)

Due to buckling, from the experimental results [30], the part of the substrate surface in glued connection would be subjected to normal stress traction from the buckled nanowire. That distributed normal force can be written as,

, (11)

where  is the time variation part of the force. It is given as [34],

 (12)

Because of the normal stress traction (along thedirection), the lateral displacement (along thedirection) on the substrate surface is [35],

, (13)

where and  are the Young’s modulus and Poisson’s ratio of the substrate; is Euler’s constant.  is the residual surface stress.

According to the divergence theorem, the strain energy in the substrate is [35],

 (14)

The potential energy of distributed vertical load due to the influence of the residual surface stress is [25],

 (15)

The mechanical work across the nanowire-substrate interface by *F*1 is derived as [25],

 (16)

Substituting Eqs. (3) and (4) into Eqs. (5), (6), (8), (14), (15) and (16), respectively, the potential energy of the out-of-surface buckling structure is,

 (17)

By minimizing Eq. (17) with respect to, one can obtain the approximate wavelength of buckled nanowire-substrate structure as [36],

 (18)

***2.2 Free vibration analysis of nanowire on a compliant substrate***

The Lagranginan of the buckled nanowire on the compliant substrate is,

 (19)

where  denotes its time derivative .

The motion of the structure is described by Lagrange's equation as:

 (20)

The governing equation of motion can be given by,

 (21)

where the coefficients, ,  and  are,



The following dimensionless parameters are introduced,

 (22)

By utilizing Eq. (22), Eq. (21) can be rewritten in the following dimensionless form, and introducing new state variables, the second-order ordinary differential equation Eq. (21) can be rewritten as the first-order ordinary non-dimensional differential equations below,

 (23)

where , . The coefficients and are,

 (24)

The first-order system of ordinary differential equations Eq. (23) describes a conservative system, whose Hamiltonian energy (function) is of the form,

 (25)

The total energy of the nanowire-substrate structure can be defined as,

 (26)

where and  denote the initial displacement and velocity.  represents the potential energy of the buckled nanowire and it is calculated as .

To investigate the nonlinear vibration of the wavy nanowire on the compliant substrate, Eq. (23) must be solved. As Eq. (23) describes a conservative system, symplectic (Partitioned) Runge–Kutta methods (PRK) are appropriate [37]. For a conservative system, PRK can preserve the symplecticity of the original problems and has the characteristics of energy-prevising and long time stability [37].

A 2-stage, 4th order symplectic Runge–Kutta method is given as follows [38],

 (27)

where  is the time step size.

## 3. Result and discussion

In this section, numerical examples are analysed to investigate the nonlinear vibration of a nanowire on an elastomeric substrate.

***3.1 Verification studies***

In order to validate the proposed formulation and numerical method developed by the authors, an example is analysed and its results are given in Fig. 2, in which the corresponding parameters used are set as ,,,,,, , and [24, 25, 39].

In Fig. 2, the errors of the Hamilton function obtained by the proposed method and the 2-stage, 4th order Runge-Kutta method using the same time step size of 0.1 are compared. From Fig. 2, it can easily be noticed that the error of the proposed method is not only smaller than that of the classical Runge-Kutta method, but also stable for longer time. Because PRK shows the crucial features of energy-preservation and long time stability, it is preferable for determining the dynamic behaviour of the structure under this study.



Figure 2. Comparisons of the absolute errors of the Hamilton energy

***3.2 Influences of surface effect on the dynamic response***

Fig. 3 shows the Hamilton energy function with negative and without surface constant. From Fig. 3, it is clearly seen that the surface effect has a great influence on the Hamilton energy. The Hamilton energy drops when the surface constants are taken into account, which can be explained in Eq. (25).



Figure 3. The Hamilton energy for various values of surface elastic modulus and residual stress

Figure 4 illustrates the potential energy and phase portraits at various values of surface constant. The straight horizontal coloured lines in Fig. 4a-1 (marked as,and), and Fig. 4b-1 (marked as,and) represent the total energy levels without surface elastic modulus and with negative surface elastic modulus, respectively. They can be calculated from Eq. (26) with different initial out-of-plane amplitude  but with the same velocity. Those total energies correspond to the same coloured trajectories in phase plane Fig. 4a-2 and Fig. 4b-2.

Letting  in Eq. (23) be zero, the analytical expressions of stable and unstable equilibrium points for the different cases can be obtained as follows,

 (28)

 (29)





Figure 4．The potential well and phase portraits of buckled nanowire substrate structure for various surface elastic modulus and residual stress: a), b); 

In Fig. 4a-1, the surface elastic modulus and surface residual stress are equal to zero. From Fig.4a-1, it is observed that there are two stable centresand , and one unstable maximum (saddle point). Fig. 4a-2 displays the corresponding phase graph. As shown in Fig. 4a-2, for the fixed point, it is interesting to note that the stable and the unstable manifolds and coincide, and form a separatrix (line with tetragons in Fig. 4a-2) between the two types of motion. The fixed point (saddle point) is a homoclinic point. When the total energy  is greater than, the nanowire-substrate structure would vibrate along the single closed trajectory (line with triangles) in Fig. 4a-2, and the separatrix is surrounded by the single closed trajectory. When the total energy  is smaller than, the structure would exhibit periodic motions around the stable centres and, respectively.

In Fig. 4b-1 and Fig. 4b-2, the values of and are taken as  and , and , respectively.

Compared with those results in Fig. 4a-1 and Fig. 4a-2, it is clear that the surface effect has a strong influence on the potential well and phase portraits. The number of unstable equilibrium points would increase to three when the surface elastic modulus and surface residual stress are taken into account.

Fig. 4b-1 demonstrates the influence of the surface effect on the potential well and phase portraits. From Fig.4b-1, it is observed that the non-zero values of surface constants are have no influence on the number of stable equilibrium points. However, except the stable centre , the locations of stable and unstable equilibrium points depends on the values of and , which can be inferred from Eq. (29). When the surface elastic modulus is negative, the locations of stable and unstable equilibrium points move further away from the initial displacement. In Fig. 4b-1, the hollow pentagrams and solid circles represent stable and unstable points with negative surface constant; solid pentagons and tetragons represent stable and unstable points with positive surface constant.

For convenience, only the phase portrait of the structure with negative surface elastic modulus is shown in Fig.4b-2, and the corresponding total energies are represented by straight horizontal lines in Fig.4b-1(marked as,and). From Fig.4b-1, it can be seen that when the total energy  is greater than, the nanowire-substrate structure would separate from the substrate, which can be found at points , and . When the total energy  is smaller than, the structure would exhibit periodic motion around the stable centres and, respectively, plotted in Fig. 4b-2.

From these results in Fig. 4, it is clear that the (nonlinear) surface effect has a strong influence on the nonlinear dynamic behaviours of the buckled nanowire-substrate structure, such as the motion trajectories, the number of unstable equilibrium point, and values of potential energy. Those trends can be inferred from Eq. (26). Furthermore, from the phenomenon of separatrix passing through the same homoclinic point, one can also find that the proposed model describes an integrable system.

To evaluate the vibration amplitude and natural frequency of the structure with pre-strain, the relationship between the amplitude and frequency needs to be obtained. However, for the nonlinear buckled structure, it is not so easy to obtain this relationship. Hence, a numerical method is needed. The numerical method reported in reference [40] is used. The amplitude is defined as . Period is a function of the free vibration amplitude of the buckled structure, and it is calculated as,

 (30)

where  and  are the horizontal coordinates of the intersection points between the closed trajectories and the horizontal axis in the phase planes.

Fig. 5 illustrates the influence of the surface elastic modulus on the vibration of the nanowire-substrate structure, and the parameters used in Fig. 5 remain the same as before.



Figure 5. The vibration amplitude-frequency () curves with different values of surface constants

In Fig. 5a, the surface elastic modulus  and the surface residual stress  are taken to be zero. From Fig. 5a, it can be seen that in the range  of intra-well motion, the frequency () decreases to zero as the amplitude increases to. However, once the total energy is greater than  (Fig. 4a-1), the frequency increases with an increase of vibration amplitude in inter-well motion. Furthermore, it is very interesting to note that once the total energy  is greater than , as shown in Fig. 4a-1, the dynamic behaviour of the buckled structure would evolve from surrounding one stable centre ( or , line with tetragons trajectory) to surrounding two stable centres ( and, line with circles trajectory), and the corresponding vibration amplitude of the line with circle would be two times greater than that of the line with tetragons trajectory. Thus there is a jumping in Fig. 5a.

Fig. 5b illustrates the variation in the frequency with amplitude at different values of  and . From Fig. 5b, it can be observed that with an increase in amplitude, the frequency decreases to zero, which can be inferred from Eq. (30). In addition, it is also seen that at the same amplitude, the frequency with the positive surface elastic modulus , is greater than that with the negative surface elastic modulus , which implies that positive surface constants can make the structure stiffer and can be explained in Eq. (30) [41].

***3.3 Effect of pre-strain on nonlinear vibration***

In this subsection, the effect of pre-strain on the nonlinear vibration of the buckled structure is analysed.



Figure 6. The potential well of buckled structure for different pre-strains

In Fig. 6, and are chosen. From Fig. 6, it is easily noticed that pre-strain  plays an important role on the locations of stable and unstable equilibrium points in Fig. 6. One can find that the locations of stable and unstable equilibrium points move further away from the initial displacement with an increase of pre-strain.



Figure 7. The phase graph of buckled structure for different pre-strains

Fig. 7 shows the influence of pre-strain on the phase portraits of the buckled structure. From Fig. 7, it can be clearly found that the pre-strain has a very important influence on the homoclinic orbits of the nanowire-substrate structure. At the same values of  and , with an increase of pre-strain, the homoclinic orbits are expanded; it is also easily found that the locations of stable and unstable equilibrium points move further away from the initial displacement with an increase of pre-strain.



Figure 8. Influence of pre-strain on the vibration amplitude

Fig. 8 illustrates the influence of pre-strain on the vibration amplitude. From Fig. 8, it can be observed that, at the same pre-strain, when the positive and negative surface elastic modulus are taken, the amplitudes are larger than that without surface effect; with the increase of pre-strain, the amplitudes also increase, which can be inferred from Eq. (30). From Fig. 8, one can also find that, at the same pre-strain, the amplitude obtained with negative surface elastic modulus is greater than that with the positive surface elastic modulus, which implies that negative surface constants can make the structure softer and can be explained in Eq. (30) [41].

Fig. 9 plots the influence of pre-strain on the static bifurcation of the nanowire-substrate structure. The expressions of abscissa  for the different cases can be obtained as follows,

 (31)

 (32)

The stability of the equilibrium points can be determined through the eigenvalues of Jacobian matrix of Eq. (23) at, which can be written as,

 (33)

From Eq. (31) and Eq. (32), it is clear that the signs of terms of , , , and , have influences on the numbers of stable and unstable equilibrium points, which are summarized in Tables 1 and 2.

In Fig. 9a, the surface elastic modulus and the surface residual stress are taken to be zero. From Fig. 9a, it is noted that when the value of  is in the region , there is only one stable equilibrium point at . When the value of  is in the region , the number of stable equilibrium points would increase to two at , which can be explained in Eq. (31). This phenomenon is a pitch-fork bifurcation. The relationships of the numbers of stable and unstable equilibrium points and the abscissa  are summarized in Table1.

|  |  |  |
| --- | --- | --- |
| Table 1 Equilibrium positions of the nanowire-substrate structure | | |
| Region | features |  |
|  |  |  |
|  |  |  |

Figure 9. Static bifurcation of nanowire-substrate structure versus pre-strain a), b)(solid line stable, hollow dashed line unstable)

In Fig. 9b and Fig. 9c, the values of and are taken as  and. The nonlinear vibration of the nanowire-substrate structure exhibits complex bifurcation. It should be stated that Fig. 9b shows a local enlarged view of Fig. 9c. From Fig. 9b, it is can be found that when the value of  is in the region, there is only one stable point; but when the value of  is in the region , there are two stable points.

|  |  |  |
| --- | --- | --- |
| Table 2 Equilibrium positions of the nanowire-substrate structure | | |
| Region | features |  |
|  |  |  |
|  |  |  |
|  |  |  |
|  |  |  |

When the pre-strain is in region , there are one stable equilibrium point, and two unstable equilibrium points . When the pre-strain is in region, there are three unstable equilibrium points  and, and two stable equilibrium points. Excluding the results in Fig. 9b, from Fig. 9c, it is clearly seen that with an increasing pre-strain, the number of stable points is two and that of the unstable points is three. The relationships of the numbers of stable and unstable equilibrium points and the abscissa  are summarized in Table 2.

In order to explain the stability of the equilibrium points more clearly, the potential wells of the buckled structure in regions,, andare plotted in Fig. 10. The solid markers, such as pentagrams and triangles, represent the stable points. The hollow markers, such as the hollow circles and pentagrams, represent the unstable points. According to Table 2, the stable and unstable points can be determined from Eq. (31).



Figure 10. The potential well of buckled structure in different regions.

***3.4 Application discussion***

The above results, though obtained from a theoretical model, actually reveal some of the physics behind the nanowire-substrate structure. It has been found that when the wavy structure is stretched, the amplitudes and periods of this wave shape would change to accommodate the deformation. Hence, they are two key factors for the design of nanowire-based stretchable electronics. From Eq. (18), it is easy to find that the surface effect can affect the buckling wavelength. From Eq. (21), it is also easy to see that the amplitude of the buckled structure is dependent on the pre-strain, the surface elastic modulus, the surface residual stress and other geometrical parameters. Thus, the wavy design can be precisely controlled by pre-strain and other physical and geometrical parameters, and the stretchability can be tailored [15], which is also a big advantage of the wavy design. The results of the nonlinear vibration of the buckled structure, such as the vibration amplitude and natural frequency, influence of pre-strain on the vibration amplitude and so on, provide a comprehensive understanding on its mechanical behaviour, and are useful to guide the design and fabrication of buckled nanowire-based stretchable electronics devices with more robust and higher dynamic performances.

## 4. Conclusions

In this paper, the nonlinear vibration of a wrinkling nanowire on a compliant substrate (as a typical strategy of stretchable electronics) is investigated. The buckled nanowire is modelled as a nonlinear Euler-Bernoulli beam combined with the surface effect, and the elastomeric substrate is modelled as a semi-infinite solid neglecting its surface elasticity and residual surface tension. By means of Lagrange’s equation, the equation of motion is derived and solved by Symplectic (Partitioned) Runge–Kutta method (PRK). Compared with the results obtained by Runge–Kutta method (RK), the accuracy and stability of PRK are illustrated to be higher. The influences of surface effect and pre-strain on the vibration of the buckled structure are analysed through several numerical examples. These results demonstrate that the surface effect and pre-strain play an important role on the nonlinear dynamic behaviours of the buckled structure. Some conclusions are given as the following:

1. When the surface elastic modulus and surface residual stress are considered, the number of unstable equilibrium points is three, which is different from when these are ignored. With an increase in amplitude, the natural frequency decreases. At the same pre-strain, the frequency obtained with the positive surface elastic modulus is greater than that obtained with negative surface elastic modulus, implying the positive surface effect can make the nanowire-substrate structure stiffer. In addition, when the negative surface elastic modulus is taken, the locations of stable and unstable equilibrium points move further away from the initial displacement.
2. When the pre-strain increases, the locations of stable and unstable equilibrium points move further away from the initial displacement, and the homoclinic orbits become expanded. At the same pre-strain, when the surface constants are taken, the amplitudes are larger than that without surface constants; at the same pre-strain, the amplitude obtained with a negative surface elastic modulus is greater than that with a positive surface elastic modulus, which implies that negative surface constants can make the structure softer.

It should be pointed out that this is the first study of dynamics of out-of-surface buckling of nanowire-based stretchable electronics

## Acknowledgments

The authors acknowledge support from the National Natural Science Foundation of China (No. 11802319, 11572254) and National key Research and Development Program of China (2017YFB1102801). Part of this work is done during the first author’s visits to the University of Liverpool.

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