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Nonlinear waves in diatomic crystals

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HIGHLIGHTS

- The suitable numbering for continualization is found for atoms in diatomic lattice.
- The coupled equations have solutions for both the acoustical and optical branches.
- Improvement of the existing continuum models for the composites is discussed.

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ABSTRACT

A possible improvement of a continuum model for diatomic crystals is examined using continuum limit of a discrete diatomic model. For this purpose, various discrete models of diatomic lattice are compared at the linearized and weakly nonlinear levels. The suitable numbering of the atoms in the lattice is found which is better adopted for continualization than the familiar pair numbering introducing two sub-lattices. The coupled governing partial nonlinear differential equations for longitudinal strain and relative distance between the atoms are obtained in the continuum limit that allows us to describe localization of the strains due to the presence of the atoms of two kinds. It is found, that the equations obtained possess two kinds of localized wave solutions, one related to the acoustical branch and the other one related to the optical branch.

0. Introduction

Recently a model has been developed to account for localization of nonlinear strain waves in a periodic two-component composite [1]. It was found that the strain waves localization strongly depends on the elastic properties of the components of the composite and the width of the lamina. Mathematically it affects the dispersion and nonlinear terms in the governing equation for longitudinal strains and provides a balance between nonlinearity and dispersion required for the localization of a strain wave. Among the materials of the composite, a bi-atomic SiC has been examined, and an important variation in the sign of the amplitude of the strain wave has been found for the composite Al–SiC. A pure continuum approach was used in [1], and both materials were assumed to be isotropic and elastic. However, it is known that the modeling of diatomic crystalline materials usually involves microstructure [2–4] while typical evidence of a microstructure is the presence of dispersion of the strain waves in media [5]. Therefore, additional dispersion may modify the findings in [1], if an improved nonlinear continuum model is developed taking into account a diatomic crystalline structure of the material.

The theory of diatomic lattices generalizes the well developed nonlinear theory of monoatomic lattices that considers not only solid lattices but also the granular media and photonic lattices, see, e.g., [2,6–10]. Usually, the diatomic lattice is a primary object of the study while a continuum limit is employed to better understand the behavior of the lattice [2,11–19]. Both

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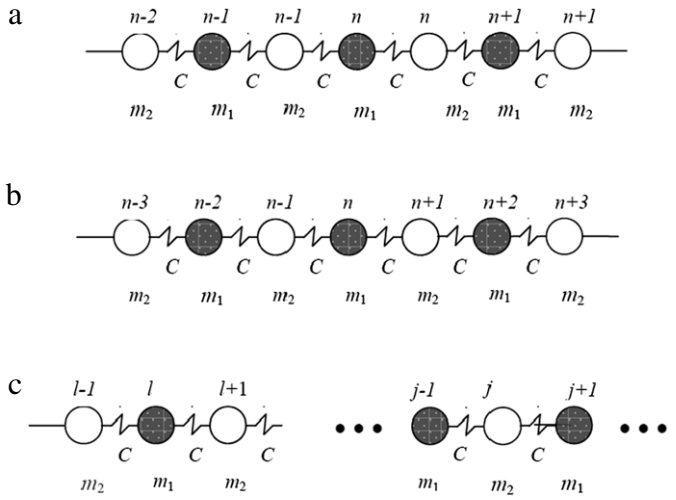

Fig. 1. Numbering of the masses in the lattice for different models: (a) pair or double numbering, (b) consecutive numbering, (c) numbering suitable even for non-neighboring masses.

linear [11–13,18] and weakly nonlinear [2,14,15,17,19] models are considered, and a weak nonlinearity is approximated by the power series in displacements. Another approach considers elastic diatomic crystalline material as a primary continuum object while the discrete lattice is used as a model that helps to improve the continuum model of the material. Thus, a direct continuum approach has been developed in [3,4] to account for diatomic materials. Also a phenomenological approach for media with microstructure, see, e.g., [20,21], may be employed for modeling diatomic crystals [22]. A comparison between the continuum model from [3] and the phenomenological models may be found in [22,23]. One of disadvantages of the pure continuum approaches is a lack of the values of the parameters of the model. These parameters may be estimated using the parameters of the discrete models when the governing partial differential equations are obtained as a continuum limit of the differential–difference equations.

In this paper, the second approach was employed to try to improve a nonlinear continuum model of the diatomic elastic material. For this purpose, first, the existing linear discrete models of diatomic lattices with different numbering of the atoms were compared to choose the most suitable model for further continualization and derivation of the governing differential equations. Then a proper discrete weakly nonlinear model was suggested, its continuum limit was obtained that resulted in the coupled partial nonlinear differential equations for a macro-displacement and an internal variable accounting for structural variations. It was found that equations obtained possess two kinds of localized wave solutions, one related to the acoustical branch and the other one related to the optical branch. The application of the results for an improvement of the theory for the composite [1] was discussed. A possible link to the direct continuum nonlinear model [3,4] was considered.

1. Discrete models for diatomic lattice

First, the linear models are considered. The Born–von Kármán model [11,12] accounts for a lattice that is a chain of the atoms with masses m_1 and m_2 interacting with each other. The interaction with only nearest neighbors is considered and it is modeled by elastic springs with equal constant stiffness C. It is assumed [11,12] that the lattice consists of two sub-lattices with atoms of each kind, and pair or double numbering is used to take it into account, see Fig. 1(a). Then the differential–difference equations of motion are

$$m_1\, u_{n,tt} = C[(v_n - u_n) - (u_n - v_{n-1})], \tag{1}$$

$$m_2\, v_{n,tt} = C[(u_{n+1} - v_n) - (v_n - u_n)], \tag{2}$$

where u and v are the displacements of the atoms with masses m_1 and m_2 respectively.

However, use of the consecutive numbering, see Fig. 1(b), results in the other equations of motion [13,19],

$$m_1\, u_{n,tt} = C[(v_{n+1} - u_n) - (u_n - v_{n-1})], \tag{3}$$

$$m_2\, v_{n+1,tt} = C[(u_{n+2} - v_{n+1}) - (v_{n+1} - u_n)]. \tag{4}$$

Finally, a numbering may be employed [6,14,18], that considers not obviously neighboring atoms, see Fig. 1(c):

$$m_1 u_{l,tt} = C[(v_{l+1} - u_l) - (u_l - v_{l-1})], \tag{5}$$

$$m_2 v_{j,tt} = C[(u_{j+1} - v_j) - (v_j - u_{j-1})]. \tag{6}$$