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Mechanical wave propagation within nanogold granular crystals

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ABSTRACT

We computationally investigate the wave propagation characteristics of nanoscopic granular crystals composed of one-dimensionally arrayed gold nanoparticles using molecular dynamics simulation. We examine two basic configurations, i.e. homogeneous lattices and diatomic lattices with mass-mismatch. We discover that homogeneous lattices of gold nanospheres support weakly dissipative and highly localized solitary wave at 300 K, while diatomic lattices have a good tuning ability of transmittance and wave speed. We establish a validated nonlinear spring contact model with the consideration of complex interactions between gold nanospheres which reveals the physical nature of wave behaviors at nanoscale. This work sheds light on the application of nanogold as a novel mechanical wave tuner, qualitatively and fundamentally different from its counterpart granular materials at meso- and macroscale.

Artificially structured phononic crystals and acoustic metamaterials have been at the frontier of science and engineering in recent years due to their novel ability to manipulate mechanical wave propagation in unprecedented ways [1,2]. The linear response of the periodic system gives rise to many common but useful properties such as the existence of band gaps. However, in the regime of nonlinearity, the wave dynamics in periodic structures become more complex, with no analogs in linear theory. Granular crystals, consisting of tightly packed elastic granules, are a typical example of nonlinear periodic phononic structures, whose nonlinearity rises from the geometry [3,4]. The simplest form of granular crystals, one-dimensional (1D) chains of identical elastic spheres, were analytically, numerically and experimentally shown to possess the concept of "sonic vacuum" where classical phonons are not supported to highly nonlinear solitary waves (Nesterenko soliton or compacton) [5–8]. The nonlinear response of 1D granular crystals can be tuned in a wide range from linearity, weakly nonlinearity to strongly nonlinearity by the application of a variable precompression [7–9]. Furthermore, by altering the geometry [10–13], material properties [14,15] and spatial distribution [16–18] of component granules, one is rendered more freedom to manipulate the propagation of mechanical signals, which makes granular crystals building blocks for a broad range of novel applications such as impact-protection devices [13,19,20], acoustic diodes [21] and switches [22], and tunable vibration filters [23,24], just to name a few. Granular crystals composed of granules with diameters at centimeter scale respond to input mechanical signals ranging from 1 to 20 000 Hz [3]. However, the frequencies of acoustic waves used in many useful applications such as ultrasonic medical imaging and surgery should reach the order of a megahertz, where downsizing the granules would be a straightforward solution.

Recently, wave propagation in microscopic granular crystals has been experimentally studied [25] and numerical works on nanoscale counterparts (lattices of buckyballs [26–28] and short carbon nanotubes [29,30]) were conducted via molecular dynamics simulation. It is shown that nanoscopic buckyball granular crystals exhibit an ultra-strong nonlinearity, mainly due to the highly nonlinear molecular repulsive forces instead of the geometry, permitting non-dispersive solitary waves with shorter wavelength and more localized energy compared to its macroscopic counterpart. Exciting as it may seem, the experimental realization of buckyball or carbon nanotube lattices is challenging due to the high-demanding measurement and manipulating equipment, the issue of chemical stability and the requirement of extremely low ambient temperature. Another fascination of granular crystals is the construction of diatomic lattices composed of alternating granules of two different properties such as shape, stiffness and mass etc., adding to the tunability of mechanical waves to a great extent. For example, in compressed diatomic chains of alternating steel and aluminum spherical granules, the existence of discrete breathers was theoretically and experimentally proved, where sustained, exponentially localized oscillations emerge at a frequency inside

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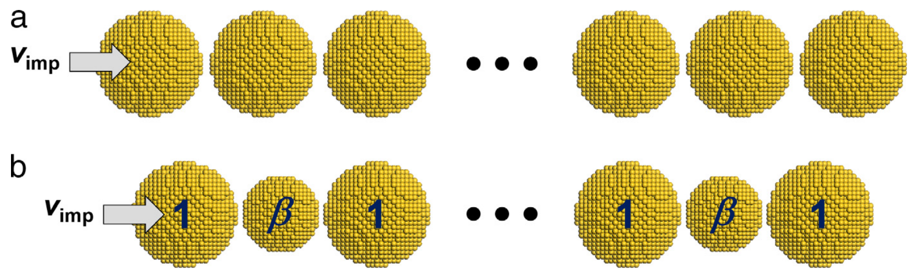

Fig. 1. Schematics of 1D nanogold granular crystals. (a) A homogeneous GNS lattice. (b) A diatomic GNS lattice.

the forbidden band of the linear Fourier spectrum [31]. For uncompressed diatomic lattices assembled by two different masses, strongly nonlinear resonances and anti-resonances are described by theory and experiments, resulting in an optimal wave attenuation and a new type of solitary wave respectively [32–34].

With the boost of nanotechnology in recent decades, gold nanoparticles have been playing an active role in fields of biology [35], medicine [36], nanocatalysis [37] and metamaterials [38–40] etc. The shape of gold nanoparticles can be well controlled during synthesis [41]. As one of the least reactive chemical elements, gold is an elite candidate for long-term use, especially in corrosive environments. In recent years, there have been plenty of work on the nanogold photonic crystals and electromagnetic metamaterials, exhibiting interesting phenomena with rich physics such as Fano resonance [40] and tunable refractive index [39].

To the best of authors' knowledge, no phononic crystals or acoustic metamaterials at the length-scale of 10^0–10^2 nm has been reported. Herein, we report a computational molecular-dynamics (MD) study of nanoscopic nonlinear granular crystals comprising one-dimensionally arrayed gold nanospheres (GNS), one of the thermodynamically stable shapes [42]. We construct two basic configurations of GNS granular crystals, namely, 1D homogeneous GNS lattices, and 1D diatomic GNS lattices with mass-mismatch, simulated at the temperature of 300 K. It is shown that 1D homogeneous GNS lattices support weakly dissipative and highly localized solitary waves at 300 K and the wave properties are quantitatively studied by establishing a nonlinear spring (NS) model. To describe the dynamics of 1D diatomic GNS lattices, the NS model is modified to account for the interaction between two GNSs with different masses. The theoretical predictions of transmission rate and average wave speed are in good agreement with the results of MD simulation.

1. Results and discussion

Configurations of nanogold granular crystals. The configurations of 1D homogeneous GNS lattice and diatomic GNS lattice are illustrated in Fig. 1, both of which consist of 25 GNSs. The spacing between adjacent GNSs equals to the sum of van der Waals radii, corresponding to the unprecompressed case of their macroscopic counterparts. Diatomic GNS lattices are characterized by a non-dimensional parameter mass ratio β, defined as the mass ratio of the light and heavy GNS ($0 < \beta \leq 1$). When $\beta = 1$, the diatomic lattice degenerates to a homogeneous one; when β approaches 0, the lattice becomes a so-called "auxiliary system" [32]. The radii of GNS in homogeneous lattice and heavy GNS in diatomic lattice are both $R_0 = 2.5$ nm. To maintain the contact homogeneity, the 1D lattice is aligned along [001] direction of GNS for the realization of pure facet–facet contact between all neighboring GNSs. The first GNS has a moderate initial velocity v_{imp} ranging from 200 to 1400 m/s, serving as a nanoscale stress wave generator (see Fig. 1). The initial temperature of the system is $T_0 = 300$ K, which strictly prohibits stable solitary wave propagation in 1D buckyball lattices [26].

Homogeneous GNS granular crystals. For homogeneous GNS lattices, a typical result of wave propagation at $T_0 = 300$ K is shown in Fig. 2, and is compared to low-temperature system at 10 K. To capture the wave behaviors, the resultant force (F_R) histories of 6th, 9th, 12th, 15th and 18th GNSs are extracted, normalized as $F_{R,N} = F_R / \left(E_{Au} R_0^2\right)$, where $E_{Au} = 79$ GPa is the Young's modulus of gold. Time is normalized by the time duration of the sound traveling the distance of the diameter, i.e. $t_N = t/(2R_0/c_{Au})$, where $c_{Au} = 2030$ m/s is the speed of sound in a gold rod. The moment of impact is shifted to $T_N = 0$. The normalized impact velocity is given as $v_{imp,N} = v_{imp}/c_{Au}$, and three impact velocities applied here are $v_{imp,N} = 0.197$, 0.296 and 0.394. According to the results shown in Fig. 2(a)–(b), stable traveling nonlinear waves are supported by homogeneous GNS lattice at $T_0 = 300$ K, and the comparison to system at 10 K reveals that the behaviors of the traveling wave are not sensitive to the temperature effect, in contrast to buckyball lattices. It is observed that the wave propagation actually has a little attenuation (<5% from 6th to 18th GNS), corresponding to the concept of weakly dissipative solitary wave in literature [43]. It is obvious from Fig. 2(a)–(b) that the waves have a nonlinear property of amplitude-dependent wave speed: the larger the amplitude, the larger the wave speed. Fig. 2(c) shows the change of system temperature upon various impact velocities. The temperature is normalized as $T_N = T/T_0$. Intuitively, higher impact velocity gives rise to higher temperature rise, but the peak value of system temperature is well below the melting point of gold (1337.33 K [44]). After reaching the peak value, the temperature decreases because part of system kinetic energy transforms to potential energy mainly due to the deformation of GNSs. During the simulation, no plastic behavior is observed and the deformation of GNSs can elastically recover after the wave passing through the system. Therefore, potential energy transforms back to kinetic energy and the temperature again increases at the end.

At macroscale or microscale, granular crystals can be described as a set of coupled nonlinear oscillators governed by Herzian contact, under the assumptions of small, elastic deformation and frictionless surfaces [45]. The Hertz law gives the compression force–overlapping distance relation of two spheres as

$$F_{ij} = \frac{4}{3}\left(\frac{1-\nu_i^2}{E_i} + \frac{1-\nu_j^2}{E_j}\right)^{-1}\left(\frac{R_i R_j}{R_i + R_j}\right)^{1/2}\delta_{ij}^{3/2}$$

where $\delta_{ij} = \left(R_i + R_j\right) - \left(x_j - x_i\right)$ is the overlapping distance; F is the compression force; R is the radius; x is the coordinate of the center of the sphere; E is Young's Modulus; ν is Poisson's ratio. The subscripts i and j denote two contacting granules. The above expression of the Hertzian contact is of decisive importance to the wave dynamics in granular crystals. However, for nanoscale contact, the breakdown of continuum theory is demonstrated [46], and the "rough" surfaces of nanoparticles consisting of crystal steps and terraces lead to more complex interaction law. Although many original investigations on nanoscale contact problem