Designing mechanical response using tessellated granular metamaterials

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Jammed packings of granular materials display complex mechanical response. For example, the ensemble-averaged shear modulus $\langle G \rangle$ increases as a power-law in pressure $p$ for static packings of spherical particles that can rearrange during compression. We seek to design granular materials with shear moduli that can either increase or decrease with pressure without particle rearrangements even in the large-system limit. To do this, we construct tessellated granular metamaterials by joining multiple particle-filled cells together. We focus on cells that contain a small number of bidisperse disks in two dimensions. We first study the mechanical properties of individual disk-filled cells with three types of boundaries: periodic boundary conditions, fixed-length walls, and flexible walls. Hypostatic jammed packings are found for disk-filled cells with flexible walls, but not in cells with periodic boundary conditions and fixed-length walls, and they are stabilized by quartic modes of the dynamical matrix. The shear modulus of a single cell depends linearly on the pressure. In fact, studies have shown that the ensemble-averaged shear modulus scales as $\langle G \rangle \sim p^0$ for all packings in single cells with periodic boundary conditions where the number of particles per cell $N \geq 6$. In contrast, single cells with fixed-length and flexible walls can possess $\lambda_c > 0$, as well as $\lambda_c < 0$, for $N \leq 16$. We show that we can force the mechanical properties of multi-cell granular metamaterials to possess those of single cells by constraining the endpoints of the outer walls and enforcing an affine shear response. These studies demonstrate that tessellated granular metamaterials provide a novel platform for the design of soft materials with novel mechanical properties.

I. INTRODUCTION

Granular materials represent an interesting class of physical systems that are composed of individual macroscopic particles that interact via dissipative, contact forces [1]. As a result of the dissipative particle interactions, granular materials come to rest in the absence of external driving, such as applied shear or vibration. Because of this, they frequently occur in amorphous states lacking long-range positional order. Further, granular systems can undergo a jamming transition, where they develop nonzero bulk and shear moduli when they are compressed to large packing fractions [2, 3].

There have been numerous computational [2, 4–15] and experimental [16–25] studies of the structural and mechanical properties of jammed granular materials. In particular, it has been shown that the shear modulus $G$ depends sensitively on the number of contacts and anisotropy of the interparticle contact network [2, 11, 12, 15, 26–28]. For example, in jammed packings of frictionless spherical particles with purely repulsive linear spring interactions, we have shown that the shear modulus of individual packings decreases with increasing pressure as long as the contact network does not change during the compression [15]. However, the range of pressure $\Delta p$ over which the contact network does not change decreases with increasing system size, $\Delta p \sim N^{-1}$, where $N$ is the number of particles in the system. Thus, in the large-$N$ limit, granular packings undergo frequent irreversible particle rearrangements to new jammed packings after each $\Delta p$ increment. During compression, each new contact network typically possesses an increased number of contacts, and thus the shear modulus increases with pressure. In fact, studies have shown that the ensemble-averaged shear modulus scales as $\langle G \rangle \sim p^{0.5}$ in the large $pN^2$ limit for jammed packings of spherical particles with purely repulsive linear spring interactions [11].

In this article, we design granular metamaterials for which the shear modulus can either decrease or increase with increasing pressure with no particle rearrangements. The lack of particle rearrangements provides robust material properties that are reversible during compression and decompression and shear strain cycling. We will leverage the recent findings that for granular packings with small $N$, particle rearrangements are rare and the shear modulus depends linearly on pressure in the absence of rearrangements. We will first consider systems in two dimensions, but these concepts can easily be extended to three dimensions.

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Gus of each cell obeys of the confining walls. We find that the shear modulus of these structures. In Sec. III, we present the methods for calculating the pressure, shear stress, and shear modulus of these structures. In Appendix A, we show that Maxwell-like counting arguments can be used to determine the minimum number of particle-particle and particle-wall contacts in jammed disk packings within single cells with fixed-length and flexible walls. In Appendix B, we determine analytical expressions for the dependence of the components of the stiffness matrix on the angle of the applied shear relative to the orientation of the confining walls. The variation in the disk shading between different cells indicates the types of cells based on their adjacent cells.

We envision tessellated granular metamaterials that are made up of many individual cells that each contain a small number of grains, i.e. \( N < 16 \), and are bounded by four freely jointed elastic walls. The disks within each cell are jammed with typically an isostatic number of contacts. See Fig. 1. The mechanical response of each cell is highly anisotropic, i.e., its shear modulus depends on the angle \( \theta \) of the applied shear relative to the orientation of the confining walls. We find that the shear modulus of each cell obeys \( G_c = G_{c0} + \lambda c p \), where \( G_c = G_{c0} \) at \( p = 0 \), and we determine the sign and magnitude of \( \lambda \) as a function \( N \), \( c \), and the ratio of the particle and wall stiffnesses. We vary the size of the tessellated granular metamaterials by adding multiple copies of individual cells together, e.g. by generating an \( n \times n \) array of cells that share the confining walls. We identify the regimes where the shear modulus of the full system is similar to that for the individual cells. In particular, we find that large tessellated granular metamaterials can possess shear moduli that decrease with increasing pressure and that these materials retain the anisotropy of the individual cells.

The remainder of the article is organized as follows. In Sec. II, we describe the computational methods, including the particle-particle, particle-wall, and wall-wall potential energies, the protocols for generating disk-filled single cells and collections of multiple cells, and the methods for calculating the pressure, shear stress, and shear modulus of these structures. In Sec. III, we present the results on how the boundary conditions, individual disk packing configuration, and the ratio of the particle to wall stiffness affect the relation between the shear modulus and pressure in single cells, as well as coupled systems composed of \( N_c = n^2 \) cells. In Sec. IV, we provide conclusions and discuss promising directions of future research, such as the mechanical response of tessellated granular metamaterials in three dimensions. We also include three Appendices. In Appendix A, we show that Maxwell-like counting arguments can be used to determine the minimum number of particle-particle and particle-wall contacts in jammed disk packings within single cells with fixed-length and flexible walls. In Appendix B, we determine analytical expressions for the dependence of the components of the stiffness matrix on the angle of the applied simple shear strain for jammed disk packings in single cells. In Appendix C, we verify that the pressure-dependence of the single-cell shear modulus is related to the second derivative of the packing fraction at jamming onset \( \phi_j \) with respect to shear strain \( \gamma \) for an example disk-filled cell with fixed-length walls.

## II. METHODS

We study individual cells containing jammed packings of \( N \) bidisperse disks: \( N/2 \) small and \( N/2 \) large disks with diameter ratio \( \sigma_1/\sigma_s = 1.4 \). We consider three types of boundary conditions for the cells as illustrated in Fig. 2: (a) periodic boundary conditions in square cells with side length \( L_0 \), (b) cells with four straight walls of fixed length \( L_0 \), and (c) cells with four flexible walls such that adjacent vertices are connected by linear springs with preferred length \( L_0 \). For boundary condition (c), the connected walls are freely jointed such that the angle between them can change without energy cost.

Within each cell, we consider frictionless disks that interact via pairwise, purely repulsive linear spring forces. The corresponding interparticle potential energy is given by

\[
U^{pp}(r_{jk}) = \frac{\epsilon_{pp}}{2} \left( 1 - \frac{r_{jk}}{\sigma_{jk}} \right)^2 \Theta \left( 1 - \frac{r_{jk}}{\sigma_{jk}} \right),
\]

where \( \epsilon_{pp} \) gives the strength of the repulsive interactions, \( r_{jk} \) is the distance between the centers of disks \( j \) and \( k \), \( \sigma_{jk} \) is the sum of the radii of disks \( j \) and \( k \), and \( \Theta() \) is the Heaviside step function. The repulsive force on disk \( j \) from disk \( k \) is

\[
j^{pp}_{jk} = -\left( \frac{dU^{pp}}{dr_{jk}} \right) r_{jk},
\]

where \( r_{jk} \) is a unit vector pointing from the center of disk \( j \) to the center of disk \( k \).

For boundary condition (a), there are only interparticle interactions. For boundary conditions (b) and (c), we also consider repulsive interactions between the disks and walls using the purely repulsive linear spring potential energy,

\[
U^{pb}(\rho_{ji}) = \frac{\epsilon_{pb}}{2} \left( 1 - \frac{\rho_{ji}}{R_j} \right)^2 \Theta \left( 1 - \frac{\rho_{ji}}{R_j} \right),
\]

where \( \rho_{ji} \) is the distance between a disk \( j \) and a wall \( i \) and \( R_j \) is the radius of disk \( j \).
where $\epsilon_{bb}$ is the strength of the repulsive interactions between the disks and walls, $r_{ji}^{bb}$ is the shortest distance between the center of disk $j$ and the $i$th wall, and $R_j$ is the radius of disk $j$. The repulsive force on disk $j$ from the $i$th wall is 

$$
\vec{f}_{ji}^{bb} = -(dU_{ji}^{bb}/dr_{ji}^{bb})\hat{r}_{ji}^{bb},
$$

where $\hat{r}_{ji}^{bb}$ is the unit vector pointing to the center of disk $j$ and perpendicular to the $i$th wall.

For the flexible wall boundary conditions, we consider interactions between the wall endpoints using the linear spring potential energy,

$$
U^{bb}(r_{i,i+1}^{bb}) = \frac{\epsilon_{bb}}{2} \left( 1 - \frac{r_{i,i+1}^{bb}}{L_0} \right)^2,
$$

where $\epsilon_{bb}$ is the characteristic energy scale of the linear spring potential, $r_{i,i+1}^{bb}$ is the distance between endpoints $i$ and $i+1$, and $L_0$ is equilibrium length for the $i$th wall.

The force on endpoint $i$ from endpoint $i+1$ in the $i$th wall is

$$
\vec{f}_{i,i+1}^{bb} = -(dU_{i,i+1}^{bb}/dr_{i,i+1}^{bb})\hat{r}_{i,i+1}^{bb},
$$

where $\hat{r}_{i,i+1}^{bb}$ is the unit vector pointing from endpoint $i+1$ to $i$.

We calculate the stress tensor $\Sigma_{i\alpha\beta}$ (with $\alpha, \beta = x, y$) of the tessellated granular metamaterials using the virial expression. For forces, the total potential energy is $U = \sum_{j<k} U^{pp}(r_{jk}^{pp})$ and stresses are generated only from interparticle forces. The total stress tensor is thus $\Sigma_{i\alpha\beta} = \Sigma_{i\alpha\beta}^{pp}$, where

$$
\Sigma_{i\alpha\beta}^{pp} = \frac{1}{A} \sum_{j=1}^{N} f_{j\alpha,i\beta}^{pp} f_{j\beta,i\alpha}^{pp},
$$

where $A$ is the area of the cell, $f_{j\alpha,i\beta}^{pp}$ is the $\alpha$-component of the force on disk $j$ from $k$, and $r_{jk}^{pp}$ is the $\beta$-component of the separation vector from the center of disk $k$ to the center of disk $j$. For cells with periodic boundary conditions, the forces between the walls and particles also contribute to the stress tensor. For cells with walls of fixed length, the total potential energy is $U = \sum_{j<k} U^{pp}(r_{jk}^{pp}) + \sum_{j=1}^{N} \sum_{i=1}^{4} U^{pb}(r_{ji}^{pb})$. In this case, the total stress tensor is $\Sigma_{i\alpha\beta} = \Sigma_{i\alpha\beta}^{pp} + \Sigma_{i\alpha\beta}^{pb}$, where

$$
\Sigma_{i\alpha\beta}^{pb} = \frac{1}{A} \sum_{j=1}^{N} \sum_{\alpha=1}^{4} f_{j\alpha,i\beta}^{pb} f_{j\beta,i\alpha}^{pb},
$$

where $f_{j\alpha,i\beta}^{pb}$ is the $\alpha$-component of the force on disk $j$ from $i$th wall of the cell, and $r_{ji}^{pb}$ is the $\beta$-component of the separation vector from the contact point between wall $i$ and disk $j$ to the center of disk $j$. For cells with physical walls, in addition to the interparticle and particle-wall interactions, the walls store potential energy. Thus, the total potential energy is $U = \sum_{j<k} U^{pp}(r_{jk}^{pp}) + \sum_{j=1}^{N} \sum_{i=1}^{4} U^{pb}(r_{ji}^{pb}) + \sum_{i=1}^{4} U^{pb}(r_{i,i+1}^{pb})$. The total stress tensor is $\Sigma_{i\alpha\beta} = \Sigma_{i\alpha\beta}^{pp} + \Sigma_{i\alpha\beta}^{pb} + \Sigma_{i\alpha\beta}^{pp}$, where

$$
\Sigma_{i\alpha\beta}^{pb} = \frac{1}{A} \sum_{j=1}^{N} \sum_{\alpha=1}^{4} f_{j\alpha,i\beta}^{pb} f_{j\beta,i\alpha}^{pb},
$$

where $f_{j\alpha,i\beta}^{pb}$ is the $\alpha$-component of the spring force from wall $i$, and $r_{ji}^{pb}$ is the $\beta$-component of the vector with the same length as wall $i$ pointing in the same direction as $\hat{r}_{ji}^{pb}$. The pressure of the cell is $P = (\Sigma_{xx} + \Sigma_{yy})/2$ and the shear stress is $\Sigma = -\Sigma_{xy}$. We use $\epsilon_{pp}/\sigma_0^2$ for the units of stress and shear modulus and $\epsilon_{pp}$ for units of energy.

To generate jammed disk packings within a single cell, we first place $N$ disks randomly in the cell at a dilute packing fraction, $\phi < 10^{-3}$. We then apply an affine isotropic compressive strain to the disk positions and decrease the length of the walls by $\Delta L$ to achieve a small packing fraction increase, $\Delta \phi/\phi = 2\Delta L/L_0 = 2 \times 10^{-3}$, followed by potential energy minimization using the fast inertia relaxation engine (FIRE) algorithm [29]. During energy minimization, the disk positions change, while the endpoints of the fixed-length walls for the boundary conditions depicted in Fig. 2 (a) and (b) are held fixed. However, the endpoints of the flexible walls in Fig. 2 (c) are allowed to move during energy minimization.

After energy minimization, we calculate the pressure $p$ of the cell. If $p$ is less than the target pressure $p_t$, we again compress the system by $\Delta \phi/\phi$ and perform energy
minimization. If \( p > p_t \), we return to the previous disk and wall configuration, compress the system by \( \Delta \phi / 2 \), and perform energy minimization. To generate cells with disk packings at jamming onset, we repeat this process until the cell pressure satisfies \( |p - p_t| / p_t < 10^{-4} \) with \( p_t = 10^{-7} \).

For all three boundary conditions in Fig. 2 (a)-(c), we generate \( 10^4 \) disk packings at jamming onset. To investigate the mechanical response of the disk-filled cells as a function of pressure, we apply isotropic compression to the cells to achieve a range of \( p_t \) values that are logarithmically spaced between \( 10^{-7} \) to \( 10^{-2} \). To ensure that the shape of the cells does not significantly deviate from a square, we fix the endpoints of the walls for all three types of boundary conditions when generating the disk-filled cells with pressures above jamming onset.

To calculate the shear modulus of a single cell \( G_c \), at an angle \( \theta \) relative to the \( x \)-axis, we first rotate the cell clockwise by \( \theta \), as shown in Fig. 2 (d). Determining \( G_c(\theta) \) allows us to assess the anisotropy of the mechanical response of single cells. We then apply successive small steps of simple shear strain \( \Delta \gamma = 5 \times 10^{-9} \) (where \( x \) is the shear direction and \( y \) is the shear gradient direction) to the disks and walls with each strain step followed by potential energy minimization. Note that after the applied simple shear strain, the walls remain fixed during energy minimization for all three boundary conditions. We obtain the shear modulus for a single cell by calculating \( G_c = d\Sigma_c / d\gamma \), where \( \Sigma_c \) is the shear stress of a single cell.

We build large-scale tessellated granular metamaterials by joining multiple copies of a given disk-filled cell with flexible walls, e.g. the collection of 36 coupled cells in Fig. 1. After joining the cells, we perform potential energy minimization with the outermost (blue) wall endpoints held fixed, while the internal (red) endpoints, as well as the disk positions, are allowed to relax. Disks within a given cell only interact with other disks and the walls of that cell. Interior wall endpoints have four connections to other walls, while exterior wall endpoints have either two or three connections to other walls. The shear modulus \( G \) of the collection of cells is calculated in the same way as that for a single cell. In particular, we first rotate the aggregate by \( \theta \) clockwise, and then we apply small successive steps of simple shear strain, \( \Delta \gamma = 5 \times 10^{-9} \), with each step followed by energy minimization, where the outer vertices are held fixed and the inner vertices, as well as the disks, are allowed to relax. The total shear stress \( \Sigma \) of the tessellated granular metamaterial is the sum of \( \Sigma^{pp} \) and \( \Sigma^{pb} \) for all cells and the unique contributions to \( \Sigma^{bb} \) for all of the cell walls. The shear modulus of the tessellated granular metamaterial is given by \( G = d\Sigma / d\gamma \).

After we apply each simple shear strain step followed by energy minimization to tessellated granular metamaterials, we calculate the displacement field \( F_{pq} \) of all cell wall endpoints. We find the strain field that minimizes the total non-affine displacement of all endpoints for a given cell and simple shear strain step [30]:

\[
F_{pq} = \sum_{s=x,y} X_{ps} (Y^{-1})_{sq}, \tag{7}
\]

where

\[
X_{ps} = \sum_{i=1}^{4} r_{ci,s}^0 r_{ci,p}^0, \tag{8}
\]

and

\[
Y_{sq} = \sum_{i=1}^{4} r_{ci,s}^0 r_{ci,q}^0. \tag{9}
\]

Here, \( r_{ci,s}^0 \) and \( r_{ci,s} \) are the \( s \)th component of the separation vector from the center of mass of a given cell.
to its ith endpoint before and after the applied simple shear strain \( \gamma \) from \( F_{xy} \) to determine the non-affine displacement field.

### III. RESULTS

In this section, we describe the results for the mechanical response of single disk-filled cells, as well as large collections of cells. In Sec. III.A, we enumerate all of the distinct \( N = 4 \) bidisperse disk packings in single cells at jamming onset for all three boundary conditions. We determine whether the shear modulus for single disk-filled cells \( G_c \) increases or decreases with pressure over the full range of \( \theta \) in Sec. III.B. We find that \( G_c \) for cells with periodic boundary conditions nearly always decreases with pressure (for all shear angles), while \( G_c \) can either decrease or increase with pressure for single cells with (both fixed-length and flexible) physical walls. We further show that the slope of the shear modulus versus pressure \( \lambda_c = dG_c/dp \) for single disk-filled cells can be tuned by varying the particle-wall interaction energy \( \epsilon_{ph} \) and wall stiffness \( \epsilon_{bb} \). Finally, in Sec. III.C, we emphasize that the sign and magnitude of \( \lambda_c \) for a single disk-filled cell can be maintained even in a large collection of disk-filled cells since the assembly prevents particle rearrangements. We then show that the mechanical response of large collections of disk-filled cells can deviate from the single-cell behavior when we allow the outer cell walls to relax and change their positions during energy minimization.

#### A. Single disk-filled cells with \( N = 4 \)

We first illustrate the different types of jammed bidisperse disk packings that occur in single cells with periodic boundary conditions and physical walls. In Fig. 3, we show all possible jammed disk-filled cells with \( N = 4 \). We find 3 distinct jammed packings for single cells with periodic boundary conditions [31], 6 distinct packings for square cells with fixed-length walls [32], and 7 distinct packings for cells with flexible walls. For \( N = 2 \), there is only one distinct jammed disk-filled cell with the disks arranged along the diagonal of the cell.

The boundary conditions of the cells affect the number of interparticle contacts at the onset of jamming. The numbers of degrees of freedom for the disk-filled cells are the following: periodic boundary conditions, \( N_d = 2N' - 1 \), fixed-length physical walls, \( N_d = 2N' + 1 \), and flexible physical walls, \( N_d = 2N' + 2 \), where \( N' = N - N_r \) and...
$N_c$ is the number of rattler disks. (See Appendix A.) For mechanically stable disk packings [33], the number of contacts must satisfy $N_c \geq N_d$. For $N = 4$, in periodic boundary conditions, we find that the jammed bidisperse disk packings are either isostatic ($N_c = N_d$, $N' = 4$, $N_c = 7$ for configuration 1) or hyperstatic ($N_c > N_d$, $N' = 4$, $N_c = 8$ for configuration 2, and $N' = 4$, $N_c = 9$ for configuration 3). In the disk-filled cells with fixed-length walls, all of the packings are isostatic ($N' = 4$, $N_c = 9$ for configurations 1-4, $N' = 3$, $N_c = 7$ for configuration 5, and $N' = 2$, $N_c = 5$ for configuration 6). In the disk-filled cells with flexible walls, most of the jammed bidisperse disk packings are hypostatic ($N_c < N_d$, $N' = 4$, $N_c = 9$ for configurations 1-5 and $N' = 3$, $N_c = 7$ for configuration 7). In contrast, configuration 6 in Fig. 3 (c) is hyperstatic ($N' = 4$, $N_c = 13$).

Hypostatic jammed packings have only been reported for packings of non-spherical particles [8, 14] and particles with shape and size degrees of freedom [34–36]. Our results indicate that jammed packings of spherical particles can also be hypostatic in cells with flexible walls. We have shown in previous studies that jammed hypostatic packings are stabilized by quartic modes [8, 14, 35], which do not occur in isostatic and hypostatic packings. Indeed, we find that hypostatic disk-filled cells at jamming onset possess $N_d - N_c$ quartic modes. For $N > 4$, we also find that jammed disk packings are isostatic in cells with periodic boundary conditions, either isostatic or hyperstatic for cells with fixed-length walls, and either isostatic, hyperstatic or hypostatic for cells with flexible walls. At large $N$ ($N > 16$), we find jammed disk packings are typically isostatic in all types of boundary conditions studied. (See Appendix A.)

For jammed disk-filled cells with flexible walls, the shape of the boundary is not typically a square, as shown in Fig. 3 (c), since the energy function for the walls does not include a bending energy term. Despite this, we show that several of the jammed configurations in the cells with fixed-length and flexible walls share the same interparticle contact networks, e.g. configuration 1 in Fig. 3 (b) and (c).

For $N = 4$, we find that rattler particles occur in jammed disk-filled cells with fixed-length and flexible walls. See configurations 5 and 6 in Fig. 3 (b) and configuration 7 in Fig. 3 (c). Rattler disks also occur for disk-filled cells with periodic boundary conditions and physical walls for $N > 4$. Since our focus is on jammed packings that do not undergo particle rearrangements during simple shear and isotropic compression, we will not include calculations of the mechanical response for cells with rattler disks.

B. Shear modulus versus pressure for a single cell

In Fig. 4 (a)-(c), we show the shear modulus $G_c(\theta)$ of single disk-filled cells as a function of pressure $p$ over the full range of shear angles $\theta$ for cells with periodic boundary conditions, fixed-length, and flexible physical walls, respectively. In contrast to the behavior for large-$N$ systems, we find that the disks do not rearrange and $G_c(\theta)$ varies continuously with $p$ over more than four orders of magnitude. For cells with periodic boundary conditions, $G_c(\theta)$ typically decreases with $p$ as shown in Fig. 4 (a). In contrast, for cells with fixed-length walls (Fig. 4 (b)) and flexible walls (Fig. 4 (c)), $G_c(\theta)$ can either decrease or increase with $p$, depending on the value of $\theta$.

As we showed previously for jammed packings of spherical particles with periodic boundary conditions, we find quite generally that $G_c(\theta)$ varies linearly with $p$ [15, 37], $G_c(\theta) = G_{c0}(\theta) + \lambda_c(\theta)p$, for disk-filled cells with periodic boundary conditions and physical walls in the absence of particle rearrangements (see the inset to Fig. 4 (a)). $G_{c0}(\theta)$ gives the single-cell shear modulus in the zero-pressure limit and $\lambda_c(\theta) = dG_c(\theta)/dp$ gives the slope [15]. In Fig. 4 (d)-(f), we plot $\lambda_c(\theta)$ as a function of $\theta$ for all $N = 4$ disk-filled cells without rattlers. We show that $\lambda_c(\theta) = \lambda_{c,a} \sin[4(\theta - \theta_0)] + \lambda_{c,dc}$ varies sinusoidally with period $\pi/2$, where $\lambda_{c,a}$ is the amplitude, $\theta_0$ is the phase shift, and $\lambda_{c,dc}$ is the mean value of $\lambda_c(\theta)$ [27]. (Previous studies have shown that the shear modulus of jammed packings of spherical particles is sinusoidal with period $\pi/2$ [11, 38].) $\lambda_c(\theta) < 0$ for nearly all $\theta$ values and disk-filled cells for periodic boundary conditions, except for configuration 2 (Fig. 3 (a)) in the range $0.2 \leq \theta/\pi \lesssim 0.3$ (Fig. 4 (d)). For disk-filled cells with fixed-length and flexible walls, we observe similar sinusoidal behavior for $\lambda_c(\theta)$, but there are large $\theta$ ranges where $\lambda_c(\theta) > 0$. Our results showing that $\lambda_{c,a} \sim \lambda_{c,dc}$ emphasize that disk-filled cells at small $N$ are highly anisotropic. For disk-filled cells with flexible walls, we do not find a correlation between $\lambda_c(\theta) > 0$ and the occurrence of quartic modes as discussed in Sec. III A.

We focus on the response of the system to simple shear
strain, but to fully describe the pressure-dependent mechanical properties for anisotropic materials, all six components of the stiffness matrix must be determined. In Appendix B, we derive the $\theta$-dependence for all six stiffness matrix elements $C_{ij}$, where $C_{33}$ gives the shear modulus for isotropic materials. In addition, our previous studies have shown that the sign of $\lambda_c$ ($\theta = 0$) is determined by the second derivative of the packing fraction at jamming onset with respect to $\gamma$ in jammed packings of spherical particles in periodic boundary conditions [15, 37]. In Appendix C, we show that this relation is still true at any $\theta$ in disk-filled cells with fixed-length walls.

As $N$ increases, the probability $P_+$ to obtain a disk-filled cell with $\lambda_c(\theta) > 0$ decreases rapidly for periodic boundary conditions. As shown in Fig. 5, we do not find $\lambda_c(\theta) > 0$ for cells with $N \geq 6$ for periodic boundary conditions. For disk-filled cells with physical walls, $P_+$ also decreases with increasing $N$, but not as rapidly as that for cells with periodic boundary conditions. These results emphasize that if one wants to tune the pressure dependence of $G_c(\theta)$ (i.e., between $\lambda_{c,\alpha} > 0$ and $\lambda_{c,\alpha} < 0$), one should employ disk-filled cells with small $N$.

We next investigate the dependence of $\lambda_c(\theta)$ on the particle-wall stiffness $\epsilon_{pp}/\epsilon_{pp}$ and wall stiffness $\epsilon_{bb}/\epsilon_{pp}$ relative to the strength of the repulsive interparticle interactions in disk-filled cells with fixed-length and flexible physical walls. In Fig. 6 (a), we show that for configuration 4 depicted in Fig. 3 (b), $\lambda_{c,a}$, $\lambda_{c,dc}$, and $\theta_0$ undergo only small variations when $\epsilon_{pp}/\epsilon_{pp}$ changes by nearly two orders of magnitude. $\lambda_{c,a}$ and $\lambda_{c,dc}$ converge for $\epsilon_{pp}/\epsilon_{pp} \geq 10$ for all $N = 4$ disk-filled cells with fixed-length physical walls (Fig. 6 (b) and (c)). For configuration 4, we find that $\lambda_c(\theta) > 0$ for a finite range of $\theta$ in the large $\epsilon_{pp}/\epsilon_{pp}$ limit. We can also fix $\epsilon_{pp}/\epsilon_{pp}$ and show that $\lambda_{c,a}$, $\lambda_{c,dc}$, and $\theta_0$ converge in the large $\epsilon_{pp}/\epsilon_{pp}$ limit. (See Fig. 6 (d)-(f).) We find that $\lambda_c(\theta) < 0$ (for all $\theta$) at large $\epsilon_{bb}/\epsilon_{pp}$ for all $N = 4$ configurations with flexible physical walls, since $\lambda_{c,dc} < 0$ and $\lambda_{c,a} < |\lambda_{c,dc}|$. These results emphasize that disk-filled cells with flexible physical walls become similar to cells with periodic boundary conditions (with $\lambda_c(\theta) < 0$) in the large $\epsilon_{bb}$-limit. Thus, particle-wall interactions are essential for $\lambda_c(\theta) > 0$.

C. Shear modulus versus pressure for tessellated granular metamaterials

We now study the pressure-dependence of the shear modulus $G(\theta)$ for tessellated granular metamaterials (Fig. 1) constructed from multiple disk-filled cells with flexible walls, $\epsilon_{pp}/\epsilon_{pp} = 1$, and $\epsilon_{bb}/\epsilon_{pp} = 0.1$. In Fig. 7...
(a), we show $G(\theta)$ versus $p$ for $N_c = 36$ cells that each contain configuration 5 from Fig. 3 (c). Similar to the results for $G_c(\theta)$ for single cells, the mechanical response of tessellated granular metamaterials shows strong shear angle dependence. In particular, for some values of $\theta$, the slope of $G(\theta)$ versus $p$, $\lambda(\theta) > 0$, and for other values, $\lambda(\theta) < 0$. In Fig. 7 (b), we show that $\lambda(\theta)$ possesses weak system-size dependence as $N_c$ is increased. $\lambda(\theta)$ for the multi-cell system in the large-$N_c$ limit converges to $\lambda_c(\theta)$ for a single cell with flexible walls with $\epsilon_{bb}/\epsilon_{pp} = 0.05$, which is half of the value for the multi-cell system. This result can be explained because each wall in the tessellated granular metamaterial is shared by its neighboring cell except for those on the exterior. Since $\lambda(\theta)$ for the tessellated granular metamaterial mimics that for single cells, with fixed outer wall endpoints during compression and shear, which causes the deviations in $G(\theta)$ versus $p$. Therefore, to ensure that tessellated granular metamaterials lock-in single-cell behavior, it is necessary to constrain all of the outer wall endpoints.

IV. CONCLUSIONS AND FUTURE DIRECTIONS

In the large-system limit, the shear modulus $G$ of static packings of spherical particles increases with pressure due to frequent particle rearrangements and non-affine particle motion that enable the packings to increase their contact number with increasing pressure. In this work, we investigate a novel class of granular materials, tessellated granular metamaterials, that allow us to control the slope of the shear modulus versus pressure by preventing particle rearrangements even in the large-system limit. We focus on tessellated granular metamaterials in two dimensions, which are collections of $N_c$ coupled cells that each contain $N$ bidisperse disks enclosed by four physical walls. In particular, we can design tessellated granular metamaterials with negative slope of the shear modulus with pressure even in the large-$N_c$ limit.

We first studied the mechanical properties of single disk-filled cells with three sets of boundary conditions: periodic boundary conditions, fixed-length physical walls, and flexible physical walls. Packings with small $N$ do not undergo frequent particle rearrangements, and thus we enumerated all possible mechanically stable disk-filled cells with all three boundary conditions.
FIG. 8. (a) Tessellated granular metamaterial with $N_c = 36$ described in Fig. 7, except now some of the wall endpoints marked by red crosses are no longer fixed after the applied isotropic compression and simple shear strain. (b) Shear modulus $G(0)$ measured at $\theta = 0$ as a function of pressure $p$ when different wall endpoints on the outer boundary are switched from fixed to mobile (blue circles: all outer wall endpoints are fixed, red crosses: endpoint 1 is mobile, magenta upper triangles: endpoint 2 is mobile, black squares: endpoint 3 is mobile, yellow diamonds: endpoint 4 is mobile, green left triangles: endpoints 1 and 3 are mobile, cyan crosses: endpoints 2 and 4 are mobile, and purple asterisks: endpoints 1-4 are mobile). (c)-(d) Tessellated granular metamaterials at $p = 0.01$ when (c) endpoint 1 is mobile, and (e) endpoints 1-4 are mobile.

for $N \leq 8$. We find that the mechanically stable disk-filled cells with periodic boundary conditions and fixed-length physical walls are either isostatic or hyperstatic, while those with flexible physical walls can be hypostatic, as well as isostatic and hyperstatic. The hypostatic disk-filled cells with flexible physical walls are stabilized by quartic modes, as found for hypostatic packings of non-spherical and deformable particles. Second, we showed that the shear modulus of single disk-filled cells depends linearly on pressure, $G_c(\theta) = \lambda_c(\theta)p + G_c(0)$. Further, the slope of the shear modulus versus pressure for single disk-filled cells is strongly anisotropic, i.e. $\lambda_c(\theta) = \lambda_{c,dc} + \lambda_{c,a}\sin(4(\theta - \theta_0))$ and $\lambda_{c,a} \sim \lambda_{c,dc}$. We find that $\lambda_c(\theta) < 0$ for single disk-filled cells in periodic boundary conditions with $N > 4$. In contrast, disk-filled cells with fixed-length and flexible physical walls and small $N$ can possess either $\lambda_c(\theta) > 0$ or $\lambda_c(\theta) < 0$. However, the probability of obtaining disk-filled cells with $\lambda_c(\theta) > 0$ vanishes in the large-$N$ limit. After studying the mechanical response of single disk-filled cells, we investigated the shear modulus of tessellated granular metamaterials formed by connecting many single disk-filled cells with flexible walls. We showed that we can lock-in the mechanical response of single disk-filled cells in tessellated granular metamaterials. The ability to lock-in the mechanical response of single cells in multi-cell systems is reduced if the outer wall endpoints are free to move during energy minimization after applied deformations. These results demonstrate that we can build large-scale granular metamaterials whose mechanical properties do not change after repeated cycles of compression and decompression, as well as positive and negative simple shear strain, since particle rearrangements are eliminated.

These findings raise many interesting directions for future research. First, we found that the mechanical response of both single and multiple-cell granular systems is highly anisotropic. To fully understand the pressure-dependent mechanical properties of anisotropic materials.
in two dimensions, we must characterize all 6 stiffness matrix components as a function of pressure. Second, for the current studies, we fixed all of the outer wall endpoints during energy minimization to enforce nearly affine simple shear of tessellated granular metamaterials. However, when the outer wall endpoints are not fixed, the individual disk-filled cells can change their shape during energy minimization that follows the applied compression and simple shear strain. Thus, it will be interesting to study and predict the pressure dependence of $G_c(\theta)$ of single disk-filled cells when the outer wall endpoints are free to move or bending ending is included between adjacent endpoints to generate cells with arbitrary shapes. Third, we have focused on tessellated granular metamaterials composed of identical single cells. In future studies, we will consider tessellated granular metamaterials composed of single cells with different disk configurations and boundaries with varied $\epsilon_{pb}$ and $\epsilon_{bb}$ to understand how the mechanical properties of single cells determine the mechanical properties of the multi-cell system. Fourth, we will extend our studies of tessellated granular metamaterials to three dimensions. In three dimensions, there are three principal simple shear directions, instead of one in two dimensions, which provides additional ways to design tessellated granular metamaterials. For example, we can create strongly anisotropic tessellated granular metamaterials by having some cells possess $\lambda_c(\theta) > 0$ in one shear direction, others possess $\lambda_c(\theta) < 0$ in another shear direction, and others possess $\lambda_c(\theta) > 0$ in the remaining shear direction.

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Appendix A: Isostaticity in a single cell

In this Appendix, we discuss the number of degrees of freedom $N_d$ in disk-filled cells for all three boundary conditions. In periodic boundary conditions, $N_d = 2N' - 2 + 1 = 2N' - 1$, where $N' = N - N_r$ and $N_r$ is the number of rattler disks. In this expression, the $-2$ comes from the two global translational degrees of freedom in periodic boundary conditions and the $+1$ comes from the size degree of freedom of the disks. For the degrees of freedom in disk-filled cells with fixed-length and flexible walls, we must include the degrees of freedom of the wall endpoints, as well as the disks: $N_d = 2N' + 2N_v - N_B - 3 + 1$. Here, $N_v = 4$ is the number of wall endpoints, $N_B$ is the number of constraints associated with the walls, the $-3$ comes from the two rigid-body translational and one rotational degree of freedom, and the $+1$ comes from the size degree of freedom of the disks. For flexible walls, four springs connect the wall endpoints, and hence $N_B = 4$. For fixed-length walls, in addition to the length constraint for each wall, the angle between any two neighboring walls is also fixed, and thus $N_B = 5$. Hence, $N_d = 2N' + 1$ for cells with fixed-length walls and $N_d = 2N' + 2$ for flexible walls. For isostatic packings, the total number of contacts satisfies $N_c = N_d$. A packing is hyperstatic when $N_c > N_d$ and hypostatic when $N_c < N_d$. We show that the probability of obtaining a hyperstatic or hypostatic disk-filled cell decreases with increasing $N$ for all three boundary conditions as shown in Fig. 9. We note that there are a finite number of hypostatic packings in disk-filled cells with flexible walls even at $N \leq 16$, which highlights the effect of soft physical walls on the structural and mechanical properties of jammed granular materials.

Appendix B: Stiffness matrix after rotation

In this Appendix, we show the angular dependence of all elements of the stiffness matrix $C$, which relates stress and strain. At a predefined orientation with $\theta = 0$, we can calculate the stiffness matrix $C(0)$. After rotating the configuration by an angle $\theta$ clockwise, the stiffness matrix becomes $C(\theta) = \hat{R}^T(\theta)C(0)\hat{R}(\theta)$, where

$$\hat{R}(\theta) = \begin{pmatrix}
\cos^2 \theta & \sin^2 \theta & -\frac{1}{2} \sin 2\theta \\
\sin^2 \theta & \cos^2 \theta & \frac{1}{2} \sin 2\theta \\
\sin 2\theta & -\sin 2\theta & \cos 2\theta
\end{pmatrix}. \quad (B1)$$
Using Eq. B1, we find the following angle-dependent stiffness matrix elements:

\[
\hat{C}_{11}(\theta) = \hat{C}_{11}(0) \cos^4 \theta + \hat{C}_{22}(0) \sin^4 \theta \\
+ \hat{C}_{33}(0) \sin^2(2\theta) + \frac{1}{2} \hat{C}_{12}(0) \sin^2(2\theta) \\
+ 2\hat{C}_{13}(0) \sin(2\theta) \cos^2 \theta \\
+ 2\hat{C}_{23}(0) \sin(2\theta) \sin^2 \theta,
\]  

(B2)

\[
\hat{C}_{12}(\theta) = \left( \frac{1}{4} (\hat{C}_{11}(0) + \hat{C}_{22}(0)) - \hat{C}_{33}(0) \right) \sin^2(2\theta) \\
+ \hat{C}_{12}(0) \left( \sin^4 \theta + \cos^4 \theta \right) \\
+ \frac{1}{2} \hat{C}_{33}(0) \sin(4\theta) + \frac{1}{4} \hat{C}_{12}(0) \sin(4\theta) \\
+ \hat{C}_{13}(0) \cos^2 \theta (2\cos(2\theta) - 1) \\
+ \hat{C}_{23}(0) \sin^2 \theta (2\cos(2\theta) + 1),
\]

(B3)

\[
\hat{C}_{13}(\theta) = -\frac{1}{2} \hat{C}_{11}(0) \sin(2\theta) \cos^2 \theta + \frac{1}{2} \hat{C}_{22}(0) \sin(2\theta) \sin^2 \theta \\
+ \frac{1}{2} \hat{C}_{33}(0) \sin(4\theta) + \frac{1}{4} \hat{C}_{12}(0) \sin(4\theta) \\
+ \hat{C}_{13}(0) \cos^2 \theta (2\cos(2\theta) - 1) \\
+ \hat{C}_{23}(0) \sin^2 \theta (2\cos(2\theta) + 1),
\]

(B4)

\[
\hat{C}_{22}(\theta) = \hat{C}_{11}(0) \sin^4 \theta + \hat{C}_{22}(0) \cos^4 \theta + \hat{C}_{33}(0) \sin^2(2\theta) \\
+ \frac{1}{2} \hat{C}_{12}(0) \sin^2(2\theta) - 2\hat{C}_{13}(0) \sin(2\theta) \sin^2 \theta \\
- 2\hat{C}_{23}(0) \sin(2\theta) \cos^2 \theta,
\]

(B5)

\[
\hat{C}_{23}(\theta) = -\frac{1}{2} \hat{C}_{11}(0) \sin(2\theta) \sin^2 \theta + \frac{1}{2} \hat{C}_{22}(0) \sin(2\theta) \cos^2 \theta \\
- \frac{1}{2} \hat{C}_{33}(0) \sin(4\theta) - \frac{1}{4} \hat{C}_{12}(0) \sin(4\theta) \\
+ \hat{C}_{13}(0) \sin^2 \theta (2\cos(2\theta) + 1) \\
+ \hat{C}_{23}(0) \cos^2 \theta (2\cos(2\theta) - 1),
\]

(B6)

\[
\hat{C}_{33}(\theta) = \frac{1}{4} (\hat{C}_{11}(0) + \hat{C}_{22}(0) - 2\hat{C}_{12}(0)) \sin^2(2\theta) \\
+ \frac{1}{2} (\hat{C}_{23}(0) - \hat{C}_{13}(0)) \sin(4\theta) \\
+ \hat{C}_{33}(0) \cos^2 (2\theta).
\]

(B7)

Eqs. B2-B7 show that generally all six elements of the reference stiffness matrix contribute to each \( \hat{C} \) element at a given angle \( \theta \). Therefore, in anisotropic materials, it is important to track all \( \hat{C} \) elements to fully characterize their mechanical properties.

FIG. 10. (a) Shear modulus \( G_c(\theta) \) for a single cell containing a monodisperse \( N = 2 \) disk packing with fixed-length walls at shear angle \( \theta = 0 \) (red squares and red solid line) and \( \pi/4 \) (blue circles and blue solid line) as a function of pressure \( p \). The squares and circles show results from the numerical simulations and analytical calculations using Eq. C1. The inset shows the \( N = 2 \) disk-filled cell at simple shear strain \( \gamma = 0 \) and \( \theta = 0 \). (b) Packing fraction \( \phi_J \) of the single cell in (a) at jamming onset as a function of \( \gamma \) at several values of \( \theta \) as indicated by the different colors and symbols. The symbols and solid lines correspond to the results from the numerical simulations and analytical calculations using Eqs. C2-C8.

Appendix C: Relation between shear modulus and mixed shear strain derivatives

In this Appendix, we verify that the pressure-dependence of the single-cell shear modulus is related to the variation of the packing fraction at jamming onset \( \phi_J \) with simple shear strain \( \gamma \) as shown in previous studies [37]. We illustrate this relationship using a single cell containing the \( N = 2 \) monodisperse disk packing with fixed-length walls in the inset to Fig. 10 (a) since \( \phi_J(\gamma) \) can be calculated analytically for this case. The shear modulus can be written in terms of three mixed
derivatives of the simple shear strain:

\[ G = \frac{d\Sigma}{d\gamma} = \frac{1}{A} \left( \frac{d}{d\gamma} \left( \frac{d\phi}{d\gamma} p \right) \right) \phi \]

(C1)

In Fig. 10 (a), we demonstrate that Eq. C1 still holds for single disk-filled cells with fixed-length walls.

The second term in Eq. C1 is proportional to \( p \), with \( \left( \frac{d}{d\gamma} \left( \frac{d\phi}{d\gamma} \right) p \right) \phi > 0 \) for single cells with \( N \geq 6 \) and periodic boundary conditions [15]. In contrast, the first and third terms in Eq. C1 do not possess strong \( p \)-dependence. Therefore, the second derivative of \( \phi_J(\gamma) \) typically determines whether \( G \) will increase or decrease with \( p \). In particular, if \( \phi_J(\gamma) \) is concave upward, \( G \) decreases with increasing \( p \), and vice versa.

For the single cells with the \( N = 2 \) monodisperse disk packing and fixed-length walls, we can analytically determine the packing fraction at jamming onset \( \phi_J \) as a function of the simple shear strain \( \gamma \) and shear angle \( \theta \):

\[ \phi_J(\theta, \gamma) = \frac{\pi (B - \sqrt{B^2 - 4AC})^2}{2A^2}, \]

(C2)

where \( A, B, \) and \( C \) are given by

\[ A = 4 \cot^2 \alpha, \]

\[ B = -4(a \cot \alpha + b(\cot \alpha \cos(2\alpha) + \sin(2\alpha))), \]

\[ C = a^2 + 2ab \cos(2\alpha) + b^2, \]

and \( a, b, \) and \( \alpha \) are given by

\[ a = \sqrt{1 - 2\gamma \sin \theta \cos \theta + \gamma^2 \sin^2 \theta}, \]

\[ b = \sqrt{1 + 2\gamma \sin \theta \cos \theta + \gamma^2 \cos^2 \theta}, \]

\[ \alpha = \frac{1}{2} \cos^{-1} \left( \frac{\gamma(\cos^2 \theta - \sin^2 \theta) - \gamma^2 \sin \theta \cos \theta}{ab} \right). \]

We verify in Fig. 10 (b) that \( \phi_J(\theta, \gamma) \) determined by the numerical simulations matches that predicted by Eq. C2. At \( \gamma = 0 \), which is where \( G_c(\theta) \) is measured throughout the main text, we find that the \( \phi_J(\gamma) \) is concave downward at \( \theta = 0 \) and concave upward at \( \theta = \pi/4 \) (Fig. 10 (b)). Thus, since \( \lambda(\theta) \) switches sign, we expect a saddle point to occur in the \( \phi_J(\gamma, \theta) \) plane between \( \theta = 0 \) and \( \pi/4 \). In future studies, we will apply a similar approach that generated Eq. C1 to obtain the pressure-dependence of all elements of the stiffness matrix.


