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Stiffness transition in anisotropic fiber nets

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We demonstrate the existence of a percolationlike stiffness transition in fiber networks with a bidisperse orientation distribution and with fiber densities clearly above the geometrical and the ordinary stiffness transition. The fibers are oriented parallel and perpendicular to a strain direction and they have a large fiber aspect ratio. The stiffness $K$ of the fiber nets can be described by a scaling relation, $K \propto \tau^{\gamma g((\epsilon - \epsilon_c)/\tau)}$, where $\tau$ is the fraction of fibers parallel to strain. $g$ is a scaling function that is roughly described by a power law $g(x) \propto x^{\gamma - 1}$ for stiffness above the transition and by a constant below the transition. The transition point is characterized by qualitative changes in the distribution of the elastic deformation energy of the fibers, the deformation mode of the fibers, the effective Poisson ratio of the nets, the distribution of elastic energy on fibers and cross links, and the ratio of elastic and viscous dissipation energy. This transition opens the possibility of extreme stiffness variations with minimal mesh manipulations in the vicinity of the transition (i.e., a stiffness gate). It is possible that this transition affects the mechanical behavior of the cytoskeleton in cells.

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I. INTRODUCTION

Fiber networks are materials made of stiff fibers connected in a more or less random way to form a mesh. If the fibers have a large aspect ratio (i.e., length to width ratio) it is possible to construct a connected material with a very low solid volume fraction. A low volume fraction enables design of materials that are very light and the network structure provides the possibility to tune properties such as strength, conductivity, and optical properties. Glass fiber and Kevlar are the classic examples.

Here we consider a particular type of fiber network. The nets we are interested in have the majority of fibers oriented either perpendicular or parallel to the direction of applied strain. As demonstrated below, this anisotropy results in an extreme mechanosensitivity at a critical point. These types of anisotropic networks also seem to play a significant role in the mechanical behavior of, for example, endothelial or aortic smooth muscle cells [1–5]. Technological examples include structures made of carbon nanotubes such as carbon nanotube sheets, also called “buckypaper” due to structural resemblance to paper. Carbon nanotube sheets are a candidate for extremely strong yet lightweight materials [6–10].

To understand the mechanical behavior of the type of fiber nets described above, we investigate the variations of stiffness caused by changes in the mesh texture. Such changes include parameters such as density, connectivity, orientation, dispersion, and strain.

A mesh has no stiffness for densities below geometric percolation. As the density reaches the percolation threshold, stiffness appears, unless the fibers are springs that do not possess any bending stiffness [11]. Close to, but above the percolation point, there is a critical regime, and above that a mesh of slender fibers enters the nonaffine regime. Finally, at high densities the affine regime appears [12–18]. A network made of fibers without bending stiffness reaches the so-called stiffness transition at a critical value for the coordination number [19].

We investigate a three-dimensional (3D) fiber mesh in the nonaffine regime with fibers oriented either parallel or perpendicular to an external unidirectional strain $\epsilon$ with only Poisson contraction in the perpendicular directions. The texture is changed via a parameter $\tau$ that determines the relative fraction of parallel and perpendicular fibers. The third important parameter is the mesh density $\rho$. We demonstrate that as these networks are stretched, they reach a critical point at which stiffness increases suddenly by several orders of magnitude. The strain at which the transition appears is governed by the parameter $\tau \rho$. The transition may appear for any mesh density clearly above the percolation transition and below the affine regime.

The mechanism behind this stiffness transition can be described as follows: Below the transition, the number of fibers parallel to the strain direction is too small and force has to be carried mainly along perpendicular filaments. This means that the stiffness of the mesh is dominated by the transverse stiffness modes of the fibers. The dominating transverse deformation mode for slender fibers is bending, which scales as $Ew^4/l^3$, where $E$ is Young’s modulus of the fiber material and $w/l$ the aspect ratio of the fibers. Above the transition point, the parallel fibers are enough to carry the majority of the load. The parallel fibers deform mainly by stretching, which means that stiffness scales as $Ew^2/l$. As the aspect ratio of the fibers becomes very small, even a single path of mainly parallel fibers crossing the mesh is enough to dominate its stiffness behavior. Consequently, for such meshes it is reasonable to expect that stiffness will display a percolationlike transition in stiffness when the ratio of parallel to perpendicular fibers is varied. We use a numerical simulation model for mechanical tension tests of 3D fiber networks [18] to demonstrate the transition. Reminiscent nonlinear strain-dependent stiffness in fiber networks has also been observed for other types of meshes as reported in, for example, Refs. [18,20].

For applications, this stiffness transition offers an opportunity to design fiber networks that can switch between a stiff and a floppy mode near the transition point with minimal
manipulations of the mesh. Such a property may be used in the design of intelligent materials functioning as stiffness gates and actuators. It also seems quite reasonable that such a transition could play a role in, for example, the stiffness response of cellular cytoskeletons. The model demonstrates, for example, why dense bundles of filaments, so-called stress fibers, in the direction of an externally applied strain on a cell [1,2] are such an efficient way to alter stiffness. In such a bundle, \( \tau \approx 1 \) and \( \rho \) are considerably increased compared to the cytoskeleton in general. Since the governing parameter for the transition is \( \tau_0 \rho \), it means that formation of stress fibers immediately takes a mesh above the transition point, which would increase stiffness of the cytoskeleton by several orders of magnitude if the starting point is at or below the transition.

II. MODELS AND METHODS

We use a recently developed a three-dimensional (3D) computational model to simulate the tension of fiber networks [18,21]. The model consists of stiff 3D fibers cross linked to each other by springs at fiber-fiber intersections. All fibers are considered to be identical and straight under zero loading conditions. Individual fibers have a finite length \( l \) and width \( w \). The fibers have a random, uncorrelated and uniform center-of-mass distribution. Substrate is applied in the \( x \) direction. The orientation distribution is such that fibers have an orientation that is limited to \( \pm 0.1 \pi \) radians to either the direction parallel to the applied strain or perpendicular. The orientation distribution is uniform in the perpendicular plane. Boundary conditions are such that the \( y \) and \( z \) directions are free, while the ends of the mesh are clamped and forced to move in the \( x \) direction (i.e., the clamped ends are free to move in the \( yz \) plane). The mass of each fiber is discretized to a set of points (of mass \( m \)) at equal distances along the fiber (10 mass points per fiber were used). Each pair of mass points belonging to different fibers and closer than some threshold \( \delta l \), are cross linked by a spring with spring constant \( k \). The force between two cross-linked mass points only depends on the distance between them. The mesh obtained through this deposition process is taken as the initial configuration. Figure 1 provides an illustration of the system.

A segment, bounded by two mass points, is modeled by an Euler-Bernoulli beam [22]. Each such elastic beam can be deformed by stretching, bending, transverse, and torsional displacements. The aspect ratio of the fibers was chosen to be \( \lambda \approx 30 \). This choice guarantees that shear deformations remain small and can be neglected. To properly describe the elastic modes for each segment, a stiffness matrix \( K \) is constructed. To fully account for the degrees of freedom for the segmental endpoints, the matrix has a size of \( 12 \times 12 \). For the stiffness matrix of the whole mesh, these segmental matrices must be expanded and added together. Details are provided in our previous papers [18,21].

Global strain is applied by moving the opposite boundaries away from each other in the \( x \) direction by \( \pm \delta x \), where \( \delta x \equiv \delta x(t) \).

The equation of motion for the deformation field of the mesh is a discrete version of Newton’s equation of motion with dissipation,

\[
M\ddot{r} + C\dot{r} + K\overrightarrow{r} = 0 . \tag{1}
\]

The term for viscous damping, \( C \), is a diagonal matrix containing the damping coefficients, and \( M \) describes the inertia of the mass points. Column vector \( \overrightarrow{r} \) contains the position vectors of all mass points. Since the time derivatives of \( \overrightarrow{r} \) remain small at all times, we use the diagonal (or so-called lumped mass and damping matrices) instead of the consistent mass and damping matrices with off-diagonal elements. We use a dynamic approach and do not try to solve for the elastic equilibrium as a unique equilibrium does not necessarily exist for a mesh that contains springs [11].

As the mass points move in discrete time steps, the segments deform and the network geometry changes. In a fiber-mesh material constructed of slender fibers with a lot of empty space between, the fibers will begin to align themselves in the direction of stretching as strain increases. This implies that the stiffness matrix evolves over time. Changes in the stiffness matrix imply that \( K \) is also a function of \( \overrightarrow{r} \) and hence the equation of motion becomes nonlinear through the third term in Eq. (1), which becomes \( \int_0^\tau K[\overrightarrow{r}(\tau')]d\overrightarrow{r}(\tau') \).

While rotations and translations of the individual segments can be large, elastic deformations remain small. This allows a simplification since we can neglect nonlinear higher-order terms in calculating the elastic deformation forces.

The computational model contains two options for fibers that collide during deformation of the mesh. Either fibers repel each other via an elastic force or they behave like ghost fibers and do not interact. The first option is, obviously, the physically more correct while the other is computationally more efficient. Both options were tested. As the total number of collisions typically remain small during stretching of a mesh, there are only minor differences between the two. Therefore most results were obtained with the second option.

The behavior of the model is invariant under parameter rescaling as long as the relations between the terms in Eq. (1) remain constant. Since the model is largely scale invariant, the parameters that are relevant when comparing with, for example, actin-myosin systems are dimensionless. These parameters are: the aspect ratio of the fibers \( \lambda \), the dimensionless density of fibers \( \delta x(t) \)
unit-volume), and the ratio between the stiffness of the fibers and the cross links. In the simulations done here, the first term in Eq. (1) is largely negligible (i.e., the dynamics of the model is controlled by the balance between elastic and damping forces). The crossover between elastic- and viscotic-dominated regimes are determined by, \( c\dot{\epsilon}/E\epsilon \), where \( c \) is the damping coefficient, \( E \), Young’s modulus of the fibers, \( \epsilon \) is strain, and \( \dot{\epsilon} \) its time derivative.

The dimensionless parameters, except for the crossover parameter, determine the relative variations in the entries of the stiffness matrix \((K\text{ matrix})\) [18,21]. For a typical mesh they can be reduced to two parameters only. These two governing parameters are the aspect ratio of a fiber segment and the stiffness ratio for the cross links and the fiber segment. The model parameters used in the simulations were chosen to give fairly similar values for these two dimensionless parameters as typical values for an actin-myosin mesh \((E = 2 \text{ GPa} [23], \ w = 7 \text{ nm} [24], \text{ mesh size } \sim 100 \text{ nm} [24], \text{ and } k \sim 0.1 \text{ pN/nm} [25])\).

In the numerical model all lengths are measured in units of \( l \) (i.e., \( l = 1 \)). The thickness of the fiber was \( w = 0.001 \text{ mass } m = 2 \times 10^{-5}, \text{ damping in the range } c = 10^{-5} - 10^{-7}, \) and Young’s modulus \( E = 10^7 - 10^9 \). The spring constant of the cross links was set to \( k = 0.6 \). Strain rate was of the order \( 10^{-2} \).

The values for actin mesh and the numerical model gives aspect ratios of the order of \( 10^3 - 10^5 \), and stiffness ratios of the order of \( 10^7 - 10^9 \).

III. RESULTS

Figure 2 shows snapshots of two different meshes [26]. The network in Fig. 2(a) contains 1000 fibers, while the network in Fig. 2(c) contains 1300 fibers. The average number of contacts per fiber is close to six in both cases. This is clearly above the percolation threshold at \( \approx 1 \) contact per fiber on average [27]. Figure 2(a) shows a mesh with \( \tau = 0.45 \) at zero strain, while Fig. 2(b) is the same mesh at strain \( \epsilon = 0.3 \). Figures 2(c) and 2(d) display snapshots for a mesh at similar strains but with \( \tau = 0.04 \). The network in Fig. 2(b) is clearly above the stiffness transition point, while the mesh in Fig. 2(d) is right at the transition point. The strained meshes in Figs. 2(b) and 2(d) shows clearly the qualitative difference in mechanical behavior under strain. In Fig. 2(d) visible gaps are opening up between the weakly connected perpendicular fibers. These gaps grow significantly to the strain of the mesh, and they are formed by rather gentle bending of the fibers. In contrast, the cross links are much more deformed in Fig. 2(b), Poisson contraction is stronger, the parallel fibers are stretched, and the perpendicular fibers are bent to a much larger degree.

Figure 3 shows the effective stiffness \( K \) of a set of meshes with different fractions of parallel fibers, as a function of strain, \( \epsilon \), for a constant mesh density \( \rho \).

If \( K(\epsilon, \tau) \) is expected to display percolation-type critical behavior it is reasonable to postulate a scaling relation of the form

\[
K \propto \tau^\alpha g[(\epsilon - \epsilon_c)/\tau^{-\beta}].
\]

where \( g \) is a scaling function, \( \epsilon_c \) the critical strain, and \( \alpha, \beta \) are scaling exponents. Equation (2) represents the general form of percolation-type scaling relations [28,29]. The function, \( g \) represents the strength of the percolating cluster, which in our case is represented by paths of fibers that are deformed by stretching as opposed to bending only. Below the transition there are no such paths and one would expect \( g(\epsilon) \) to be roughly a constant and right above the transition a power law, \( g(\epsilon) \sim \epsilon^{-7} \). Equation (2), with \( g \) a constant for strain below \( \epsilon_c \), and a power law above \( \epsilon_c \), is fitted to simulation data in Fig. 3(a). The best fits are given by \( \gamma \approx 1.65 \). The fitted parameters \( \alpha, \beta, \) and \( \epsilon_c \) are summarized in Fig. 3(b).

As is evident from Figs. 3 and 4, the scaling relation Eq. (2) describes very well the simulation results for the stiffness of anisotropic fiber networks. This equation can be used for collapsing the simulated \( K(\epsilon) \) for different \( \tau \) onto a single curve. The results are displayed in Fig. 4. In Fig. 4(a) the fitted values for the individual curves, represented by the markers in
Fig. 3. (a) Stiffness, $K$, as a function of strain, $\epsilon$. Curves obtained for different $\tau$ ranging from 0.1 to 0.8 are displayed. Simulation data is shown by markers and fits to Eq. (2) by lines. The function $g$ is set to be a constant at strain below a critical value and a power law $\chi^{1.65}$ at strain above the critical point. The exponent $1.65$ is a fit. (b) Fitted values, as a function of $\tau$, for the parameters $\alpha$, $\tau^{0.65}$, and $\epsilon_c$ in Eq. (2). The fitted lines represent $\alpha \approx 1.1$, $\beta \approx 0.3$, $\epsilon_c \approx \tau^{-1.2}$.

Fig. 3(b), are used to perform the data collapse. In Fig. 4(b) the averaged values, represented by the lines in Fig. 3(b), are used for the collapse. The collapse in Fig. 4(a) works excellently, except for a minor cross-over region observed close to the critical point. Obviously, the collapse using the averaged values in Fig. 4(b) does not work quite as well as in Fig. 4(a), but still reasonably well.

Figures 3 and 4 are obtained for a constant mesh density $\rho$. In order to investigate the effect of changes on density, the elastic energy $W$ was recorded at constant strain for three different densities, $\rho$, and varying $\tau$. Notice that for a constant strain $W \propto K$. The result is displayed in Fig. 5(a). The energy is scaled by $\rho$. $\tau$ is scaled by $\rho_0/\rho$, where $\rho_0 = 100$. The data points in Fig. 5 fall on a single curve indicating that $\tau$ should be replaced by $\tau \rho$ in Eq. (2) for the case of varying $\rho$.

The fact that $\tau \rho$, rather than just $\tau$, governs the transition indicates that it is not the fraction of fibers in the parallel direction that is important. It is the density of fibers in this direction that induces the transition. The scaling by $\rho$ on the vertical axis is simply a consequence of the stiffness being approximately proportional to the density of fibers.

To investigate finite-size effects, three different sizes for the lowest density in Fig. 5(a) were studied. The mesh size was increased from $V_0 = 2.5 \times 2.5 \times 1.5$ to $2V_0$ and $4V_0$. No significant changes in the dependence of $W/\rho$ on $\tau \rho$ could be observed. This result is displayed in Fig. 5(b).

Notice also that the exponents in Eq. (2) differ clearly from the exponent of bond bending rigidity transition, $3.75$ [30].

To further investigate the characteristics of the transition, the distribution of the deformation energy on the fibers was calculated. For $\tau$ below the transition, the energy distribution follows a power law with an exponential large energy cutoff ($W_f^{-0.35} \exp[-W_f/10^{-6}]$) [31]. Such a distribution indicates that below the transition, the elastic energies are randomly scattered low numbers. The energies have almost the same distribution as if they would be given by $W_f \propto 10^{-6}$, with $\alpha$ a uniform random variable limited by some extreme values. Such a distribution would give $N(W_f) \propto 1/W_f$. At and above the transition point, the power law vanishes and a log-normal-like distribution appears.

The variations in the average fiber deformations were recorded for different values of $\tau$. In particular, the deformation angle $\phi$, which measures the deformation mode, was introduced. If a fiber is deformed perpendicular to, but not stretched or compressed along, its axis, then $\phi = \pi/2$. At the other limit when a fiber is only deformed along its axis $\phi = 0$.

To test the changes in the distribution of the angle $\phi$, a set of meshes with $\tau$ ranging from very small values well below
the transition to significantly above it were simulated. The resulting distributions fell into two distinct categories. The distributions in Fig. 6(b) are colored such that the blue lines are distributions below the transition and red ones above: the only significant change in the distribution of $\phi$ occurs right at the transition point. Below the transition there is a peak at $\cos(\phi) = 0$ and a rapid decay as $\cos(\phi) \to 1$: fibers below the transition prefer to deform by bending, while the fibers above the transition are stretched to a considerably larger degree.

This effect can also be seen by recording the maximum stretch of the fiber segments and comparing it to the average strain of the mesh. If fibers only bend the mesh can be strained without stretching the fibers and therefore the parameter, $\epsilon_{fm}$, which is the relation between the maximum stretch of the segments and the average mesh strain is very low below the transition point. It increases rapidly close to unity at the transition, as can be seen in Fig. 6(c). Also the ratio of the stretching energy of the fibers to the entire elastic deformation...
energy, including bending, behave in a similar fashion. This is demonstrated in Fig. 6(d). This figure displays $E_{\text{stret}}/E_{\text{elast}}$ as a function of mesh strain $\epsilon$.

Figure 6 can be interpreted as follows: Networks below $\tau_c$ are so soft that the observed stiffness is, to a large degree, a result of viscous damping. It is only when a mesh reaches the transition point and fiber can no longer only be bent that elastic stiffness become dominant. This means that the stiffness differences at the transition in Figs. 4 and 5 would actually be even larger if the already low strain rate would be further decreased.

As the fibers mainly deform by bending below and by stretching above the transition, while the deformation mode of the cross links remain unaffected, we also expect that the elastic deformation energy of the fibers in relation to the elastic deformation energy of the cross links increases with $\tau$ and that this increase would be most significant at the transition.

To test the above, the ratio of elastic energy and the viscous damping energy was measured as a function of $\tau$. As expected, Fig. 7(a) shows that this fraction increases with $\tau$ and that it exceeds unity roughly at the transition point. Figure 7(b) shows the ratio of the elastic energy of the fibers and the cross links, which follows a similar behavior, but with a more distinct transition at the critical point.

IV. SUMMARY AND DISCUSSION

We have demonstrated that stretched fiber networks with an anisotropic fiber orientation distribution display a stiffness transition that depends on the ratio of perpendicular to parallel fibers ($\tau$). For a small fraction of parallel fibers and at small strains, the mesh stiffness is dominated by the bending stiffness of fibers, which is considerably weaker than the tensile stiffness of the fibers. At a critical point that depends on $\tau$, the fiber density ($\rho$), and mesh strain ($\epsilon$), the fiber mesh can no longer be stretched by only bending the fibers and a crossover to a significantly larger stiffness appears. This crossover is described by a scaling function of the form $\tau^{\alpha}g[(\epsilon - \epsilon_c)/\tau^\beta]$, which indicates that there exists, apart from the rigidity transition, a critical stiffness transition, which appears in anisotropic networks well above the percolation and rigidity transition. Notice that the rigidity transition appears at the same density as the percolation transition for fibers with bending stiffness.

The stiffness transition has a number of potential applications, in particular in the design of smart mechanosensitive materials. Since at the transition the stiffness changes with minimal mesh manipulations, it is possible to envision using this property as a mechanosensitive gating mechanism. In light of this investigation, it is quite obvious why stress fibers in eucaryotic cells are so efficient in increasing stiffness of cells in a particular direction [1,2]. The filaments in stress fibers are strongly oriented in the strain direction and are closely packed together to form a dense bunch. It is also evident that once stress fibers begin to disintegrate, a threshold will be reached when they no longer significantly contribute to cell stiffness. Close to this threshold it is likely that cells can change their stiffness very rapidly and with minimal changes to the cytoskeleton.

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