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Mechanical Response of Common Millet (*Panicum miliaceum*) Seeds under Quasi-static Compression: Experiments and Modeling

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Abstract

The common millet (*Panicum miliaceum*) seedcoat has a fascinating complex microstructure, with jigsaw puzzle-like epidermis cells articulated via wavy intercellular sutures to form a compact layer to protect the kernel inside. However, little research has been conducted on linking the microstructure details with the overall mechanical response of this interesting biological composite. To this end, an integrated experimental-numerical-analytical investigation was conducted to both characterize the microstructure and ascertain the microscale mechanical properties and to test the overall response of kernels and full seeds under macroscale quasi-static compression. Scanning electron microscopy (SEM) was utilized to examine the microstructure of the outer seedcoat and nanoindentation was performed to obtain the material properties of the seedcoat hard phase material. A multiscale computational strategy was applied to link the microstructure to the macroscale response of the seed. First, the effective anisotropic mechanical properties of the seedcoat were obtained from finite element (FE) simulations of a microscale representative volume element (RVE), which were further verified from sophisticated analytical models. Then, macroscale FE models of the individual kernel and full seed were developed. Good agreement between the compression experiments and FE simulations were obtained for both the kernel and the full seed. The results revealed the anisotropic property and the protective function of the seedcoat, and showed that the sutures of the seedcoat play an important role in transmitting and distributing loads in responding to external compression.

Keywords: Common Millet, Seed, Suture, Anisotropy, Compression, Finite Element

1. Introduction

Through years of evolution and natural selection, biological armors in various species of fauna and flora have adapted to provide mechanical protection and flexibility that accommodate growth, deformation, and locomotion. Extensive research has been motivated to study interesting micro/nano structures of biological armors and their mechanical response. These include the brick-mortar structures of nacre (Ji and Gao, 2004; Barthelat et al., 2007; Barthelat and Espinosa, 2007; Dunlop and Fratzl, 2010; Bonderer et al., 2008; Podsiadlo et al., 2007; Munch et al., 2008; Rajabi et al., 2014), multilayered protective exoskeletal materials including crustaceans (Raabe et al., 2005), insects (Barbakadze et al., 2006) fish scales (Bruet et al., 2008; Browning et al., 2013; Yang et al., 2013; Zhu et al., 2012), mechanical interlocks in the turtle carapace (Krauss et al., 2009; Damiens et al., 2012; Achrai and Wagner, 2015), and biological sutures in vertebrate skulls, stickleback fish, diatom and ammonites (Song et al., 2010; Li et al., 2011, 2012 and 2013). This research has advanced the development of numerous biomimetic materials, such as nacre-inspired composites across all length scales (Podsiadlo et al., 2007; Munch et al., 2008; Barthelat and Zhu, 2011; Valashani and Barthelat, 2015; Zhang et al., 2015), as well as diatom suture and ammonite suture inspired interfaces fabricated via 3D printing (Lin et al., 2014a and 2014b). A thorough review of these developments can be found in the most recent review papers (Chen et al., 2012; Studart, 2012; Meyers et al., 2008; Meyers et al., 2011; Chen and Pugno, 2013; Ulrike et al., 2015). Here, we are particularly interested in a flora armor system, the seedcoat of common millet (*Panicum miliaceum*), which shows a remarkable network of jigsaw-puzzle shaped articulation between the microscale building blocks.

Due to their high survivability and adaptability, common millet (*Panicum miliaceum*) is an ancient crop to humans and spreads all over the world. The outer coat is composed of jigsaw-puzzle shaped epidermis cells articulating together to form a compact coat that protects the seed inside (Lu et al., 2009). The seedcoat of *Panicum miliaceum* are composed of inorganic silica phytoliths and organic biopolymers. Phytoliths are common components in the grass family (Poaceae). Lu et al., reported that deposited silica phytoliths of the seedcoats of both foxtail millet and common millet were well observed after removal of the organic phase (Lu et al., 2009). While the kernel is composed of micro-scale polyhedron starch cells with starch granules within each cell (Zarnkow et al., 2007).

In biology, the micromorphology of the seed coat epidermis cells serves as a diagnostic signature (Danin et al., 2008; Lu et al., 2009). For example, the variety of micromorphology of seed coats has been used to distinguish between foxtail millet (*Setaria italica*) and common millet (*Panicum miliaceum*) (Lu et al., 2009), and to distinguish between different species within the same *Portulaca* family (Danin et al., 2008). The intercellular boundaries of the epidermal cells are joined by thin, wavy suture interfaces. This indicates that the seedcoat is in fact a composite material with relatively stiff building blocks articulated

via a compliant network of thin interfacial tissue. This type of natural composite was also observed in armors at a much larger scale, such as the scale armor of the box fish (*Ostracion lentiginosum*) (Meunier and Francillon-Vieillot, 1995; Yang et al., 2015), and turtle carapace (Krauss et al., 2009; Damiens et al., 2012; Achrai and Wagner, 2015). Theoretical models have been developed for interdigitating suture interfaces of varying profiles, with analytical expressions derived for the stiffness, strength and local stress distributions for rectangular and triangular suture interfaces (Li et al., 2011 and 2012), and for a suture of arbitrary geometry (Li et al., 2013). These models have also been applied to and validated with experimental results from 3D printed prototypes of various suture interface geometries (Lin et al., 2014a and 2014b).

Similar to other seed systems, common millet seeds undergo various environmental threats, such as mechanical damages by birds or insects, infection by bacteria, virus and fungi, imbibition damage due to drought or heavy rain (Sheahan, 2014). Common millet is known to have high water use efficiency which allows it to grow in dry regions with good drought-tolerance. As the most important reproductive organ for plants, seeds are well protected by the seedcoats. The functions of a seedcoat are multifaceted: it protects the seed (embryo and endosperm) from mechanical damage (insects, abrasion and crushing) and infection by bacteria, virus particles and fungi. It also prevents the seed from dehydration, freezing and fire. In addition, it provides a time delay factor for the germination of the seed until the conditions for survival of the seedling are favorable. In literature, both individual and bulk seeds from different species have been studied, such as individual black pepper seeds (Murthy and Bhattacharya, 1998), sunflower seeds (Gupta and Das, 2000), and safflower seeds (Baumler et al., 2006). For bulk seed studies, the physical properties of bulk quantities of minor millets were also determined, including common millet, with linear relationships identified for density, coefficients of static and internal friction, and hardness for a given moisture content (Balasubramanian and Viswanathan, 2010). Bulk grain properties and the dependence on moisture content have also been studied (Molenda and Stasiak, 2002), where the mechanical properties were obtained from the elastic unloading response of a uniaxial compression (oedometric) test. Numerical finite element (FE) models were also developed to simulate the bulk confined compression of seeds using an explicit algorithm, investigating the seed interactions during loading (Petru et al., 2014).

However, most of this research has been focused on determining the macroscale seed geometry and the dependence of environment conditions on the overall mechanical properties, and is primarily guided towards oil expression, and storage, handling and processing applications e.g. dehulling. Few efforts have been made on quantifying the relation between the microstructure and the intrinsic mechanical properties of the material. While the microstructure property relationship is the key guideline for biomimetic design, in the current research field on seeds, a gap exists in characterizing the mechanical behavior of seeds and

their application to bio-inspired designs for new materials. The present study is aimed at narrowing this gap by building a bridge by exploring the structured property relationship of a characteristic system, individual seeds of common millet (*Panicum miliaceum*).

In this study, the periodic microstructure of the seedcoat of common millet (*Panicum miliaceum*) was characterized using scanning electron microscopy (SEM). Nanoindentation was also performed to obtain the Young's modulus of the stiff epidermis cells. To investigate the mechanical response of the seeds under compression, macroscale uniaxial compression tests were performed to obtain the load-displacement response of seeds, with and without the seedcoat. To explore the microstructure property relationship, a multiscale simulation approach was utilized. First, both analytical and the microstructural based FE model of a representative volume element (RVE) of the seedcoat was developed to determine the effective anisotropic mechanical properties of the seedcoat; subsequently the effective properties were input to the macroscale model of the seed to simulate the compressive behavior of the whole seed. The FE results were further validated by the macroscale experiments.

2. Materials and Methods

2.1. Microstructure of seed coat

The SEM image (Fig. 1a) of the entire seed shows an ellipsoidal shape. The SEM images were obtained using a Tescan Lyra3 GMU Combined FE-SEM/FIB field emission microscope at the University of New Hampshire. The maximum length scale of a common millet seed is approximately 3 mm. In this paper, two coordinates are defined and shown in Fig. 1a: one is a global coordinate system is defined as x - y - z , with the x direction along the longer axis of the seed, and the y direction along the shorter axis of the seed, and z direction is along the height of the seed. The other is a local coordinate system 1-2-3 defined on the top surface of the seedcoat, with direction 1 along the transverse direction of the seedcoat and the direction 2 along the longitudinal direction of the seedcoat. The in-plane microstructure of the seedcoat is shown in Fig. 1b, where the jigsaw-puzzle-like epidermis cells are primarily rectangular and the intercellular boundaries form a remarkable wavy suture network. One representative epidermal cell is highlighted in Fig. 1b. The longer edges b of the rectangular epidermis cells are oriented along the longitudinal direction 2 on the seedcoat, and the shorter edges a of the rectangular epidermis cells are oriented along the transvers direction 1. The dimensions of total 10 epidermis cells were measured from the SEM images. From the measurement, length b is in a range of $39.94 \pm 4.11 \mu\text{m}$ and length a is in a range of $11.40 \pm 0.70 \mu\text{m}$. The length aspect ratio b/a of the epidermis cell is then in a range of $\sim 3.53 \pm 0.83$. The neighboring epidermis cells roughly overlap in a half cell length with each other. Image processing software ImageJ was used to measure the coordinates of suture skeletonized points (x_i, y_i) to calculate the wavelength and amplitude of the suture geometry. Measured from the SEM images of the 10

epidermis cells, the vertical wavy sutures between the epidermis cells have wavelength λ_2 in a range of $7.51 \pm 0.58 \mu\text{m}$ and an amplitude A_2 in a range of $3.76 \pm 0.78 \mu\text{m}$; the horizontal suture interface has a wavelength, λ_1 and amplitude A_1 in a range of $4.25 \pm 1.02 \mu\text{m}$ and $2.68 \pm 0.70 \mu\text{m}$, respectively; and the thickness of the thin suture interfacial layer is in a range of $0.50 \pm 0.27 \mu\text{m}$.

The structure of seed was evaluated using Skyscan 1173 (Kontich, Belgium) micro-tomography scanner (μ -CT) with the following parameters: 0.25 mm aluminium filter, 5-frames averaging, 0.2° rotation step, $6 \mu\text{m}$ resolution, 90 kV voltage, and 88 μA current. The acquired images were processed using a commercial program (SkyScan NRecon V1.6) and the whole seed structure was 3-dimensionally observed using CTVol (Skyscan, Kontich, Belgium). A micro-CT image of the sample transverse cross-section (y-z plane) is shown in Fig. 1c, which demonstrates that the kernel is wrapped by the seed coat with a small gap in-between. SEM images of the cross-sections of broken seedcoats at different locations were taken, with one example shown in Fig. 1d. The out-of-plane thickness of the seedcoat is in the range of $\sim 20\text{--}50 \mu\text{m}$. Fig.1d also shows a thin layer ($\sim 5\text{--}8 \mu\text{m}$) underneath the jigsaw puzzle layer. From the literature (Lu et al., 2009) this layer is an organic lamella and is much softer than the puzzle layer. There should also be a very thin organic cutin layer on the very top of the seedcoat (Zarnkow et al., 2007), although it is hard to tell from Fig.1d. The puzzle layer is the major part of the seedcoat and the major load carrying component of the seedcoat.

2.2. Nanoindentation on the cross-section of the seedcoat

Nanoindentation was performed on the cross-section (y-z plane in Fig.1a) of the seed coat. Seeds were first soaked in PBS for 24 hours and were then embedded in a room-temperature curing epoxy (Fixmaster Fast Cure Poxy Pak Epoxy). The seed-epoxy blocks were sectioned using a low speed diamond saw (No. 11-1280 ISOMET, Buehler, USA) running at 700–800 rpm. The sectioned samples were again adhered to a steel puck by super glue (Scotch) and were polished successively with $6 \mu\text{m}$ and $1 \mu\text{m}$ silica nanoparticles on a soft pad and again with 500 nm silica nanoparticles on microcloth. The samples were then sonicated for 10 seconds in distilled water three times and gently dried. Nanoindentation experiments were conducted on the sample cross-section in ambient conditions using a NanoTest system (NanoTest NTX) using a Berkovich (trigonal pyramid) diamond probe tip. The applied load function was divided into five segments as follows: The first segment consisted of a 5 second hold at zero force allowing for tip-sample equilibration. Segment two was a constant loading rate of $200 \mu\text{N/s}$ until the maximum set peak load of $1000 \mu\text{N}$, was reached. The third segment, a hold period of 5 s, would then follow. The fourth segment decreased the load at a constant unloading rate of $200 \mu\text{N/s}$. The fifth segment would conclude the experiment with a 5 s hold at zero force. The seedcoat layer of the cross-sectioned seed samples were indented and the inter-indentation spacing was $10 \mu\text{m}$, so as to ensure there were no

interactions between adjacent indentations. The probe tip area function and frame compliance were calibrated prior to each set of experiments using a fused quartz sample. Load versus indentation depth curves from multiple experiments using the same maximum load and from different sample locations were then averaged.

The effective stiffness of the epidermis layer of three randomly chosen specimens was measured using nanoindentation experiments for the cross-section direction. Using the Oliver-Pharr method (Pharr et al., 1992), indentation moduli were obtained as 7.0 ± 3.9 GPa from 25 indentation data on one seed sample. In order to confirm the sample variation, further nanoindentation experiments were carried out ($n=3$). The indentation moduli of other seed samples were not statistically different among specimens, indicating that sample variation for indentation modulus was not significant ($p > 0.05$).

In order to estimate Young's modulus and yield stress, nanoindentations were simulated via two dimensional nonlinear FE models with ABAQUS, by following a similar method by Bruet et al. (2008). Two-dimensional, axisymmetric FE models were used with appropriate symmetric boundary conditions, assuming an isotropic material model. The 3D geometry of a Berkovich indenter was approximated as a 2D, conical-like axisymmetric indenter with the radius equal to the tip radius of the Berkovich indenter; the tip cross-sectional area was the experimentally measured Berkovich tip area function (TAF).

2.3. Analytical modeling of the effective anisotropic mechanical properties of the seedcoat

The seedcoat was modeled as a two-phase composite: a hard phase (epidermal cell) and soft intercellular suture layer. As shown in Fig. 2, in the local coordinate, the wavy morphology of the suture line in longitudinal direction 2 is represented by a sinusoidal curve $y_2 = A_2 \sin\left(\frac{2\pi}{\lambda_2}x\right)$, with amplitude A_2 and wavelength λ_2 . The local suture morphology represented in Fig. 2 is that of a rectangular geometry. The suture line along the transverse direction 1 is also represented by a sinusoidal curve $y_1 = A_1 \sin\left(\frac{2\pi}{\lambda_1}x\right)$, with amplitude A_1 and wavelength λ_1 . The microstructure of the seedcoat was then separated into two major areas: **S2** suture area along direction 2 (blue layers in Fig. 2); and major epidermis cell area **M** (yellow layers in Fig. 2). Then generally, the seedcoat can be equivalent to a composite with alternating in-plane layers of **S2** and **M**, as shown in Fig. 2. The volume fraction of area **S2** is $f_{S2} = \frac{A_2}{a}$, and the volume fraction of **M** is $f_M = 1 - f_{S2}$.

In order to get the effective mechanical properties of each in-plane layer **M**, area **M** was further separated into two sub-areas: **S1**, suture area along the transverse direction 1, and area **H**, the area with only the hard phase. The effective volume fraction of area **S1** in area **M** is $f_{S1} = \frac{a-A_2}{a} \frac{A_1}{b}$, and the effective volume fraction of area **H** in area **M** is $f_H = 1 - f_{S1}$.

The constitutive equation of the seedcoat can be expressed as:

$$\bar{\epsilon} = \mathbf{S} : \bar{\sigma}, \quad (1)$$

where, $\bar{\sigma}$ and $\bar{\epsilon}$ are the effective stress and strain tensors, respectively, in vector form using Voigt notation, and $\mathbf{S}$ is effective compliance tensor of the seedcoat. For an orthotropic material, the nonzero components of the leading diagonal of the compliance tensor include $S_{1111} = \frac{1}{\bar{E}_{11}}$, $S_{2222} = \frac{1}{\bar{E}_{22}}$, $S_{3333} = \frac{1}{\bar{E}_{33}}$, $S_{2323} = \frac{1}{\bar{G}_{23}}$, $S_{3131} = \frac{1}{\bar{G}_{13}}$ and $S_{1212} = \frac{1}{\bar{G}_{12}}$. The off-diagonal components include $S_{1122} = -\frac{\bar{\nu}_{21}}{\bar{E}_{22}}$, $S_{1133} = -\frac{\bar{\nu}_{31}}{\bar{E}_{33}}$ and $S_{2233} = -\frac{\bar{\nu}_{32}}{\bar{E}_{33}}$, where $(\bar{E}_{11}, \bar{E}_{22}, \bar{G}_{12})$ are the effective in-plane moduli, and $(\bar{E}_{33}, \bar{G}_{13}, \bar{G}_{23})$ are the out-of-plane moduli. $(\bar{\nu}_{12}, \bar{\nu}_{21})$ are the effective in-plane Poisson's ratios, and $(\bar{\nu}_{13}, \bar{\nu}_{31}, \bar{\nu}_{23}, \bar{\nu}_{32})$ are the out-of-plane Poisson's ratios. The effective orthotropic compliance matrix, $\mathbf{S}$, of the entire seedcoat can be obtained by calculating the effective stiffness tensors in each sub-areas, and then assembling them in a hierarchical manner. First, the anisotropic effective mechanical properties of areas **S1** and **S2** can be obtained by applying the theoretical suture model (Li et al., 2011, 2012, and 2013), then the effective properties of area **M** can be obtained via the rule of mixtures. Eventually, all components in the effective compliance matrix can be obtained. The specific equations for each step are shown subsequently.

Areas **S1** and **S2** are suture areas. The anisotropic effective mechanical properties of them can thus be obtained by jointly applying the analytical suture model (Li et al., 2011, 2012, and 2013) and the rule of mixtures (Voigt and Reuss laws) as:

$$\bar{E}_{11}^{S2} = E_h (f_{S2}')^2 \left[(1 - f_{S2}') \left(\frac{E_h}{G_i} \sin^2 \theta_2 \cos^2 \theta_2 + \frac{E_h}{E_i} \sin^4 \theta_2 \right) + f_{S2}' \right]^{-1}, \quad (2)$$

$$\bar{E}_{22}^{S2} = \left[(1 - f_{S2}') \left(\frac{\cos^2 \theta_2 \sin^2 \theta_2}{G_i} + \frac{\cos^4 \theta_2}{E_i} \right) + \frac{f_{S2}'}{E_h} \right]^{-1}, \quad (3)$$

$$\bar{G}_{12}^{S2} = \frac{f_{S2}'^2 C E_i E_h}{f_{S2}' C C^b E_i + (1 - f_{S2}') (1 + C^r) E_h}, \quad (4)$$

$$\bar{\nu}_{12}^{S2} = f_{S2}' \nu_h + (1 - f_{S2}') \nu_i, \text{ and} \quad (5)$$

$$\bar{\nu}_{21}^{S2} = \bar{\nu}_{12}^{S2} \frac{\bar{E}_{22}^{S2}}{\bar{E}_{11}^{S2}}, \quad (6)$$

where, f_{S2}' is the volume fraction of the hard phase in area **S2**, and is equal to $f_{S2}' = 1 - \frac{\mathcal{L}_2 t}{(2A_2 + t)\lambda_2}$. $\mathcal{L}_2$ is the arc length of the sinusoidal wave y_2 within one wavelength, and equal to $\mathcal{L}_2 = \int_0^{\lambda_2} \sqrt{1 + \left(\frac{dy_2}{dx} \right)^2} dx$, where t is the in-plane thickness of the wavy layer. Similarly, the volume fraction of the hard phase in area **S1** is f_{S1}' . E_i and G_i are the Young's modulus and shear modulus of the soft interface, respectively, and E_h is the Young's modulus of the hard phase. Additionally, $\theta_2 = \tan^{-1} \frac{\lambda_2}{4A_2}$, $C = \frac{G_i}{E_i} + (1 - \nu_i^2)^{-1} (\tan \theta_2)^{-2}$, $C^b = \frac{3E_h}{4[f_{S2}' G_h + (1 - f_{S2}') G_i]} + \frac{5}{16} (\tan \theta_2)^{-2}$, and $C^r = \frac{3G_i}{2[f_{S2}' G_h + (1 - f_{S2}') G_i]} + \frac{9G_i}{8E_h} (\tan \theta_2)^{-2}$ (Li et al., 2012).

By applying the rule of mixtures, the effective out-of-plane properties in area **S2** were derived as:

$$\bar{E}_{33}^{S2} = f_{S2}' E_h + (1 - f_{S2}') E_i, \quad (7)$$

$$\bar{G}_{13}^{S2} = \bar{G}_{23}^{S2} = \left(\frac{f_{S2}}{G_h} + \frac{1-f_{S2}}{G_i} \right)^{-1}, \quad (8)$$

$$\bar{\nu}_{32}^{S2} = \bar{\nu}_{31}^{S2} = f_{S2}' \nu_h + (1 - f_{S2}') \nu_i, \text{ and} \quad (9)$$

$$\bar{\nu}_{23}^{S2} = \bar{\nu}_{13}^{S2} = \bar{\nu}_{31}^{S2} \frac{\bar{E}_{11}^{S2}}{\bar{E}_{33}^{S2}}. \quad (10)$$

Similarly, the effective in-plane mechanical properties of suture area **S1** were derived as:

$$\bar{E}_{11}^{S1} = \left[(1 - f_{S1}') \left(\frac{\cos^2 \theta_1 \sin^2 \theta_1}{G_i} + \frac{\cos^4 \theta_1}{E_i} \right) + \frac{f_{S1}'}{E_h} \right]^{-1}, \quad (11)$$

$$\bar{E}_{22}^{S1} = E_h (f_{S1}')^2 \left[(1 - f_{S1}') \left(\frac{E_h \sin^2 \theta_1 \cos^2 \theta_1}{G_i} + \frac{E_h \sin^4 \theta_1}{E_i} \right) + f_{S1}' \right]^{-1}, \quad (12)$$

$$\bar{G}_{12}^{S1} = \frac{f_{S1}'^2 c E_i E_h}{f_{S2}' c^b E_i + (1 - f_{S2}') (1 + c^r) E_h}, \quad (13)$$

$$\bar{\nu}_{21}^{S1} = f_{S1}' \nu_h + (1 - f_{S1}') \nu_i, \text{ and} \quad (14)$$

$$\bar{\nu}_{12}^{S1} = \bar{\nu}_{21}^{S1} \frac{\bar{E}_{11}^{S1}}{\bar{E}_{22}^{S1}}, \quad (15)$$

where, $\theta_1 = \tan^{-1} \frac{\lambda_1}{4A_1}$, $c = \frac{G_i}{E_i} + (1 - \nu_i^2)^{-1} (\tan \theta_1)^{-2}$, $c^b = \frac{3E_h}{4[f_{S2}' G_h + (1 - f_{S2}') G_i]} + \frac{5}{16} (\tan \theta_1)^{-2}$, and $c^r = \frac{3G_i}{2[f_{S2}' G_h + (1 - f_{S2}') G_i]} + \frac{9G_i}{8E_h} (\tan \theta_1)^{-2}$ (Li et al., 2012).

The effective out-of-plane mechanical properties of suture area **S1** were derived as:

$$\bar{E}_{33}^{S1} = f_{S1}' E_h + (f_{S1}') E_i, \quad (16)$$

$$\bar{G}_{13}^{S1} = \bar{G}_{23}^{S1} = \left(\frac{f_{S1}}{G_h} + \frac{1-f_{S1}}{G_i} \right)^{-1}, \quad (17)$$

$$\bar{\nu}_{32}^{S1} = \bar{\nu}_{31}^{S1} = f_{S1}' \nu_h + (1 - f_{S1}') \nu_i, \text{ and} \quad (18)$$

$$\bar{\nu}_{23}^{S1} = \bar{\nu}_{13}^{S1} = \bar{\nu}_{31}^{S1} \frac{\bar{E}_{11}^{S1}}{\bar{E}_{33}^{S1}}. \quad (19)$$

Since area **M** can be equivalent to a composite with alternating layers **H** and **S1** (Fig. 2), the in-plane effective mechanical properties of layer **M** can be obtained via the rule of mixtures as:

$$\bar{E}_{11}^M = f_H E_h + (1 - f_H) \bar{E}_{11}^{S1}, \quad (20)$$

$$\bar{E}_{22}^M = \left(\frac{f_H}{E_h} + \frac{1-f_H}{\bar{E}_{22}^{S1}} \right)^{-1}, \quad (21)$$

$$\bar{G}_{12}^M = \left(\frac{f_H}{G_h} + \frac{1-f_H}{\bar{G}_{12}^{S1}} \right)^{-1}, \quad (22)$$

$$\bar{\nu}_{12}^M = f_H \nu_h + (1 - f_H) \bar{\nu}_{12}^{S1}, \text{ and} \quad (23)$$

$$\bar{\nu}_{21}^M = \bar{\nu}_{12}^M \frac{\bar{E}_{22}^M}{\bar{E}_{11}^M}. \quad (24)$$

The out-of-plane effective mechanical properties of layer **M** can also be obtained via the rule of mixtures as:

$$\bar{E}_{33}^M = f_H E_h + (1 - f_H) \bar{E}_{33}^{S1}, \quad (25)$$

$$\bar{G}_{13}^M = \left(\frac{f_H}{G_h} + \frac{1-f_H}{\bar{G}_{13}^{S1}} \right)^{-1}, \quad (26)$$

$$\bar{\nu}_{32}^M = \bar{\nu}_{31}^M = f_H \nu_h + (1 - f_H) \bar{\nu}_{31}^{S1}, \text{ and} \quad (27)$$

$$\bar{\nu}_{23}^M = \bar{\nu}_{13}^M = \bar{\nu}_{31}^M \frac{\bar{E}_{11}^M}{\bar{E}_{33}^M}. \quad (28)$$

Eventually, by taking the entire seedcoat as a composite with alternating in-plane layers of **S2** and **M**, the effective mechanical properties of the seedcoat can be obtained as:

$$\bar{E}_{11} = \left(\frac{f_{S2}}{\bar{E}_{11}^{S2}} + \frac{1-f_{S2}}{\bar{E}_{11}^M} \right)^{-1}, \quad (29)$$

$$\bar{E}_{22} = (1 - f_{S2}) \bar{E}_{22}^M + f_{S2} \bar{E}_{22}^{S2}, \quad (30)$$

$$\bar{G}_{12} = \left(\frac{f_{S2}}{\bar{G}_{12}^{S2}} + \frac{1-f_{S2}}{\bar{G}_{12}^M} \right)^{-1}, \quad (31)$$

$$\bar{\nu}_{21} = (1 - f_{S2}) \bar{\nu}_{21}^M + f_{S2} \bar{\nu}_{21}^{S2}, \text{ and} \quad (32)$$

$$\bar{\nu}_{12} = \bar{\nu}_{21} \frac{\bar{E}_{11}}{\bar{E}_{22}}. \quad (33)$$

The effective out-of-plane mechanical properties of the entire seedcoat can also be derived as:

$$\bar{E}_{33} = (1 - f_{S2}) E_h + f_{S2} \bar{E}_{33}^{S2}, \quad (34)$$

$$\bar{G}_{13} = \bar{G}_{23} = \left(\frac{f_{S2}}{\bar{G}_{13}^{S2}} + \frac{1-f_{S2}}{\bar{G}_{13}^M} \right)^{-1}, \quad (35)$$

$$\bar{\nu}_{31} = \bar{\nu}_{32} = (1 - f_{S2}) \bar{\nu}_{31}^M + f_{S2} \bar{\nu}_{31}^{S2}, \text{ and} \quad (36)$$

$$\bar{\nu}_{13} = \bar{\nu}_{23} = \bar{\nu}_{31} \frac{\bar{E}_{33}}{\bar{E}_{11}}. \quad (37)$$

2.4. Finite element simulations of the in-plane mechanical behavior of the seedcoat

To numerically obtain the in-plane anisotropic effective moduli of the seedcoat, FE simulations of a representative volume element (RVE) were performed under three in-plane loading cases: (Case 1) uniaxial tension in transverse direction 1, (Case 2) uniaxial tension in longitudinal direction 2, and (Case 3) simple in-plane shear, as shown in Figs. 3a, b, and c, respectively.

In the FE models, periodic boundary conditions were used for all three cases and 2D plain stress elements (CPS4R) were used. Both hard and soft phases were modeled as linear elastic isotropic materials. The Young's modulus E_h of the isotropic hard phase was 6 GPa , as obtained from nanoindentation (Section 2.2). Experimentally, it is challenging to measure the properties in the thin suture layer, so in the FE models, the stiffness of the thin layer was assumed isotropic with Young's modulus E_i varied from 6 MPa to 6 GPa . The Poisson's ratios of the hard phase and soft phase were $\nu_h =$

0.3 and $\nu_i = 0.4$, respectively. The Poisson's ratios were chosen based on the overall properties of ceramic and organic materials reported in (Greaves et al., 2011, Dri et al., 2013). In addition, it was found that the effective stiffness's $\bar{E}_{11}$, $\bar{E}_{22}$ and shear modulus $\bar{G}_{12}$ are largely insensitive to a large change in Poisson's ratio of both the hard and soft phases. The dimensions of the RVE were the average values of all geometric variables measured from the SEM images. Specifically, in the RVE, the wavelength and amplitude of the sutures in area **S2** were $7.51 \mu\text{m}$ and $3.76 \mu\text{m}$, respectively. The wavelength and amplitude of the sutures in area **S1** were $4.25 \mu\text{m}$ and $2.68 \mu\text{m}$, respectively. To avoid self-penetration between the sutures in junction areas of **S2** and **S1**, the amplitude was slightly reduced in those areas. The average edge lengths of the epidermis cells were $a = 11.40 \mu\text{m}$ and $b = 39.94 \mu\text{m}$. The thickness of the suture interface was uniformly set as $0.50 \mu\text{m}$. The in-plane moduli were obtained from these FE simulations and were compared with the analytical predictions (Section 2.3). The results will be shown in Section 3.2.

2.5. Quasi-static compression experiments on seeds and kernels

To accurately capture the geometry and relative length scales of the seed (with the seedcoat) and kernel (without the seedcoat), prior to compression testing, the seed geometry (major diameter, D_{S1} , minor diameter, D_{S2} , and height, h_s , as shown in Fig. 4) were measured for a sample of 10 seeds with seedcoat. The geometry of the kernel (major diameter, D_{K1} , minor diameter, D_{K2} , and height, h_K , as shown in Fig. 4) were also measured from 10 kernels.

The average major diameter (D_{S1}), minor diameter (D_{S2}) and height (h_s) with the standard deviation of the seeds were $2.728 \pm 0.091 \text{ mm}$, $2.102 \pm 0.054 \text{ mm}$ and $1.657 \pm 0.056 \text{ mm}$, respectively. The kernels were more spherical in shape so only the height h_K was measured with the average being $1.567 \text{ mm} \pm 0.055 \text{ mm}$. The difference in the height of the two set of samples is due to the thickness of the seedcoat and possible small gap between the inner surface of the seedcoat and the kernel.

Compression testing was performed with a Zwick/Roell (zwickiLine) testing machine, instrumented with a 100 N load cell. The compression testing setup is shown in Fig. 5. Experiments were performed at ambient conditions. Individual seeds and kernels were placed between two steel platens and compressed at a quasi-static displacement rate of 0.02 mm/min. The tests were stopped when the load started to drop. A total of ten seed and kernel samples each were tested.

2.6. Hertzian contact model for kernel property evaluation

As the material properties of the inner kernel were unknown, a Hertzian contact model (Johnson, 1985) was used to evaluate the stiffness of the kernel. Here, the contact problem of a sphere compressed with a platen is a special case of the classic Hertzian model of contact between two elastic spheres when the

radius of one sphere goes to infinity. The relationship between the total displacement of the sphere between two planes, α , and the applied force, P is given for this special case of contact as (Puttock and Thwaite, 1969):

$$\alpha = (3\pi)^{2/3} P^{2/3} \left[\left(\frac{1-\nu_k^2}{\pi E_k} \right) + \left(\frac{1-\nu_p^2}{\pi E_p} \right) \right]^{2/3} \left(\frac{1}{D_k} \right)^{1/3} \quad (38)$$

where, E_k and ν_k are the Young's modulus and Poisson ratio of the kernel, respectively; and E_p and ν_p are the Young's modulus and Poisson ratio of the steel platens, respectively. The Young's modulus and Poisson ratio of the steel disks were 205 GPa and 0.28, respectively. The kernel was assumed to be spherical with diameter $D_{K1} = D_{K2}$ equivalent to the average measured kernel height h_k .

The kernel was assumed to be linear elastic, isotropic and homogeneous. The stiffness, E_k (assuming $\nu_k = 0.3$) was calculated by matching the prediction from Eq. (38) and the experimental kernel contact force-displacement history, to a small displacement level. To negate the size effect, the force and displacement were normalized by the individual kernel heights, where the normalized force was $\bar{P} = P/D^2$ and the normalized displacement was $\bar{\alpha} = \alpha/D$. E_k was calculated as 506 MPa, which was taken as the average stiffness for a given linear range of small displacement from $\bar{\alpha} = 0.002$ to $\bar{\alpha} = 0.004$. The normalized force $\bar{P}^{2/3}$ is linearly related to the normalized displacement $\bar{\alpha}$. Based on Eq.38, the inverse slope C^{-1} of $\bar{P}^{2/3}$ vs $\bar{\alpha}$ curve is:

$$\frac{1}{C} = (3\pi)^{2/3} \left[\left(\frac{1-\nu_k^2}{\pi E_k} \right) + \left(\frac{1-\nu_p^2}{\pi E_p} \right) \right]^{2/3} \quad (39)$$

Thus, the stiffness of the kernel, E_k could be found numerically. This evaluation was also validated from FE simulations on the quasi-static compression of kernels in Sections 2.7 and 3.4.

2.7. FE simulations of the compression of kernels and seeds

To study the mechanical behavior of the seeds and kernels under compression, FE models of seeds (with seedcoat) and the kernel (without seedcoat) were developed. The kernel was modeled as a deformable ellipsoid with dimensions of approximately 97% of the seedcoat dimensions. As shown in Fig. 6, the seed model included the kernel model with the addition of the seedcoat to simulate the compressive behavior of the entire seed. The seedcoat was meshed with shell elements with reduced integration (S4R). The thickness was taken as an average measurement from SEM evaluation, as 50 μm . A small gap between the inner surface of the seedcoat and the kernel exists ($\sim 13 \mu\text{m}$). For both models, the kernel and kernel with seedcoat were placed between two discs that were discretized with rigid elements (R3D3/R3D4). The kernel was meshed with 3D continuum elements (C3D4) and had an elastic isotropic material property with the Young's modulus and Poisson ratio of 506 MPa and 0.3, respectively. This was found from the preceding section discussing the Hertzian contact model fit to the experimental

kernel compression data. Good agreement was found between the FE results and the experimental data, thus this choice of kernel material property was justified.

The seedcoat had an orthotropic elasticity material model with the in-plane elastic constants being calculated for a given interface stiffness, E_i , from the FE suture composite model discussed in Section 2.4. The out-of-plane elastic constants were derived in Section 2.3 given the properties of the hard phase found from nanoindentation testing, and a given interface stiffness, E_i . An iterative scheme was undertaken to vary the interface stiffness to study the dependence on the overall response. A mesh sensitivity study was also undertaken to ensure the results were independent of the approximate mesh size.

Simulations were performed in ABAQUS under quasi-static displacement rate, and a surface-to-surface contact assignment was made between the rigid plates and the respective seedcoat / kernel surfaces. The contact definition used a hard normal and a tangential friction coefficient of 0.25, reported for millet seeds with low moisture content (Balasubramanian and Viswanathan, 2010). The seed and kernel models are shown in Fig. 6. The force-displacement response was outputted from the simulation and validated with the experimental data. The results will be shown in Section 3.4.

3. Results and Discussion

3.1. Nanoindentation results

The averaged experimental load-depth data for the outer epidermis layer was fitted to an isotropic, elastic-perfectly plastic FE numerical model as shown in Fig. 7. The FE models were discretized with four-node bilinear axisymmetric quadrilateral elements (CAX4R) and mesh convergence studies were assessed to determine the optimal mesh (1540 elements) for accurate solutions. The 2D simulations were found to have more than 97 % accuracy as compared to the fully 3D simulations. The Berkovich indenter was assumed as a rigid conical-like indenter. Large deformation theory and frictionless contact between the indenter and material were assumed. The deformation mode was chosen as quasi-static. All of the nanoindentation simulations were conducted to a maximum load of 1000 μN in accordance with the experiments. The Young's modulus was thus determined by a best fit to the averaged loading experimental data. The results gave a Young's modulus value of 6 GPa for the epidermis cell.

3.2. Effective in-plane anisotropic moduli of the seed coat

The results of the FE simulations of the seedcoat RVE and the analytical prediction of the in-plane moduli of the seedcoat (Section 2.3) are shown and compared in Fig. 8. It shows that generally, since E_h was fixed as 6 GPa, when E_h/E_i increases (i.e. when E_i decreases), all component of the moduli decrease. As shown in Figs. 8a and 8c, the effective properties obtained from the FE simulations of an

RVE are quite consistent with the analytical predictions, especially for the transverse stiffness $\bar{E}_{11}$ and in-plane shear stiffness $\bar{G}_{12}$. For the longitudinal stiffness $\bar{E}_{22}$, when $E_h/E_i < 10$, the analytical prediction (Eq.30) provided in Section 2.3 is very accurate, because when E_i is large, the stiffness of area **S1** is comparable to that of area **H**, therefore, both layer **M** and layer **S2** are mainly in tension along direction 2, and this deformation mechanism can be accurately captured by the rule of mixtures. However, when $E_h/E_i > 10$, the analytical prediction under-predicts the longitudinal stiffness. This is because when E_i becomes smaller, the area **S1** becomes softer and area **S1** will in significant tension while area **S2** will experience significant shear, similar to the deformation mechanism of nacre (Ji and Gao, 2004; Barthelet et al., 2007). The deformation mechanism of the entire seedcoat is close to that of rectangular sutures with flat tips (Lin et al., 2014a). Therefore, when $E_h/E_i > 500$ the dash line based on the rectangular suture model (see **Appendix**) accurately captures the longitudinal stiffness, as shown in Fig. 8b. For the range of $10 < E_h/E_i < 500$, the FE results shows a combination/transition between the two different deformation mechanisms.

The FE results of the in-plane anisotropy ratio defined as $\bar{E}_{22}/\bar{E}_{11}$ is plotted as a function of E_h/E_i in Fig. 9. It can be seen that generally when E_h/E_i increases, the degree of anisotropy increases nonlinearly. When $E_h/E_i < 50$, the in-plane anisotropy ratio is close to 1, indicating quasi-isotropic property in this range. When E_h/E_i increases beyond 50, the in-plane anisotropy ratio increases dramatically. For example, when $E_h/E_i = 100$, $\bar{E}_{22}/\bar{E}_{11}$ is about 2, and when E_h/E_i increases to 100, $\bar{E}_{22}/\bar{E}_{11}$ increase to 5. For many biological materials, the stiffness ratio between the hard phase and soft phase is between $\sim 10^2$ - $\sim 10^3$ (Ulrike et al., 2015). In this range of E_h/E_i , the seedcoat is expected to show significant in-plane anisotropy. During germination process, due to hydration, the interfacial layer becomes softer, and the seedcoat more likely becomes more anisotropic and therefore to facilitate the germination by tearing along the longitudinal direction (Zarnkow et al., 2007).

The FE contours of in-plane normal stresses, shear stress and maximum in-plane stress for the seedcoat RVE under three in-plane loading cases are shown in Fig. 10. The cases with $E_i = 60\text{MPa}$ ($E_h/E_i = 100$) at small deformation (0.1% strain) are shown as the representative examples. It can be seen that under transverse tension (Fig. 10a), stresses in both directions 1 and 2 are larger in area **S2** than area **M**, indicating the hard phase in suture area **S2** are the major load carrier under transverse loads. While under longitudinal loads (Fig. 10b), compared with area **M**, the suture area **S2** barely takes any load, although suture area **S1** is actively sharing the longitudinal loads with sub-area **H**. Thus it can be concluded that the suture area mainly takes the transverse load and takes little longitudinal loads, while the suture area **S1** actively takes the longitudinal load and takes little transverse load. Under in-plane shearing load (Fig.

10c), the hard phase around the softer wavy suture layer is the major load carrier. The region of hard phase far from the suture region shows a relatively lower stress field.

3.3. Experimental compression results

The load-displacement results for nine full seed and eight kernel samples are shown in Fig. 11. The curves are up to the initial load drop indicating damage initiation. The average load-displacement curve is slightly nonlinear, which is consistent with the prediction from Hertzian contact problem (Eq. 38). The load-displacement curves of the whole seed shows a low stiffness regime due to the elastic deformation (mainly bending) of the seedcoat, and upon further loading, the hard kernel provides increased stiffness up to the failure point. A similar behavior was observed in the idealized load-displacement response reported for the uniaxial compression of nearly spherical black pepper seeds (Murthy and Bhattacharya, 1998).

As shown in Fig.11, comparing between the experimental seed and kernel results, the kernels show a larger range in both force and displacement before damage initiation occurs. Also, the kernels have an increased stiffness response compared to the full seeds, and fail at a lower displacement and load level. In addition, the curves for kernel have a large variation (standard deviation ~45%) due to the variation of sample size and more importantly, the imperfections such as micro cracks or damage; while the curves for full seed have a relatively small variation (~20%), although the variation in sample size is similar for kernels and full seeds. This reveals that the seedcoat offers protection to the kernel in three aspects. First, the existence of the seedcoat increases the average strain to damage initiation of the seeds from 6.13% to 8.41%, indicating the seedcoat absorbs energy first and delays the deformation of the kernel; second, because of the seedcoat, the load to damage initiation of full seeds is ~27.6% higher than the kernel without protection from the seedcoat, indicating the seedcoat increases the strength in compression and damage tolerance of the seeds; and third, with the seedcoat, the response of individual full seed is less deviated from each other, indicating more robust mechanical performance of the seeds with less influence from size and imperfection of the kernel.

3.4. FE results on compression tests

FE simulations with various E_i (from 60MPa to 600 MPa) were performed, it was found that the load-displacement curves of the seed are not highly sensitive to E_i . Given the Young's modulus of the hard phase, $E_h = 6$ GPa, and an suture layer stiffness of $E_i = 60$ MPa, the derived elastic constants for the seedcoat material model are shown in Table. 1.

Table. 1 – Material constants for elastic orthotropic seedcoat material model

$\bar{E}_{11}$ (MPa)	$\bar{E}_{22}$ (MPa)	$\bar{E}_{33}$ (MPa)	$\bar{G}_{12}$ (MPa)	$\bar{G}_{13}$ (MPa)	$\bar{G}_{23}$ (MPa)	$\bar{\nu}_{12}$	$\bar{\nu}_{13}$	$\bar{\nu}_{23}$
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1323	2650	5421	813	202	202	0.14	0.31	0.31
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Figure. 12 shows the comparison between the full seed and kernel experimental results with the respective FE model. For the FE kernel response and comparison with the experimental results (Fig. 12a), the model reproduces the experimental results very well and accurately matches the average overall stiffness. This validates the kernel stiffness value obtained by the Hertzian contact fit to the initial loading region of the experimental kernel data. It should be noted that the higher apparent stiffness of the kernel model compared to the seed model is due to the gap between the seedcoat and kernel. Thus, there is a delay during indentation before the kernel starts to be loaded. Comparing the FE full seed response with the respective experimental data (Fig. 12b), again there is good agreement between the results but the overall stiffness of the FE model is higher than that of the experimental results. This might be due to the non-elastic mechanical behavior of the real material and/or microcracks or damage evolution in the kernel and the seedcoat before the first load drop, which was not captured by the current elastic FE model without damage.

Fig. 13 shows the stress contours for the outer seed coat from the full seed FE model at relatively large deformation (6.15% overall strain), corresponding to a total loading platen displacement of 0.1 mm which is just below the range of damage initiation of the seeds. It is apparent there is a large gradient of tensile and compressive normal stresses at the contact site with the loading platen, and the stresses on the outer and inner surfaces of the seedcoat at the same location flips sign, indicating bending deformation of the seedcoat in the contact area. This locally varying stress distribution in longitudinal and transverse directions indicates the effect of anisotropy of the seedcoat. It can be seen that the transverse stress S_{11} is the dominant stress component. Therefore, the stress distribution of the maximum principle stress is similar to that of S_{11} . The elongation in particular of the maximum in-plane principal stress along the longitudinal direction of the seedcoat reveals how the stress concentrates along this major axis, due to the larger S_{11} stress component. While, as shown in Fig.10a, in responding to the transverse load, sutures in the **S2** area is the major load carrier and plays a very important role in distributing load and absorbing energy.

4. Conclusion and discussion

The goal of this paper was to study the quasi-static compressive response of common millet seeds (*Panicum miliaceum*). This was split into five separate parts: (1) characterization of the periodic microstructure of the seedcoat using SEM, (2) nanoindentation of the seedcoat to identify the material properties of the hard phase material, (3) analytical derivation of the in-plane and out-of-plane seedcoat material properties, and FE simulations of a 2D RVE for the periodic suture model under three in-plane

loading cases, (4) quasi-static compression testing of individual kernels and full seeds, and (5) FE simulations for the kernel and full seed under compression.

From the microstructure of the seedcoat obtained from SEM, a characteristic RVE for the periodic suture composite model was defined. This allowed the in-plane and out-of-plane material constants to be derived, given the elastic constants for the hard phase material found from nanoindentation testing of the seedcoat, and the interfacial material properties. This allowed a fully orthotropic material model to be defined for the seedcoat. Individual seeds and kernels were tested in quasi-static compression, with the average experimental kernel response being used with a Hertzian contact fit to find the Young's modulus of the kernel. FE models of the kernel and full seed were developed using ABAQUS.

The experimental results of the seeds and kernels showed that the seedcoat delayed the onset of damage initiation for the full seed, further showing the protective nature of the seedcoat. For the FE results, the kernel model exhibited a closer fit to the experimental data than the full seed FE model did. Investigation of the stress profiles for the seedcoat at large deformation showed an increase in the local stresses at the contact site and due to the anisotropic mechanical properties of the seedcoat, the stress in the transverse direction is the dominant stress component under compression. Investigation of the maximum in-plane stresses showed a stress concentration along the longitudinal direction on the seedcoat, caused by the larger transverse stress component. The FE results from the hierarchical computation clarified the different functions of each area/subarea on the seedcoat: the suture area (**S2**) along the longitudinal direction in the seedcoat actively takes the transverse load, while the middle part of the epidermis cells (area **H**) mainly take the longitudinal loads, and the suture area (**S1**) along the transverse direction also takes the longitudinal load.

The preceding experimental, numerical and analytical results reveal that the anisotropy of the seedcoat significantly affects the spatial stress distribution on the seedcoat, and therefore its protective function. The seedcoat protects the kernel by increasing the damage and imperfection tolerance, and therefore increases the overall strength and the effective strain to crushing of the seeds. In addition, the results indicate that the seedcoat sutures play a very important role in resisting indentation loads, and sutures in different areas are responsible for resisting loads in different directions. For this specific seed, the transverse stress is the critical stress component in resisting the indentation load. Modeling the seedcoat as a full composite including the details of the microstructure via a hierarchical computation strategy is a promising avenue to explore. This study also enables further applications on the development of a plethora of bioinspired materials, such as plates and shells for body armors or vehicle armors or flexible and tough thin sheets with tunable anisotropic mechanical properties.

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Contribution of authors

Hasseldine, and Gao have close contribution to the mechanical characterization part of the paper.

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Appendix:

Prediction of the in-plane longitudinal stiffness of the seedcoat by the rectangular suture model with tips

As shown in Fig. 8b, when the stiffness of the interfacial layer E_i becomes small ($E_h / E_i > 100$), the rule of mixture significantly over-predicts the overall effective longitudinal stiffness of the seedcoat. This is because when E_i becomes small, the effective in-plane longitudinal stiffness $\bar{E}_{22}^{S1}$ in the suture area **S1**

becomes much smaller than the stiffness E_h (6GPa) in area **H**. Thus, under in-plane longitudinal tension, the deformation mechanism in suture area **S2** is dominated by shear instead of tension. This deformation mechanism can be captured by the general trapezoidal suture model with tips (Lin et al., 2014a). The suture area **S1** is equivalent to the tip area in that model, the suture area **S2** is equivalent to the vertical soft interfacial layer of the rectangular suture interface in that model, and area **H** is equivalent to the rectangular teeth in that model. If we assume the area **H** is rigid, then the rigid tooth model (RTM) (Lin et al., 2014a) can be used. Therefore, by applying the RTM rectangular suture model with tips, the effective stiffness of the seedcoat can be derived as:

$$\bar{E}_{22}^{RTM} = (1 - f_{S2}) \left(\frac{0.5b}{2A_2} \right)^2 \bar{G}_{12}^{S2} + (1 - f_H)(1 - f_{S2}) \bar{E}_{22}^{S1} \left(\frac{0.5b}{2A_1} \right)^2, \quad (A1)$$

in which, the first term accounts for the contribution from the effective shearing resistance of the suture area **S2**, and the second term is due to the effective longitudinal tension resistance in the suture area **S1**.

The prediction from Eq. (A1) are compared with the prediction from the rule of mixture and the FE results in Fig. 8b. It can be seen that when E_h / E_i increases beyond 500, Eq. (A1) accurately captures the effective longitudinal stiffness $\bar{E}_{22}$ of the seedcoat. While when $E_h / E_i < 500$, Eq. (A1) over-predicts the longitudinal stiffness, this is because area **H** was assumed rigid in deriving Eq. (A1). The rule of mixtures considers the deformation in area **H**, and therefore it accurately predicts the longitudinal stiffness in the range of $E_h / E_i < 10$. There is a transition range, $10 < E_h / E_i < 500$, in which, the FE data fall between the two limits predicted by the two analytical models (Eq. 38 and Eq. A1) derived from the two different deformation mechanisms.

List of Figures:

Fig. 1 – (a) SEM image of an entire common millet (*Panicum miliaceum*) seed with seed coat. The global coordinate system is defined as x - y - z , with the x direction along the longer axis of the seed, and the y direction along the shorter axis of the seed, and z direction is along the height of the seed. The local coordinate system 1-2-3 defined on the top surface of the seed coat, with the direction 1 along the transverse direction of the seed coat and the direction 2 along the longitudinal direction. (b) SEM image showing the in-plane microstructure of the seedcoat. a and b are the shorter and longer edge of epidermis cell, representatively. λ_i and A_i ($i=1, 2$) are the wavelength and amplitude of wavy sutures of epidermis cell in directions 1 and 2, where the white dash frame indicating the midlines of the wavy boundary of an epidermis cell; (c) microCT slice showing the x - y plane of an entire common millet (*Panicum miliaceum*) seed with seedcoat, indicating a small gap between the seedcoat and kernel (d) the SEM image of the cross-section of a broken seedcoat to show the thickness of the seedcoat.

Fig. 2 – Schematic graph of the composite plate model of the entire seedcoat with sinusoidal sutures (left), and a zoom-in graph of two neighboring representative volume elements (RVE) (right) to represent the in-plane (1-2) and out-of-plane (1-3) structures of the model (the coordinates of x - y - z and 1-2-3 are consistent with those defined in Fig.1a), in which the microstructure of the seedcoat is separated into two major areas: S2 suture area along direction 2 (blue layers); and major epidermis cell area M (yellow layers). M is further separated into two sub-areas: S1, suture area along the transverse direction 1; and area H, the area with only the hard phase.

Fig. 3 - Schematic drawings of the seedcoat RVE under different in-plane loading conditions (the coordinates of 1-2 is consistent with the local coordinates defined in Figs.1a and 1b), (a) uniaxial tension in direction 1, (b) uniaxial tension in direction 2, and (c) in-plane simple shear.

Fig. 4 – (a) Photos of the seed with seedcoat and the kernel with seedcoat peeled off, and (b) major dimensions defining the geometry of the seed and kernel (the coordinates of x - y - z is consistent with the global coordinate defined in Fig.1a), in which D_{S1} , D_{S2} , h_S are the major diameter, minor diameter and height of the full seed, respectively; and D_{K1} , D_{K2} , h_K are the major diameter, minor diameter and height of the kernel, respectively.

Fig. 5 – Setup of the uniaxial compression experiments (the coordinates of x - y - z is consistent with the global coordinate defined in Fig.1a).

Fig. 6 – The FE models of seed and kernel (the coordinates of x - y - z is consistent with the global coordinate defined in Fig.1a with the x direction along the longer axis of the seed, and the y direction along the height of the seed, and z direction is along the shorter axis of the seed.) for (a) side view, and (b) top view.

Fig. 7 – Average nanoindentation load-depth curves of the seedcoat layer (The horizontal error bar represents one experimental standard deviation at the load of 0.75 mN).

Fig. 8 – Comparison of the numerical and analytical results of the effective in-plane moduli for the seedcoat RVE (the symbols represent the FE results and the lines represent the analytical results) for (a) $\bar{E}_{11}$, (b) $\bar{E}_{22}$, and (d) $\bar{G}_{12}$. E_h/E_i is the stiffness ratio between hard phase and soft interfacial layer.

Fig. 9 – FE results of the in-plane anisotropy ratio. E_h/E_i is the stiffness ratio between hard phase and soft interfacial layer.

Fig. 10 – FE contours of normal stress (S_{11} and S_{22}), shear stress (S_{12}) and the maximum in-plane principle stress when $E_t = 60 \text{ MPa}$ for (a) tension in direction 1, $\varepsilon_{11} = 0.1\%$, (b) tension in direction 2, $\varepsilon_{22} = 0.1\%$, and (c) shear, $\varepsilon_{12} = 0.1\%$. (The coordinates of 1-2 is consistent with the local coordinates defined in Figs.1a and 1b, and the scale bar represents $10 \mu m$)

Fig. 11 - Experimental compression results of individual seeds up to damage initiation for full seeds and kernels. The solid color lines represent the load-displacement curves of kernel. The dash color lines represent the load-displacement curves of seed.

Fig. 12 – Experimental compressive results to damage initiation of individual seed / kernels for (a) kernels with FE kernel model results, and (b) full seeds with FE seed model results. The solid lines in the figure represent the experimental results. The dash lines represent the simulation results.

Fig. 13 – FE stress contours for seedcoat viewed from the top view (x-z plane, the coordinates of x-z is consistent with the global coordinate defined in Fig.1a) for large deformation (0.1 mm), plotted for the outer and inner shell surfaces.

Highlights

- The seedcoat of *Panicum miliaceum* shows remarkable micro-scale suture networks
- Sophisticated composite plate model was first developed for the seedcoat
- First experimental-numerical study on a single *Panicum miliaceum* seed and kernel

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