A non-classical computational method for modelling functionally graded porous planar media using micropolar theory

5 Abstract

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6 The current study proposes a computational-based method to employ the non-classical micropolar 7 continuum for modelling plates with in-plane functionally graded porosities. Initially, a 8 homogenisation method is developed to derive the micropolar parameters of porous heterogenous 9 plates based on strain energy equivalence in various designed deformations simulated via finite 10 element analysis. The modelling procedure is further augmented to accommodate structures with functionally graded porosities. The established method offers an effective framework for studying 11 12 the mechanical behaviour of porous plates with various porosity distributions and a wide range of aspect ratios. Results indicate that the micropolar theory-based modelling surpasses traditional 13 Cauchy theory in accurately predicting the stiffness and displacement distribution of the FG porous 14 structures. The novelty of this study lies in the integration of micropolar theory with the 15 16 homogenisation of graded porosity patterns, offering enhanced predictions for materials with microstructural features. Additionally, a custom finite element formulation is developed in 17 18 COMSOL to implement micropolar elasticity, significantly improving the computational 19 efficiency to account for complex geometry, loading, and boundary conditions. To show the 20 applicability of the method, the modelling is used to design a dental implant with its functional 21 property mimicking that of the natural bone to avoid stress-shielding while ensuring proper 22 occlusivity.

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- 24

25 Keywords: Modelling Functionally Graded Porosity; Micropolar and Cauchy continua; Finite 26 Element Analysis; Equivalent Porous-Cellular Materials; Homogenisation.

27 1 Introduction

28 The customisable properties [1], high specific surface area, and lightweight nature of porous 29 materials have made them key elements in various engineering applications. In recent decades, 30 porous materials have been widely used in many industrial sectors, including aerospace, civil 31 engineering, and biomedical applications such as porous implants and meshes for guided bone 32 regeneration [2], [3], [4]. Particularly, functionally graded porous structures [5], characterised by 33 a graded distribution of porosity, can provide customised mechanical properties along spatial 34 gradients [6], [7]. The mechanical behaviours of porous FG structures are of interest in the current literature in terms of static, vibration, and buckling problems, specifically in beams, plates, and 35 36 shells [8], [9], [10], [11], [12].

37 The thermo-mechanical behaviour of two-directional functionally graded porous-auxetic 38 metamaterial has been the topic of a study by Behravanrad and Jafari [10], where, through a 39 numerical finite difference scheme, the effects of porosity and auxeticity have been investigated. 40 Li et al. [9] studied the mechanical response of porous FG plates based on first-order shear 41 deformation theory and isogeometric analysis. Gao et al. [13] developed a mathematical model to study wave propagation in graphene platelets-reinforced porous FG plates integrated with 42

44 FG porous sandwich beams using the 2D plane stress finite element method. Ramteke et al. [15]

45 investigated the nonlinear eigenfrequency characteristics of the doubly curved multi-directional

46 FG porous panels by using the finite element method (FEM). Wu et al. [16] analysed the free and

47 forced vibrations of porous beams using FEM. Chen et al. [17] studied the static and dynamic

48 properties of a porous beam.

49 Besides the FEM approaches, isogeometric analysis (IGA), originally established by Hughes et al.

50 [18], is also used to study FG porous structures, especially when dealing with complex geometries

51 such as "triply periodic minimal surface (TPMS)". In IGA, the same non-uniform rational B-

splines (NURBS) basis functions that are used to model the exact geometry will be implemented
 to approximate the FE solution.

54 Nguyen-Xuan et al. [19] proposed an approach based on IGA and higher-order shear deformation

theory (HSDT) to study the functionally graded TPMS plate. The use of higher-order shear

56 deformation theories is to capture the nonlinear distribution of shear terms through the thickness

57 of the plate and satisfy the zero-shear strains/stresses without using shear correction factors.

The approach is further extended to study graphene platelets-reinforced FG TPMS [20]. In another recent work, Nguyen et al. [21] have integrated non-local strain gradient with IGA to enable the

60 consideration of softening and hardening and size-dependent phenomena in micro/nanostructures.

61 Another approach to increasing the accuracy of the results and the ability to capture microstructural

62 features is to use generalised continua where additional degrees of freedom are endowed to each

63 material point in addition to the standard displacement. In micropolar theory as an important

64 category of generalised continua, the rotation of the material point is introduced as the additional

degree of freedom, which is called microrotation to be distinguished from macro-rotation (local rigid rotation). Micropolar theory, also known as Cosserat, represents a significant advancement

67 in the field of continuum mechanics, particularly in the modelling of materials that exhibit complex

behaviours not adequately described by classical theories. This theory was first introduced by E. and F. Cosserat [22] and has since evolved by C. Eringen [23], [24], and W. Nowacki [25] to address various applications in engineering and materials science. W. Nowacki and C. Eringen have significantly shaped the understanding of this advanced theoretical framework. Eringen's work explored the concept of micro-polar elasticity and provided a robust mathematical framework that has been widely adopted in various fields [26]. Nowacki further enriched this theory by studying its implications in dynamic systems and wave propagation [27]. Elastic

micropolar theory has been successfully used in many applications [28], [29] to describe
heterogeneous materials [30], such as porous materials [31], [32], [33], [34], [35], cellular
materials [36], composites [37], [38], lattices [39], foams [40], [41], [42], and even nanostructures

78 [43], [44].

In the current literature, to study the structures with FG porosities, classical Cauchy continuum and non-local higher-order theories such as strain gradient theory are implemented. In these studies, the relative density is commonly taken as the dominant factor, and the relation between the elastic modulus and the density originally stems from a direct FEM calculation [45] or a micromechanics estimation [46], such as the modified rule of mixture [47] and Halpin Tsai [48] or available experiments [49].

In the present study, we advance this field by integrating non-classical micropolar theory to model
 porous plates that have in-plane functionally graded porosities. Compared to classical Cauchy
 theory, micropolar theory can better contemplate the internal structure of cellular solids [50] as it

88 uses field description at the coarse level and preserves the memory of the material underlying 89 structure at the fine level through internal scale parameters [44], [51], [52]. In this study, a 90 homogenisation scheme is proposed based on the strain energy equivalence to determine the 91 material constants of the equivalent continuum where the material parameters can consider the 92 effect of both the size and shape of the pores. The collected data for various porosities determines 93 the function for each material parameter in terms of the pore dimensions. Further, using the 94 established homogenised model, the mechanical response of porous plates with various porosity 95 distributions and a broad range of aspect ratios is investigated.

96 From a computational perspective, this study contributes by implementing a custom finite element method using the weak form of partial differential equations (PDE) in COMSOL Multiphysics to 97 98 solve the micropolar elasticity problem. This is a notable advancement, as commercial FEM 99 software typically does not support micropolar elasticity by default. Our custom formulation 100 allows for the simulation of complex boundary conditions and loading scenarios, offering more 101 precise predictions of mechanical responses. Additionally, the homogenisation scheme employed 102 reduces computational complexity, enabling the study of large-scale porous structures without the 103 burden of directly simulating their intricate microstructures. The combination of micropolar theory 104 with advanced FEM not only enhances the computational efficiency but also provides a more 105 accurate comparative analysis with classical Cauchy models, further underscoring the advantages 106 of non-classical theories for FG porous materials.

107 To show the applicability of the proposed framework, it is implemented to design a biomedical 108 prothesis used in dentistry called guided bone regeneration (GBR) mesh. GBR meshes are used in dentistry as mechanical barriers to isolate and protect the area of bone loss from the surrounding 109 110 tissue while allowing new bone growth (Fig. 1a). While various types of barriers have been used 111 for GBR, the design and mechanical properties of the GBR mesh can greatly influence its 112 effectiveness in promoting bone growth [53]. GBR meshes are designed to be porous to facilitate 113 the diffusion of fluids, oxygen, nutrients, and bioactive substances for cell growth, and an 114 appropriate pore size can ensure the desirable occlusivity of the GBR membrane [54], [55].

115 To implant GBR meshes, they are fixed to the underneath mandible bone using biocompatible 116 screws (Fig. 1b). Since these screws are located in critical loading areas, higher stiffness is required 117 in the corresponding locations on the GBR mesh, and therefore, smaller pore sizes are more 118 desirable. The importance of improving stiffness near fixing areas becomes more crucial when 119 using biodegradable resorbable materials made of natural or synthetic polymers [56], such as PLA 120 [57] or PLA composites [58]. The stiffness of these materials is much lower than that of metals 121 like titanium alloy (Ti6Al4V) that are widely used in dentistry [59]. However, the use of 122 bioresorbable materials is receiving great attention as it mitigates the need for a post-surgery to 123 remove the GBR mesh after the bone regeneration process [60].



124 125 126

a.

Fig. 1a. Implementation of a porous GBR mesh b. Fixing GBR mesh to the underneath mandible bone using biocompatible screws

127 On the other hand, bone has a heterogenous porous structure with microstructural features, for 128 which non-classical micropolar models are proven to better describe microstructure-related scale 129 effects on macroscopic effective properties [61], [62]. Lakes and co-workers [63], [64], [65], [66], 130 [67] also conducted a series of experiments and studies on bones and found that micropolar theory 131 provides better predictions of bone response than Cauchy elasticity. Such scale effects are most 132 pronounced near bone-implant interfaces and in areas of high strain gradients [68]. In the current 133 work, based on the developed framework, a design is suggested for the GBR mesh that can mimic 134 the natural FG structure of the bone.

135 The remainder of this paper is structured as follows: Section 2 presents the homogenisation 136 procedure implemented for extracting the equivalent material parameters for both micropolar and

137 Cauchy continua. Section 3 describes the developed mechanical models for plates with an in-plane

138 FG distribution of porosities. In Section 4, the obtained models are used to study the mechanical

response of FG porous plates with different distributions of porosities. The findings are compared to the response of the detailed porous structure for a wide range of senset ratios. The supress his

to the response of the detailed porous structure for a wide range of aspect ratios. The approach is used to propose an FG design for a dental GBR mesh in Section 5. Finally, Section 6 summarises

142 the key findings and outlines future research directions in the field of porous FG structures.

143 2 Homogenisation

144 For modelling the FG porous plates with different microstructures (pore patterns), a multiscale

approach [5] is proposed in which an equivalent homogenised material represents the porous

146 heterogeneous structure. The equivalent model is described in the framework of both micropolar

147 and classical (Cauchy) continua.

For the determination of the constitutive parameters of the equivalent models, the primary hypothesis is that the strain energy stored in the heterogeneous porous structure (micro-level) under prescribed boundary conditions is equal to that of the homogenous equivalent continuum description (macro-level). In the current work, at the micro-level, the classical Cauchy continuum is used, while at the macro-level, two different continuums (micropolar continuum and Cauchy continuum) are implemented, and the results are compared in describing FG porous structure (Fig. 2).



155 156 157

Fig. 2 The homogenisation procedure from classical Cauchy continuum at the micro-level to micropolar continuum and Cauchy continuum at the macro-level

- 158 The homogenisation procedure has been applied and thoroughly described before in [2]. For the
- 159 sake of completeness, only the major equations are reported below. The homogenised constitutive
- 160 parameters are further used in Section 3.2 to model functionally graded porous structures.

161 2.1 Homogenised Micropolar and Cauchy models

162 2.1.1 Micropolar Theory

163 The micropolar theory is governed by the following linearised kinematic equations:

$$\varepsilon_{ij} = u_{i,j} + e_{ijk}\phi_k$$

$$\mu_{kj} = \phi_{k,j}$$
(1)

164 where u_i and ϕ_k stand for the components of displacement and micro-rotation vectors, ε_{ii} and μ_{ki}

- 165 denote the components of strain and curvature tensors with e_{ijk} being the usual third-order
- 166 permutation symbol.
- 167 If body forces (p_i) and body couples (q_k) are also considered, the equilibrium equations take the
- 168 following form:

$$\sigma_{ij,j} + p_i = 0$$

$$\mu_{kj,j} - e_{ijk}\sigma_{ij} + q_k = 0$$
(2)

169 Where σ_{ij} and μ_{kj} are the components of the non-symmetric stress and couple-stress tensors, 170 respectively.

- 171 In the linearised 2D framework, there are two displacements and one rotational component that
- 172 can be collected in the two following vectors:

$$\mathbf{u}^{\mathrm{T}} = \begin{bmatrix} u & v \end{bmatrix}$$

$$\boldsymbol{\phi} = \begin{bmatrix} \phi \end{bmatrix}$$
 (3)

and the strain and curvature vectors will be:

$$\boldsymbol{\varepsilon}^{T} = \begin{bmatrix} \varepsilon_{11} & \varepsilon_{22} & \varepsilon_{12} & \varepsilon_{21} \end{bmatrix}$$

$$\boldsymbol{\kappa}^{T} = \begin{bmatrix} \kappa_{1} & \kappa_{2} \end{bmatrix}$$
(4)

174 Where $\varepsilon_{11}, \varepsilon_{22}, \varepsilon_{12}, \varepsilon_{21}$ are the in-plane normal and shear strains, and κ_1, κ_2 are the micropolar 175 curvatures.

176 The stress and couple stress vectors are also represented as:

$$\boldsymbol{\sigma}^{T} = \begin{bmatrix} \sigma_{11} & \sigma_{22} & \sigma_{12} & \sigma_{21} \end{bmatrix}$$

$$\boldsymbol{\mu}^{T} = \begin{bmatrix} \mu_{1} & \mu_{2} \end{bmatrix}$$
(5)

177 where σ_{ij} (*i*, *j* = 1,2) represents the normal (*i* = *j*) and shear stress (*i* ≠ *j*) components, and μ_1 , μ_2

- are the couple stresses or micro-couples.
- 179 The micropolar anisotropic constitutive equations can be represented as:

$$\begin{bmatrix} \boldsymbol{\sigma} \\ \boldsymbol{\mu} \end{bmatrix} = C \begin{bmatrix} \boldsymbol{\varepsilon} \\ \boldsymbol{\kappa} \end{bmatrix}$$
(6)

- 180 where **C** is the constitutive stiffness matrix, which due to hyperelasticity is symmetrical [69].
- 181 The geometries considered here for the 2D periodic porous model (such as the one shown in Fig.

182 2) are symmetric with respect to a 90° rotation. These symmetries in the 2D model imply a special

183 kind of orthotropic structure named "ortho-tetragonal" [37]. For the equivalent homogenised

184 ortho-tetragonal material, the constitutive equations can be presented in Voigt's notation as:

$$\begin{bmatrix} \sigma_{11} \\ \sigma_{22} \\ \sigma_{12} \\ \sigma_{21} \\ \mu_1 \\ \mu_2 \end{bmatrix} = \begin{bmatrix} A_{1111} & A_{1122} & 0 & 0 & 0 & 0 \\ A_{1122} & A_{1111} & 0 & 0 & 0 & 0 \\ 0 & 0 & A_{1212} & A_{1221} & 0 & 0 \\ 0 & 0 & A_{1221} & A_{1212} & 0 & 0 \\ 0 & 0 & 0 & 0 & D_{11} & 0 \\ 0 & 0 & 0 & 0 & 0 & D_{11} \end{bmatrix} \begin{bmatrix} \varepsilon_{11} \\ \varepsilon_{22} \\ \varepsilon_{12} \\ \varepsilon_{21} \\ \kappa_1 \\ \kappa_2 \end{bmatrix}$$
(7)

- 185 2.1.2 Identification of Equivalent Micropolar Material Parameters
- 186 Since micropolar and Cauchy continua use different degrees of freedom, a kinematic map is
- 187 required to link the two levels of description. Here, we followed the mapping proposed by Forest

and Sab [30] for a square representative volume element (RVE).

$$u^{*} = \varepsilon_{11}x + \varepsilon_{12}^{SYM}y - \frac{\kappa_{2}}{2}y^{2} - \kappa_{1}xy - \frac{10}{L^{2}}\theta(y^{3} - 3yx^{2})$$

$$v^{*} = \varepsilon_{12}^{SYM}x + \varepsilon_{22}y + \frac{\kappa_{1}}{2}x^{2} - \kappa_{2}xy + \frac{10}{L^{2}}\theta(x^{3} - 3xy^{2})$$
(8)

Eq. (8) expresses the approximate microscopic displacement field within the RVE (u^*, v^*) as a function of the macroscopic strain measures $(\mathcal{E}_{11}, \mathcal{E}_{22}, \mathcal{E}_{12}^{SYM}, \theta, \kappa_1, \kappa_2)$ at the material point on the macro-level.

192 After determination of the kinematic map, to find the micropolar material parameters in Eq. (7),

193 first we calculate the response of the porous plate subjected to various loadings using FEM. In

each case, the corresponding micropolar material parameters are found so that the equivalent

195 material stores the same strain energy density when subjected to the identical loading, i.e.,

$$U_{FEM} = U_{Micropolar} \tag{9}$$

196 Where $U_{Micropolar}$ is the strain energy density of the equivalent micropolar continuum calculated 197 using the following relation:

$$U_{Micropolar} = \frac{1}{2} \Big[\varepsilon_{11}\sigma_{11} + \varepsilon_{22}\sigma_{22} + \varepsilon_{12}^{SYM}\sigma_{12}^{SYM} + \theta\sigma_{12}^{ASM} + \kappa_{1}\mu_{1} + \kappa_{2}\mu_{2} \Big] \\ = \frac{1}{2} \big[\varepsilon_{11}(A_{1111}\varepsilon_{11} + A_{1122}\varepsilon_{22}) + \varepsilon_{22}(A_{1122}\varepsilon_{11} + A_{1111}\varepsilon_{22}) + \varepsilon_{12}^{SYM}(\frac{A_{1212} + A_{1221}}{2}\varepsilon_{12}^{SYM}) + \theta(\frac{A_{1212} - A_{1221}}{2}\theta) + \kappa_{1}(D_{11}\kappa_{1}) + \kappa_{2}(D_{11}\kappa_{2}) \Big]$$
(10)

198 And U_{FEM} is the strain energy density of the porous plate calculated using the finite element 199 method:

$$U_{FEM} = \frac{1}{2} \int_{RVE} \sigma_{ij}^{p} \mathcal{E}_{ij}^{p} dV$$
(11)

200 Where σ_{ii}^{p} and ε_{ii}^{p} are stress and strain in the porous structure.

To evaluate the components of the micropolar stiffness tensor ($A_{1111}, A_{1122}, A_{1212}, A_{1221}, D_{11}$), different boundary conditions are designed to represent uniaxial, biaxial, symmetric shear, bending, and rotational deformations. The applied tests, the corresponding material parameters obtained from each test, and the applied boundary conditions are described in Fig. 3. The boundary conditions to create each test are obtained using the micro-filed descriptions u^*, v^* in terms of macro-field strain measures presented in the kinematic map, i.e., Eq. (8).

Test 1 Uniaxial	Test 2 Biaxial	Test 3 Symmetric Shear	Test 4 Rotation	Test 5 Curvature
	$egin{array}{c} E_{\scriptscriptstyle XX} \ E_{\scriptscriptstyle YY} \end{array}$		θ	
A ₁₁₁₁	A ₁₁₂₂	A ₁₂₁₂	, A ₁₂₂₁	<i>D</i> ₁₁
$u^* = x$	$u^* = x$	$u^* = y$	$u^* = \frac{10}{L^2} \left(y^3 - 3yx^2 \right)$	$u^* = -x y$
$v^* = 0$	$v^* = y$	$v^* = x$	$v^* = \frac{10}{L^2} \left(3xy^2 - x^3 \right)$	$v^* = \frac{x^2}{2}$

208

Fig. 3 Designed FEM tests for finding micropolar material parameters.

209 More details on how to apply the boundary conditions and calculate each parameter can be found 210 in [2].

To find the homogenised Cauchy model, an analogous approach is followed in the framework of

212 Cauchy theory, which requires the definition of only three constitutive components. In this case,

213 the homogenisation is straightforward because there is no need to define a kinematic map.

Alternatively, such properties can be deducted from the micropolar one [70].

215 **2.2 Finite Element Model**

216 The finite element implementation at both macro (micropolar) and microlevels (Cauchy) is

217 described in this section. Since commercial FE codes do not yet support the micropolar continuum,

218 we implement the weak form of partial differential equations (PDE) numerically in COMSOL

219 Multiphysics. By using PDE modelling in COMSOL instead of traditional FE modelling, no user

subroutines are required and various complex geometries, boundary conditions, and loadings can

- 221 be applied in a user-friendly graphical interface.
- Regarding meshing and discretisation, the porous structure was discretised using first-order (linear) triangular elements. The thickness of the plate was assumed to be *W*/100, and therefore a 2D plane stress formulation for linear elastic media was adopted. The mesh of homogenous equivalent models is made of structured quadrilateral first-order (linear) elements. Note that the same approximation order for both displacements and micro-rotation were used.
- The weak form is formulated based on the virtual work principle for a micropolar continuum with $\frac{1}{228}$ using $\frac{1}{228}$ and $\frac{1}{228}$ as set of kinematically admissible displacement and rotation fields, such that:
- 228 **u** and ϕ as a set of kinematically admissible displacement and rotation fields, such that:

$$\int_{\Omega} \delta \boldsymbol{\varepsilon}^{T} \boldsymbol{\sigma} \, d\Omega + \int_{\Omega} \delta \boldsymbol{\kappa}^{T} \boldsymbol{\mu} \, d\Omega = \int_{\Omega} \delta \boldsymbol{u}^{T} \boldsymbol{p} \, d\Omega + \int_{B} \delta \boldsymbol{u}^{T} \boldsymbol{t} \, dB + \int_{\Omega} \delta \boldsymbol{\phi}^{T} \boldsymbol{q} \, d\Omega + \int_{B} \delta \boldsymbol{\phi}^{T} \boldsymbol{m} \, dB, \quad \forall \, \delta \boldsymbol{u}, \delta \boldsymbol{\phi}$$
(12)

- 229 Where Ω is the entire computational domain, δ denotes the variational operator with *t* and *m* 230 the traction and couple-traction vectors applied on the boundary *B*.
- 231 Displacement and microrotations are approximated by interpolating the nodal values \tilde{u} and $\tilde{\phi}$,
- 232 considered primal unknowns, using the shape functions as follows:

$$\boldsymbol{u} = \boldsymbol{N}_{\boldsymbol{u}} \tilde{\boldsymbol{u}}, \quad \boldsymbol{\phi} = \boldsymbol{N}_{\boldsymbol{\varphi}} \tilde{\boldsymbol{\phi}}$$
(13)

For quadrilateral elements, with first-order (linear) discretisation for both displacements and micro-rotation, the shape function matrices will be:

$$N_{u} = \begin{bmatrix} N_{1} & 0 & N_{2} & 0 & N_{3} & 0 & N_{4} & 0 \\ 0 & N_{1} & 0 & N_{2} & 0 & N_{3} & 0 & N_{4} \end{bmatrix}$$

$$N_{\varphi} = \begin{bmatrix} N_{1} & N_{2} & N_{3} & N_{4} \end{bmatrix}$$
(14)

Also, the micropolar strains and curvatures given in Eq. (1) can be written as:

$$\varepsilon = Lu + M\phi$$

$$\kappa = \nabla\phi$$
(15)

236 Where ∇ is the gradient operator in the 2D framework, and L and M are:

$$\boldsymbol{L} = \begin{bmatrix} \frac{\partial}{\partial x} & 0 & \frac{\partial}{\partial y} & 0\\ 0 & \frac{\partial}{\partial y} & 0 & \frac{\partial}{\partial x} \end{bmatrix}^{T}, \quad \boldsymbol{M} = \begin{bmatrix} 0\\0\\+1\\-1 \end{bmatrix}$$
(16)

237 By substituting Eq. (13) in Eq. (15), we have:

$$\boldsymbol{\varepsilon} = \boldsymbol{L}\boldsymbol{N}_{\boldsymbol{u}}\tilde{\boldsymbol{u}} + \boldsymbol{M}\boldsymbol{N}_{\boldsymbol{\varphi}}\tilde{\boldsymbol{\phi}} = \begin{bmatrix} \boldsymbol{L}\boldsymbol{N}_{\boldsymbol{u}} & \boldsymbol{M}\boldsymbol{N}_{\boldsymbol{\varphi}} \end{bmatrix} \begin{cases} \tilde{\boldsymbol{u}} \\ \tilde{\boldsymbol{\phi}} \end{cases} = \boldsymbol{B}_{\boldsymbol{\varepsilon}}\boldsymbol{d}$$

$$\boldsymbol{\kappa} = \nabla\boldsymbol{N}_{\boldsymbol{\varphi}}\tilde{\boldsymbol{\phi}} = \begin{bmatrix} \boldsymbol{0} & \nabla\boldsymbol{N}_{\boldsymbol{\varphi}} \end{bmatrix} \begin{cases} \tilde{\boldsymbol{u}} \\ \tilde{\boldsymbol{\phi}} \end{cases} = \boldsymbol{B}_{\boldsymbol{\kappa}}\boldsymbol{d}$$
(17)

238 Where *d* is the unknown vector of nodal displacements and the matrices B_{ε} and B_{κ} contains the 239 derivatives of shape functions.

240 The constitutive matrix for 2D ortho-tetragonal micropolar material in Eq. (7) will then become:

$$\boldsymbol{\sigma} = \boldsymbol{D}_{\varepsilon} \boldsymbol{B}_{\varepsilon} \boldsymbol{d} \quad \boldsymbol{\mu} = \boldsymbol{D}_{\kappa} \boldsymbol{B}_{\kappa} \boldsymbol{d} \tag{18}$$

Where:

$$\boldsymbol{D}_{\varepsilon} = \begin{bmatrix} A_{1111} & A_{1122} & 0 & 0 \\ A_{1122} & A_{1111} & 0 & 0 \\ 0 & 0 & A_{1212} & A_{1221} \\ 0 & 0 & A_{1221} & A_{1212} \end{bmatrix}, \quad \boldsymbol{D}_{\kappa} = \begin{bmatrix} D_{11} & 0 \\ 0 & D_{11} \end{bmatrix}$$
(19)

In the absence of body forces and couples, the algebraic finite element problem reads:

$$\delta d^{T} \underbrace{\int_{\Omega} (\boldsymbol{B}_{\varepsilon}^{T} \boldsymbol{D}_{\varepsilon} \boldsymbol{B}_{\varepsilon} + \boldsymbol{B}_{\kappa}^{T} \boldsymbol{D}_{\kappa} \boldsymbol{B}_{\kappa}) d\Omega}_{\boldsymbol{K}} = \delta d^{T} \underbrace{\int_{B} \begin{bmatrix} \boldsymbol{N}_{u}^{T} \boldsymbol{t} \\ \boldsymbol{N}_{\phi}^{T} \boldsymbol{m} \end{bmatrix}}_{\boldsymbol{F}} dB , \forall \delta d$$
(20)

243 Where *K* and *F* indicate the elemental stiffness matrix and the nodal force vector.

The elemental stiffness matrix K is then assembled into the global stiffness matrix, K_{Global} , by summing contributions from all elements and aligning the global degree of freedoms:

$$\boldsymbol{K}_{Global} \left\{ \begin{matrix} \boldsymbol{U} \\ \boldsymbol{\Phi} \end{matrix} \right\} = \left\{ \begin{matrix} \boldsymbol{T} \\ \boldsymbol{M} \end{matrix} \right\}$$
(21)

246 Where U and Φ are the global displacement and microrotation vectors, and T and M are the 247 global force and moment vectors.

For the benefit of readers, we also present how to practically implement the weak form of the equations in the COMSOL PDE framework.

250 We start from the balance equations and multiply each of them by its corresponding test functions,

denoted here as u_i^{test} and ϕ_k^{test} , and integrate over the entire computational domain *D*.

$$\int_{\Omega} (\sigma_{ij,j} u_i^{test} + p_i u_i^{test}) d\Omega + \int_{\Omega} (\mu_{kj,j} - e_{ijk} \sigma_{ij} + q_k) \phi_k^{test} d\Omega = 0$$
(22)

- It should be noted that the test functions are inherently the virtual displacement introduced previously in Eq. (12).
- By applying the divergence theorem and considering B as the surface boundary, the weak form equations can be defined:

$$(-\int_{\Omega} \sigma_{ij} u_{i,j}^{test} d\Omega + \int_{B} \sigma_{ij} u_{i}^{test} n_{j} dB + \int_{\Omega} p_{i} u_{i}^{test} d\Omega) + (-\int_{\Omega} \mu_{kj} \phi_{k,j}^{test} d\Omega + \int_{B} \mu_{kj} \phi_{k}^{test} n_{j} dB - \int_{\Omega} e_{ijk} \sigma_{ij} \phi_{k}^{test} d\Omega + \int_{\Omega} q_{k} \phi_{k}^{test} d\Omega) = 0$$

$$(23)$$

256 Where the domain and surface contributions can be rearranged as:

$$\int_{\Omega} (-\sigma_{ij} u_{i,j}^{test} + p_i u_i^{test} - \mu_{kj} \phi_{k,j}^{test} - e_{ijk} \sigma_{ij} \phi_k^{test} + q_k \phi_k^{test}) d\Omega$$

$$+ \int_{B} (\sigma_{ij} u_i^{test} n_j + \mu_{kj} \phi_k^{test} n_j) dB = 0$$
(24)

257 In PDE COMSOL, the domain contribution specifies the governing equations, while the surface 258 contribution should be defined in weak form as the boundary conditions. This is the main leverage 259 of implementing micropolar theory through the PDE framework developed in the current work: 260 By properly defining the weak form of governing equations and boundary conditions, constitutive equations, and kinematic relations, one can benefit from the developed capacity of COMSOL for 261 discretisation, definition of shape functions, as well as derivation and assemblage of stiffness 262 263 matrix.

264 3 **Functionally graded porous plates**

265 3.1 **Geometrical Modelling**

266 Consider a porous rectangular plate with length L, width W, and height (thickness) h, as presented 267 in Fig. 4.



Fig. 4 The coordinates and geometry of the porous rectangle plate and the 2D model

270 The Cartesian coordinates (x, y, z), located in the mid-plane, are used to define the displacements 271 u, v, and w in the length, width, and thickness directions. The porosity distributions can occur in 272 the in-plane directions, such as x-direction and y-direction, as well as the thickness [71]. Four 273 different kinds of porosity distributions in the y-direction (Types 'V', 'A', 'X', and 'O', see Fig. 274 5), which are standard in the literature [48], are used here to study the mechanical behaviour of the

275 FG porous plate.



Fig. 5 Four different types of porosity distribution through the in-plane y-direction

278 For type 'V', the porosity distribution is linearly varied in the y-direction from a small pore size 279 of 0.01 W at y = 0 to the pore size of 0.09 W at y = W. Therefore, the maximum and minimum 280 values of effective stiffness parameters correspond to the bottom and the top surfaces, respectively. 281 For type 'A', the porosity distribution linearly varies in the v-direction from a pore size of 0.09 W 282 at y = 0 to the pore size of 0.01 W at y = W. Therefore, contrary to the type 'V', the minimum and 283 maximum values of effective stiffness parameters correspond to the bottom and the top surfaces, 284 respectively. Type 'X' consists of two piecewise linear parts where the smallest pore size is located 285 on the midline and the largest size on the top and bottom parts. Reversely to type X, for type 'O', the largest pore size is located on the midline and the smallest size on the top and bottom parts. 286 287 Various porosity distributions can be considered as a function of vertical location (y). The variation

of the pore size through the FG structure for the four porosity distributions in the current work is represented in Fig. 6.





Fig. 6 The variation of pore sizes through height for each porosity distribution

Based on the distribution of porosity, the variation of the pore size (l_p) along the y direction can be described as $l_p = g_*(y)$ where the subscript * refers to the type of porosity distribution. Considering the minimum pore size as 0.01 *W* and the maximum as 0.09 *W*, the functions for each type of porosity distribution are as follows:

$$l_{p} = g_{V}(y) = \frac{0.09}{W} y + 0.05 \quad (V)$$

$$l_{p} = g_{A}(y) = -\frac{0.09}{W} y + 0.05 \quad (A)$$

$$l_{p} = g_{X}(y) = \frac{0.09}{W} |y| + 0.09 \quad (X)$$

$$l_{p} = g_{O}(y) = -\frac{0.09}{W} |y| + 0.09 \quad (O)$$
(25)

In which |y| is the absolute (positive) value of the vertical position (y), and y origin is located at W/2.

298 **3.2** Equivalent homogenised models for FG porous plates

Fig. 7 shows how the equivalent homogenised FG porous structure is derived by considering the homogenisation procedure developed for unit cells with uniform porosity [2]. First, a parametric study is conducted to find the equivalent mechanical parameters (Cauchy and micropolar) of uniform porous plates with various pore sizes. In the parametric study, the pore density (i.e., the number of pores per unit length) is kept constant and the pore sizes are changed from 0.01 *W* to 0.09 *W* to find the required equivalent parameters for each section of FG porous structure.



305

Fig. 7 A graphical abstract of the methodology for developing equivalent homogenised models of FG porous plates







Fig. 8 The flowchart for the implementation algorithm of the present work

For studying the FG patterns, we choose the pore size to vary in the range of 0.01L to 0.09L. When the pore size exceeds 0.09L, the reduction of material thickness between the pores can lead to local buckling or instability under loading, which may not be fully captured by the homogenised model. Also, very small pore sizes less than 0.01L can pose challenges related to meshing and discretisation, particularly near the discontinuities, which may reduce the numerical accuracy.

In the applications, we consider polylactic acid (PLA) as base material of the porous plate. PLA is a biodegradable and non-toxic material that is approved by the FDA for bioresorbable medical implants and therefore is widely used in the biomedical sector [58], [72]. The material properties considered for PLA are listed in Table 1.

320

Table 1 Material properties of the base material (PLA) [57], [73]

Young's Modulus	3.775	GPa
Poisson Ratio	0.3	-
Density	1120	kg/m ³

In Fig. 9, the equivalent micropolar and Cauchy parameters for the pore sizes ranging from 0.01W

- 322 to 0.09W are presented.
- 323 These data are then utilised to find curve-fitted functions, $f_i(l_p)$, for each material parameter with
- 324 respect to the pore size, l_p .
- The obtained functions for equivalent constitutive parameters (in Pa) are as follows: $A_{1111} = f_1(l_p) = -41264l_p^4 + 11339l_p^3 - 1107.1l_p^2 + 4.4412l_p + 4.1318$ $A_{1122} = f_2(l_p) = -1152l_p^4 + 2240.8l_p^3 - 357.8l_p^2 + 3.1343l_p + 1.2268$ $A_{1212} = f_3(l_p) = -21.30l_p^4 + 3013.50l_p^3 - 506.03l_p^2 + 2.26l_p + 1.94$ $A_{1221} = f_4(l_p) = 7501.8l_p^4 + 926.53l_p^3 - 281.96l_p^2 + 2.2673l_p + 0.9298$ $D_{11} = f_5(l_p) = -3355.3l_p^4 + 879.59l_p^3 - 83.344l_p^2 + 0.2526l_p + 0.3249$
- 326 And the functions for equivalent constitutive parameters for Cauchy theory are those described in
- 327 Eq. (13) for $C_{1111} = A_{1111}$, $C_{1122} = A_{1122}$ and $C_{1212} = (A_{1212} + A_{1221})/2$.



328 Fig. 9 The equivalent micropolar (a.-e.) and Cauchy (a., b., and f.) material parameters for pore sizes ranging from 0.01W to 0.09W.

330 Now, by considering the relationship between homogenised material parameters and pore sizes

331 $(f_i(l_p))$ as well as the functionality of pore sizes versus locations $(l_p = g_*(y))$ in each FG porous

pattern, it is possible to determine the constitutive functions for each FG structure by employingthe composition operator:

$$A_{\#\#\#\#} = f_i(g_*(y)) \tag{27}$$

334 Where $A_{\#\#\#\#}$ represents the constitutive parameters of the homogenised micropolar/Cauchy model

335 (see Eq. (26)).

336 4 Numerical Results and Discussion

337 4.1 Geometry, loading, and boundary conditions

338 The usefulness of micropolar model is more evident when concentrated forces are applied and/or 339 geometric discontinuities are present [38]. Also, micropolar theory is more effective compared to 340 the Cauchy theory when structures are intended to withstand shear loads as normal stiffness properties are the same between micropolar and Cauchy theories $C_{1111} = A_{1111}$ and $C_{1122} = A_{1122}$. 341 342 Therefore, to evaluate the effectiveness of micropolar theory and its proficiency to Cauchy theory 343 in describing the mechanical performance of FG porous structures, two loading scenarios are 344 considered: a distributed shear load and a vertical indentation load. The distributed shear load is 345 applied on the top surface of the porous plate/beam (p = 1000 N/m), while the bottom surface of 346 the structure is fixed. Various length scales (L/W) were investigated for four types of porosity distributions by comparing the results for L/W < 1, L/W = 1, and L/W > 1 (Fig. 10). In all the 347 348 structures, L is fixed as 1.

Fig. 10 The geometry and loading considered for evaluation of the mechanical response of porous plates. L is the length (horizontal length) and W is the width (vertical length).

352 4.2 Comparison of displacement distribution for porous and homogenised models

349 350

351

To get insight into the mechanical response within the plate, the normalised displacement on the midline (y = W/2) is compared for the porous model versus homogenised models while considering various porosity distributions. The effect of the three aspect ratios L/W = 0.55, L/W = 1, and L/W= 1.55 is also studied. All the displacements are normalised by *L*. The results are summarised in Fig. 11 for four types of porosity distributions: Types A, V, X, and O, respectively. Here, "DT", "MP" and "CHY" denote detailed porous models, micropolar homogenised models, and Cauchy homogenised models, respectively.

а.

L/W = 1

d.

L/W = 0.55

L/W = 1.55

Fig. 11 The comparison of the normalised displacement magnitude on the midline for the porous model versus homogenised micropolar and Cauchy models for FG porous structure with porosity distribution of **a**. Type A, **b**. Type V, **c**. Type X, **d**. Type O with aspect ratios of L/W = 0.55, L/W = 1, and L/W = 1.55.

363 The results for the studied cases show that micropolar homogenised models can better predict the

displacement distribution of the FG porous structure compared to the Cauchy homogenised model

365 for all porosity patterns. The advantage of micropolar to Cauchy theory is more prominent in the

366 case of A and X patterns.

- 367 In Fig. 12, the normalised displacement contour lines are compared for the case of L/W = 1 for all
- the four porosity patterns of types A, V, X, and O, respectively.

369

360

Fig. 12 Comparison of normalised displacement contours of the porous model versus homogenised micropolar and Cauchy
 models for FG porous structure with porosity distribution a. Type A, b. Type V, c. Type X, d. Type O, and L/W = 1. The values of contour lines are reported in a. for better presentation of the differences.

As shown in Fig. 12, both homogenised models can follow the displacement contours of the detailed porous model. In Fig. 12*a*, the arrows show the distance between the displacement isolines in the porous model and the corresponding predicted iso-line by each homogenised model. As it can be seen, the performance of the homogenised micropolar model is better as the displacement iso-lines are closer to the porous FG structures for the micropolar homogenised models compared to Cauchy ones.

379 4.3 Aspect ratio effect

380 To evaluate the aspect ratio effect on the stiffness of the porous structures and the capability of the

381 homogenised models in predicting stiffness, the maximum deflection (normalised displacement at

point A in Fig. 10) is compared for porous and equivalent micropolar and Cauchy models for 10

aspect ratios and the four FG patterns.

The results are presented in Table 2 and Fig. 13. Overall, the obtained results for homogenised micropolar and Cauchy models are consistent with the porous model. However, according to Table 2, compared to Cauchy theory, the micropolar model better predicts the mechanical behaviour of porous structures, especially for very small aspect ratios such as AR = 0.55. As aspect ratio

- increases, the difference between the porous response and micropolar prediction decreases.
- 389

Table 2 Comparison of the normalised displacement magnitude (in μ) obtained from the porous model and predicted by homogenised micropolar and Cauchy models for the loading and geometry demonstrated in Fig. 10. (% error) shows the difference between values resulted from the homogenised model and the detailed porous model.

Distribution	L/W	Porous	Micropolar	(% error)	Cauchy	(% error)
	0.55	10.50	11.20	(6.67)	11.50	(9.52)
٨	1.00	5.04	5.34	(5.95)	5.51	(9.33)
A	1.55	3.58	3.76	(5.03)	3.95	(10.34)
	2.00	3.20	3.33	(4.06)	3.55	(10.94)
	0.55	12.61	13.14	(4.18)	13.53	(7.27)
v	1.00	6.98	7.17	(2.65)	7.47	(7.00)
Λ	1.55	5.53	5.56	(0.67)	5.91	(6.88)
	2.00	5.16	5.11	(-0.85)	5.51	(6.80)
	0.55	6.93	7.12	(2.70)	7.33	(5.77)
V	1.00	4.29	4.31	(0.36)	4.47	(4.09)
v	1.55	3.63	3.56	(-2.10)	3.75	(3.18)
	2.00	3.47	3.34	(-3.74)	3.56	(2.53)
	0.55	10.07	10.42	(3.44)	10.58	(5.02)
0	1.00	5.58	5.69	(1.94)	5.78	(3.46)
0	1.55	4.45	4.46	(0.35)	4.56	(2.51)
	2.00	4.16	4.13	(-0.74)	4.25	(2.16)

390

396 397 Fig. 13 Comparison of maximum normalised displacement (normalised displacement at Point A in Fig. 10) in the porous and homogenised models for different aspect ratios and porosity distribution of a. Type A, b. Type X, c. Type V, d. Type O

398 4.4 The effect of different porosity distributions

399 To study the effect of different porosity distributions, the maximum deformations of the 400 homogenised models for four types of porous FG structures are compared.

401 402

Fig. 14 Comparison of the maximum normalised displacement (normalised displacement at Point A in Fig. 10) of the FG porous 403 plate for porosity distribution Type 'A', Type 'V', Type 'X', and Type 'O' for various aspect ratios.

404 As can be inferred from Fig. 14 for aspect ratios less than approximately 1.5, it is important to take 405 functional porosity into account when predicting the plate's mechanical response; however, in 406 higher aspect ratios, the overall porosity plays a more important role. This becomes clearer by comparing the maximum displacement for two distribution types A and V reported in Table 3, 407

408 with the overall same porosity. As shown in the table, the difference between maximum 409 displacement is high for L/W=0.5 and decreases for L/W=1.5 and 2.

410 Table 3 Comparison of the maximum normalised displacement (normalised displacement at Point A in Fig. 10) for porosity 411 distributions Type 'A' and Type 'V'. The values in the parentheses show the difference between the A and V distributions for each 412 AR.

Distribution	Domosity	Volume	Max Normalised Displacement					
Distribution	Folosity	Fraction	L/W	′=0.5	L/W	=1.5	L/V	V=2.0
Type A	20.14 %	0.79858	10.50	(520())	3.58	(10/)	3.20	(70/)
Type V	20.14 %	0.79858	6.93	(52%)	3.63	(1%)	3.47	(/%)

413

414

415 **4.5 Indentation of a Vertical Load**

416 To provide further evaluation of the proposed model, another loading scenario is studied in this

417 section for all the FG patterns. Fig. 15 shows the loading and boundary condition on an FG plate

418 with the O pattern as an example.

419

420 Fig. 15 The geometry, loading, and boundary conditions for the vertical indentation on an FG porous structure with porosity 421 distribution Type O

422 The maximum normalised displacement observed in the FG porous structures with different 423 patterns and the predicted values by the micropolar and Cauchy continua are compared in Fig. 16. 424 This figure shows that in all the patterns, the prediction of the micropolar theory is closer to the 425 real porous structure compared to the Cauchy predictions.

427
 428 Fig. 16 Comparison of maximum normalised displacement resulted from the vertical indentation in the porous and homogenised
 429 models for different porosity distributions of Type A, Type X, Type V, and Type O.

- 430 Besides in Fig. 17, the contour of the normalised displacements for the FG porous structure with
- 431 V pattern and the homogenised micropolar and Cauchy models are compared. As can be seen, the
- 432 load penetration reflected in the displacement contours is better captured by the micropolar model
- 433 compared to the Cauchy one.

434 435

436

437 5 Case Study: FG porous design in GBR dentistry meshes

438 From a mechanical and physiological perspective, it is important that bone scaffolds mimic the 439 mechanical characteristics of the host bone to prevent a phenomenon known as stress shielding. 440 Stress-shielding happens when an over-rigid implant reduces the stress in its adjacent bone. Since 441 loading is necessary to promote bone remodelling, this could prevent bone regeneration and result 442 in bone resorption. Conversely, an extremely flexible implant may cause undue stress on the bone, 443 impairing the consolidation of the bone-implant interphase and ultimately resulting in the death of 444 bone cells [74]. Therefore, based on the developed framework in the current work, the following design is suggested for the GBR mesh made from bioresorbable PLA. 445

446 By mimicking the FG natural structure of the bone, an FG structure of type O is suggested, as

shown in Fig. 18, so that the central part of the GBR mesh possesses mechanical properties close

- to cancellous (trabecular) bone while providing a proper occlusivity and the part near fixing areas
- 449 (the screw's location) as near as possible to cortical (compact) bone to provide required load-
- 450 bearing capacities.

451 452

Fig. 18 a. The usual porous GBR meshes implemented with uniform porosity b. FG porous structure (Type O) design

However, the experimental micropolar parameters for mandible cancellous bone are not available
in the literature. Also, it should be noted that these parameters can vary depending on different
factors such as the patient's age, gender, and health status [75].

456 An estimate of the mechanical parameters of mandible cancellous bone is reported in Table 2

- 457 retrieved from [75], [76], and considering $A_{1111} = \frac{E(1-\nu)}{(1+\nu)(1-2\nu)}$ and $A_{1122} = \frac{E\nu}{(1+\nu)(1-2\nu)}$ from 458 linear elasticity for isotropic materials [77].
- 458 Inteal elasticity for isotropic in

459

Table 4 Mechanical parameter data available for mandible cancellous bone adapted from [75], [76]

Parameter		Value	Unit
Young's Modulus	Ε	0.907	GPa
Poisson Ratio	V	0.3	-
A_{1111}		1.84	GPa
A ₁₁₂₂		0.79	GPa

460 According to the studied configurations in the current work, pore sizes of 0.075W can provide

461 mechanical parameters near those of the cancellous bone in Table 4. This is suggested as the pore

size in the middle of the GBR mesh.

463 For the GBR parts around the fixing area, a minimum pore size of 0.01W is suggested to allow for

464 enough permeability for the nutrients. Considering that *W* is around one centimetre for dental GBR

465 meshes, the pore size of 0.01W is in favour with the experimental observation of Gutta et al. [55],

466 where they reported that macro-pores of more than 1 mm promote better bone regeneration [60].

467 However, it should be noted that the micropolar parameters corresponding to the pore size of 0.01L

468 in a PLA porous plate are lower than that of the cortical bone. The micropolar parameters of the

469 compact bone retrieved from an experimental report [78], [79], are presented in Table 5. However,

this can be remedied by locally reinforcing the base material in these areas; a suggestion is to use

471 nano-reinforcements such as silver nanoparticles. Introducing a nano-reinforcement like silver

472 nanoparticles into PLA [80] will enhance its mechanical properties [81] and endow antimicrobial 473 features to the material, which is of great interest in GBR meshes [82]. For instance, as reported 474 in [81], adding 21.8% weight fraction of silver nanoparticles to PLA will improve the Young's 475 modulus by 2.75 times, and this will roughly increase all the parameters with the same order, thus making the parameters of the porous structure with 0.01L close to the ones reported in Table 5. 476 477 The full investigation of the effect of nano-reinforcement and the design of functionally graded 478 materials (FGM) in conjugation with functionally graded porosities can be the topic of future 479 investigations.

- 480
- 481

Table 5 Micropolar stiffness matrix components for bone extracted from experimental data [2]

_		
Parameter	Unit	Value
A_{1111}	GPa	12.00 ~ 43.43
A_{1122}	GPa	4.00
A_{1212}	GPa	21.10 ~ 36.77
A_{1221}	GPa	-13.05 ~ 2.67
D_{11}	kN	3.24

482

483 6 Conclusions

484 In the current work, non-classical micropolar and Cauchy continua are proposed to model porous 485 plates with functionally graded distribution of porosities within the plane. A multiscale approach 486 is developed based on the equivalence of strain energy to find the material properties of 487 homogenous continua equivalent to heterogenous FG porous structures. To evaluate the effectiveness of the method, the mechanical response of FG porous plates with diverse porosity 488 489 distributions, 'V', 'A', 'X', and 'O', and a broad range of aspect ratios is compared to the prediction 490 of the equivalent models. To show the applicability of the developed framework, it is used to 491 design a biomedical prothesis used in dentistry called guided bone regeneration (GBR) mesh.

492 The main findings are summarised as follows:

- The micropolar theory-based modelling can better predict the displacement distribution of the FG porous structure for all porosity patterns compared to the Cauchy-based modelling. The competence of micropolar to Cauchy theory is more prominent in case of A and X patterns. In all cases, the prediction of micropolar theory becomes closer to the porous structure as the aspect ratio increases.
- For aspect ratios less than approximately 1.5, it is important to take functional porosity into account when predicting the FG plate's mechanical response; however, in higher aspect ratios, the overall porosity plays a more important role.
- As a biomedical application of the proposed modelling, it is used to suggest a GBR mesh that tries to mimic the FG natural structure of the bone. The FG porous configuration is suggested so as the central part possesses mechanical properties close to mandible cancellous (trabecular) bone to provide the proper occlusivity and the part near fixing areas provides higher stiffness.
- 506

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513

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