COMPDYN 2025
10th ECCOMAS Thematic Conference on
Computational Methods in Structural Dynamics and Earthquake Engineering
M. Papadrakakis, M. Fragiadakis (eds.)
Rhodes Island, Greece, 15-–18 June 2025

EXPLORING THE MECHANICAL RESPONSE OF A DISCRETE-BASED HEURISTIC MOLECULAR MODEL WITH NONLINEAR CONSTITUTIVE RESPONSE FOR IMPACT PROBLEMS

Luis C.M. da Silva[1], Nicola Zani[2], and Siro Casolo[1]

[1]Politecnico di Milano
Department of Architecture, Built Environment and Construction Engineering, Piazza Leonardo da Vinci, 20133, Milan, Italy
e-mail: {luiscarlos.martinsdasilva,siro.casolo}@polimi.it

[2] University of Florence
Department of Civil and Environmental Engineering, Piazza Brunelleschi 6, 50121 Florence, Italy
e-mail: nicola.zani@unifi.it

Keywords: auxetic material, heuristic molecule, Cosserat, Poissons ratio, RBSM, concentrated loading

Abstract. *The mechanical response of an auxetic material obtained by an original periodic microstructure is investigated when loaded by a concentrated loading. This is intended to provide an initial insight for applications to localised impact problems. The unit cell is designed using a plane heuristic molecule approach which is based on a Rigid-Body-Spring-Model (RBSM) that includes both centred and non-centred bond-springs between specifically shaped heuristic atoms. A linear static analysis is firstly presented, then this is extended to include non-linear constitutive laws for the bonds. Bond elastic stiffness is calibrated through energy equivalence with a macro-scopic elastic and isotropic Cosserat continuum. Non-linear bond laws are proposed to model potential bond-atom contact under compression and elastic-perfectly plastic behaviour under tension. Parameters that govern the contact onset are explored to assess its influence on the macro-scale mechanical response of the material layer under concentrated loading. While this parametric study is exploratory, we discuss the advantages of the proposed microstructure for impact applications, by observing its ability to disperse tension-induced damage away from the impact zone conditioned by the bond deformation for contact onset.*

1 INTRODUCTION

The use of discrete approaches for the design of internal geometries in architected materials is currently being explored [9]. Discrete approaches are well established for the modelling of microstructures with exotic properties, as for instance pantographic structures [4, 5] or auxetic foams [3], but also to develop functional materials for different fields of application. Matlack et al. [6] developed a material with weakly interacting 2D unit cells, enabling the creation of Veselago lenses, zero-dispersion bands, and topological surface phonons. Wang et al. [8] used periodic and discrete 2D unit cells to evaluate the wave propagation properties of metamaterials.

It was demonstrated in [2] that the use of a discrete model based on an heuristic molecule (HM) can, depending on the topology adopted, allow the modelling of materials with either a positive or negative Poisson's ratio ν. It has been also demonstrated that a micropolar HM can feature an isotropic response under a linearized assumption for the spring-based bonds under uni-axial and a deviatoric deformation modes. Such findings were further explored under non-linear geometric hypothesis, and that isotropy tends to be lost under progressively large deformations [3]. Besides the ability of the micropolar heuristic molecular model to be used as a mathematical tool to predict the mechanical response of materials with $-1.0 \leq \nu \leq 0.33$ (under Plane-Stress), one highlights that the discrete nature of the approach provides a unique framework to design microstructures with a-priori targeted mechanical properties.

To explore the possibility of design different microstructures with targeted mechanical properties, we investigate here the response of different HMs for different case studies in respect to macro-scale Cauchy-type materials, i.e. "simple materials" as designated by Noll [7]. Then, by including material non-linearity, we apply it for the study of an impact-like concentrated loading. Non-linearity is lumped in the bonds that follow an elastic-perfectly plastic behaviour under tension and an elastic-hardening law in compression in order to model of a potential bond-atom contact. Parameters that govern the contact onset are explored to assess its influence on the macro-scale mechanical response of a material layer under impact. While this study has an exploratory nature, we discuss the advantages of the designed auxetic microstructure, by observing its ability to disperse tension-induced damage away from the impact zone and reduce indentation.

2 BOND-BASED HEURISTIC MOLECULAR MODEL

A linearized and two-dimensional micropolar bond-based heuristic molecular model is briefly described. It is based on the hypothesis of pair-potentials and further details can be found in [2, 3]. A plane solid material consists of a finite number of heuristic molecules (HM). Each HM is made by heuristic atoms that possess a specific polygonal shape and that are significantly more rigid than the other components of the system. These atoms are disposed according to a regular lattice arrangement and only adjacent atoms interact via bonds characterized by an elastic potential through bond-spring elements. The complete set of centred and non-centred bonds include axial bonds, cyan (horizontal and vertical) and red (diagonal) springs, and shear bonds, which are non-centered and orthogonal to the direction of the bonded atoms and are represented by magenta and green springs. These bond types are shown in Figure 1. The corresponding generalised stiffnesses are named as follows: k_c (cyan bonds), k_r (red bonds), k_m (magenta bonds), k_g (green bonds).

2.1 Linearized kinematics and deformation energy

The kinematic mapping χ between a given reference (undeformed) configuration $\mathbf{X}$ and a deformed one $\overset{\star}{\mathbf{X}}$ is given as $\chi : \mathbf{X} \rightarrow \overset{\star}{\mathbf{X}}$. The relative Lagrangian displacements and rotations are given as $\mathbf{U} = \overset{\star}{\mathbf{X}} - \mathbf{X}$ and $\mathbf{\Psi} = \overset{\star}{\mathbf{\Phi}} - \mathbf{\Phi}$, respectively. For an arbitrary bond b, within the material domain Ω, that links atoms i and j, the bond vector $\mathbf{d}_b$ is given in Eq. (1) and the deformed bond vector $\overset{\star}{\mathbf{d}}_b$ in Eq. (2).

$$\mathbf{d}_b = (\mathbf{x}^j + \mathbf{r}_b^j) - (\mathbf{x}^i + \mathbf{r}_b^i) \quad , \tag{1}$$

$$\overset{\star}{\mathbf{d}}_b = (\overset{\star}{\mathbf{x}}^j + \overset{\star}{\mathbf{r}}_b^j) - (\overset{\star}{\mathbf{x}}^i + \overset{\star}{\mathbf{r}}_b^i) \quad , \tag{2}$$

where $\mathbf{r}_b^i$ and $\mathbf{r}_b^j$ represent the rigid arms of the bond b with respect to atoms i and j, respectively. The vectors $\overset{\star}{\mathbf{r}}_b^i$ and $\overset{\star}{\mathbf{r}}_b^j$ denote the rigid arms of the atoms after the deformation of the bond b. The relative displacement vector of bond b, linking atoms i and j, is described as δ_b and is determined according to the global reference frame by $\boldsymbol{\delta}_b = \overset{\star}{\mathbf{d}}_b - \mathbf{d}_b$. The bonds experience simple axial deformations and resemble axial springs. The strain energy for an arbitrary bond b with stiffness k_b and direction $\boldsymbol{\xi}_b$ in the reference configuration has a quadratic dependence on the variation of the initial bond length:

$$\mathcal{U}_{b_\xi}(\boldsymbol{\delta}_b) = \frac{1}{2} k_b (\boldsymbol{\xi}_b \cdot \boldsymbol{\delta}_b)^2 \quad . \tag{3}$$

2.2 Relation with a reference continuum FE model

The constitutive response of the HM can be established as related to a micropolar continuum through energy equivalence. This allows to establish a mathematical bridge that eases the design process of micro-structures according to desired continuum macroscopic mechanical properties. The constitutive response in isotropic linear elasticity is described by:

$$\begin{Bmatrix} S_{11} \\ S_{22} \\ S_{12} \\ S_{21} \\ M_{13} \\ M_{23} \end{Bmatrix} = \begin{bmatrix} \mathsf{C}_{1111} & \mathsf{C}_{1122} & 0 & 0 & 0 & 0 \\ \mathsf{C}_{1122} & \mathsf{C}_{2222} & 0 & 0 & 0 & 0 \\ 0 & 0 & G+G_c & G-G_c & 0 & 0 \\ 0 & 0 & G-G_c & G+G_c & 0 & 0 \\ 0 & 0 & 0 & 0 & 2Gd^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2Gd^2 \end{bmatrix} \begin{Bmatrix} E_{11} \\ E_{22} \\ E_{12} \\ E_{21} \\ K_{13} \\ K_{23} \end{Bmatrix} \quad , \tag{4}$$

in which $\mathsf{C}_{1111} = \mathsf{C}_{2222} = \frac{2G}{1-\nu}$ and $\mathsf{C}_{1122} = \frac{2G\nu}{1-\nu}$ for a Plane-Stress (PS) problem; the Cosserat shear modulus G_c governs the specific skew-symmetric contribution to the shear elastic response; and d is the internal characteristic length associated to in-plane bending. Through the equivalence of strain energy density between the HM and a PS continuum, the stiffness of the bonds is determined. A total of five kinematic modes are considered: in-plane bending, the micropolar, uniaxial, deviatoric, and hydrostatic modes [2, 3]. The elastic stiffness for bonds is subsequently calculated:

$$k_c^{\mathsf{PS}} = G\Big(\frac{d}{\|\mathbf{r}_c\|}\Big)^2 \quad , \quad k_r^{\mathsf{PS}} = G\frac{1+\nu}{1-\nu} - k_c \quad , \quad k_m^{\mathsf{PS}} = -2G\frac{\nu}{1-\nu} + k_c \tag{5}$$

$$k_g^{\mathsf{PS}} = G - k_c \quad , \quad G_c^{\mathsf{PS}} = \frac{1-3\nu}{1-\nu} G \quad .$$

2.3 Design of the internal periodic unit-cell of 2D materials

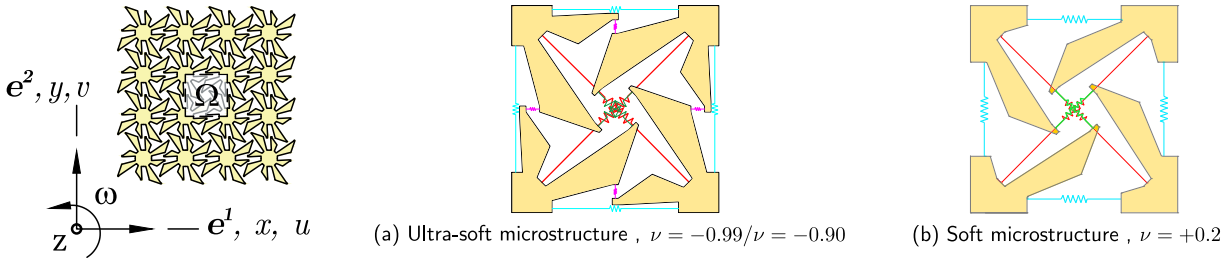
The heuristic bond-based molecular model can be used for the design of two-dimensional materials with a periodic unit-cell. The unit-cell is retrieved from the proposed HM model and following the relations derived, according to a micropolar continuum, for the stiffness of bonds.

From the HM model and to guarantee that all bonds have a non-negative stiffness, the range of possible Poisson's ratio can be written in terms of k_c according to Eq. (6):

$$k_c \in \,]0, G] \;\rightarrow\; \nu^{\mathsf{PS}} \in \left[\, \tfrac{k_c - G}{k_c + G} \;,\; \tfrac{k_c}{2G + k_c} \,\right] \;. \tag{6}$$

For the limit case where cyan bonds are nonexistent, i.e. $k_c = 0$, the microstructure can display a limit of Poisson's ratio $\nu^{\mathsf{PS}} = -1$. Therefore, by removing the cyan bonds, one can obtain either a ultra-soft auxetic material with $E \approx 0$ MPa, or a material with null Poisson's ratio.

For the auxetic microstructure, it has been envisaged to obtain a $\nu = -0.99$ nd $\nu = -0.90$ for which the cyan bonds are defined to have, respectively, $k_c = 0.001G$ and $k_c = 0.01G$. For the proposed auxetic internal structures and through Eq. (4), all the possible bonds exist as shown in Figure 1(a). The design of the HM topology for a material with standard Poisson's ratio of $\nu = +0.2$ can be also obtained and following several combinations for the stiffness of bonds. Here, a value of $k_c = \frac{G}{2}$ was chosen to remove the magenta bonds as, according to Eq. (5), $k_m = 0$. The defined topology is shown in Figure 1(b).



(a) Ultra-soft microstructure , $\nu = -0.99/\nu = -0.90$ (b) Soft microstructure , $\nu = +0.2$

Figure 1: Examples of topologies for microstructures designed according to the RBSM approach.

3 APPLICATION

The proposed heuristic molecular model is applied to predict the mechanical response of either auxetic and standard materials, at the macro-scale. First, it is demonstrated how two materials designed with the micropolar molecular modelling can feature an alike response with classical beam theories when subjected problems governed by bending. Then, it is demonstrated how the response of such materials is also alike under linear conditions for an impact like static loadings.

3.1 Benchmark 1: shear deformability and micropolar effects

The maximum deflections of solid beams with the same Young's modulus E but very different Poisson's ratios and slenderness ratio λ, subjected to a uniform distributed loading, have been compared as a first benchmark. A simply supported and a cantilever beam have been studied assuming that the internal structure is designed according to a HM micropolar molecular model. Two different HM materials are designed, i.e. having a Young's modulus E and a

$\nu = +0.10$ or a $\nu = -0.99$. The design of the internal geometries of such materials through the molecular model is achieved by considering a $k_b = G$ for a $\nu = +0.10$ and a $k_b = 0.001G$ for a $\nu = -0.99$.

Figure 2 presents the ratio of maximum vertical displacement $\overline{\delta}$ between a very auxetic material and the material with standard Poisson coefficient. For slender beams with $l = 10h$ such that $\lambda^{-1} = 0.05$, there are differences in the deflection of both materials. The decrease of slenderness leads to a reduction of the maximum deflection for the beams made with an auxetic microstructure. This trend is expected due to the auxetic and micropolar characteristic of this internal structure. The relative contribution of the shear deformation is larger for squat beams and, as $G \to \infty$ when $\nu \to -1.0$, the shear deformation is very small with respect to the $\nu = +0.1$ case. Second, due to the role played by the coupled-stress stiffness which is very significant since G is very large when $\nu = -0.99$.

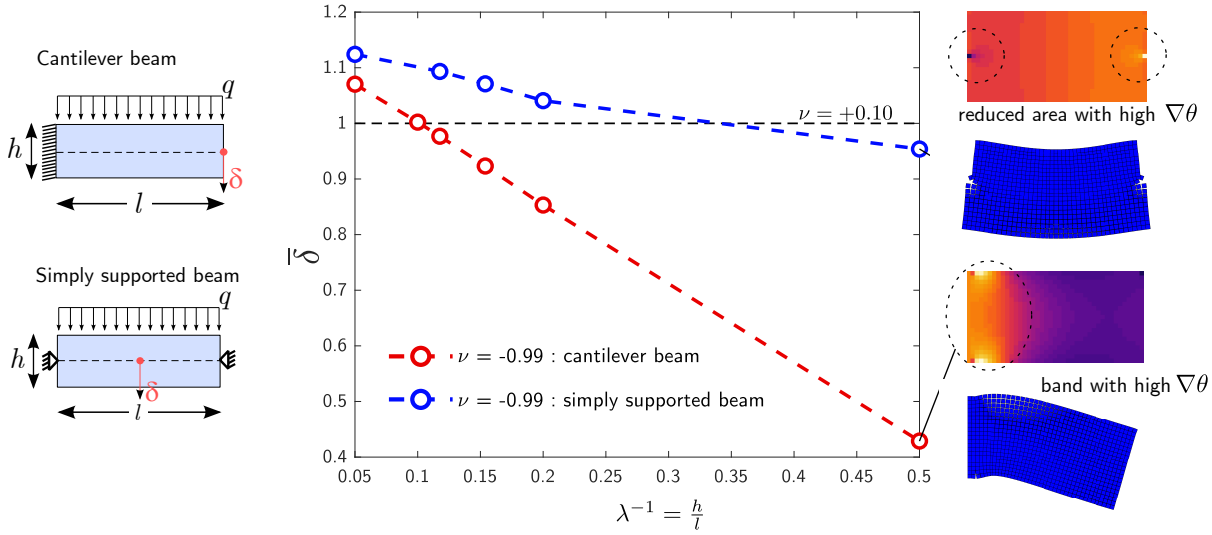
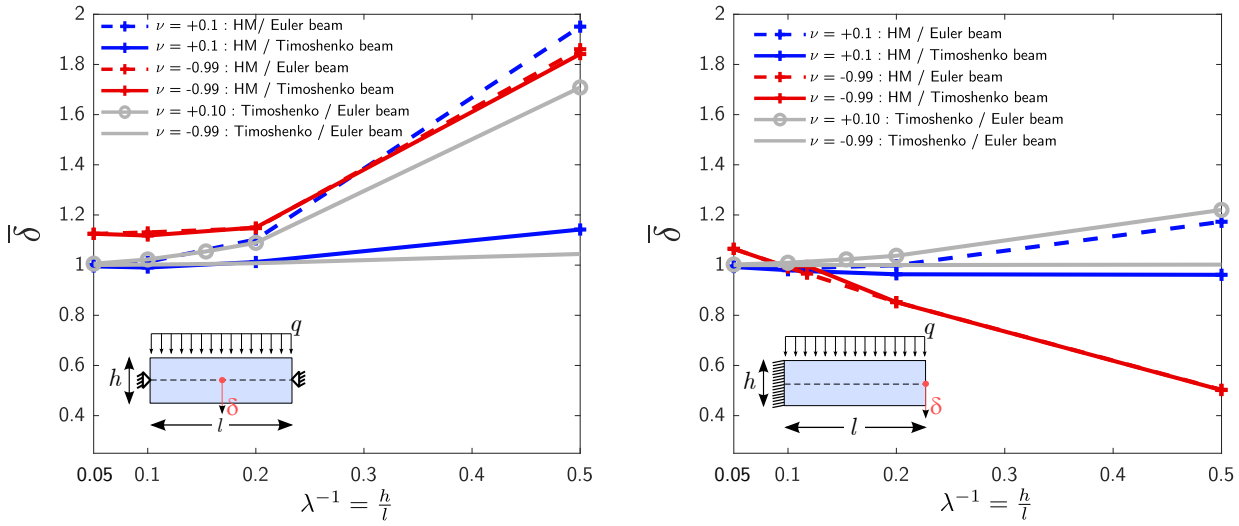


Figure 2: Ratio of vertical deflection in respect to a HM with $\nu = +0.10$ and $\nu = -0.99$ for different h/l ratios.

Note that the effect of the boundary condition is also more evident for a squat beam as demonstrated in Figure 2. In the cantilever beam, the band in the vicinity of the support has a significant curvature that leads to the activation of an extra bending stiffness term related with the coupling stress between rigid elements. This is also clear from the deformed shapes presented for both beams. This effect was demonstrated for block-based materials in [1], where the increase of stiffness due to the latter effect is indirectly concluded by the increase of the fundamental frequency of the beam.

A further analysis is conducted to compare the response between the use of a micropolar microstructure with the one found with classic Euler and Timoshenko beam theories. The maximum deflection obtained for each analysed case is normalized according to the Euler-beam result, as shown in Figure 3. For both materials, the classic Euler-Bernoulli beam theory underestimates the displacement in respect to a Timoshenko beam theory for increasing length values l of the beam (gray lines). This trend is expected and kept for the heuristic molecule (HM) model in the simply supported beam and for the cantilever beam when $\nu = +0.10$. Here, a different trend is observed when $\nu = -0.99$. This is related to the addressed coupled-stress effect that is more evident for low slenderness values. The extra bending stiffness provided by the auxetic and micropolar microstructure is able to reduce the maximum deflection of $\approx 50\%$ in respect

to a Cauchy-type material. At last, as expected, when $\nu \to -1.0$ the $\delta_{Timoshenko} \approx \delta_{Euler}$ since the shear correction term of a classical Timoshenko theory is reduced by a factor provided by $(1+\nu)$.



(a) simply supported beam (b) cantilever beam

Figure 3: Ratio of vertical deflection between the HM and Euler/Timoshenko beam theories for different beam slenderness values λ.

3.2 Benchmark 2: impact-like problem

The HM model is applied to design two numerical examples subjected to a concentrated, impact-like, load. The impact is modelled as a quasi-static concentrated load applied in a 2D rectangular layer of material with dimensions $3h \times h$ m^2 (base x height) supported along the bottom edge. Two materials are designed using the HM model, i.e. a material with $\nu = +0.20$ and another with $\nu = -0.90$, and their mechanical response is compared. It is assumed first that both materials have the same Young's modulus and behave linearly. Results from Figure 4(a) show that the auxetic microstructure is stiffer and requires around 59% more force for the same vertical displacement in respect to the standard material. Difference is reduced significantly if the axial stiffness of the latter is increased, see Figure 4(b) for a $E_{standard} = 1.50 E_{auxetic}$.

A quite different response is observed between both microstructures when material non-linearity is modelled. It is hypothesized that the shear displacement bond-springs (magenta and green) and the diagonal axial bond-springs (red) have a elastic-perfectly plastic behaviour under tension and compression and with a yielding strain of $\varepsilon_y = 5 \times 10^{-3}$. On the other hand, the axial bonds (cyan) have an elastic-perfectly plastic behaviour under tension with $\varepsilon_y = 5 \times 10^{-3}$, while an elastic-hardening behaviour is assumed in compression. It is assumed that the hardening stiffness of the axial (cyan) bonds is equal to G in order to simulate contact (initial stiffness found from Eq. 5). The onset of the hardening law is governed by an input-scalar b, such that the threshold deformation is provided as $\varepsilon_h = b\varepsilon_y$.

From Figure 4(c)-(d), it is evident that the auxetic material is able to withstand a force that is significantly greater. The role of contact under compression plays an important role. For larger values of the constitutive parameter b, the onset of contact occurs for a larger deformation of the axial (cyan) bonds and, therefore, both the energy absorbed from contact and the resisting impact force decrease. The auxetic microstructure allows to have a lower indentation

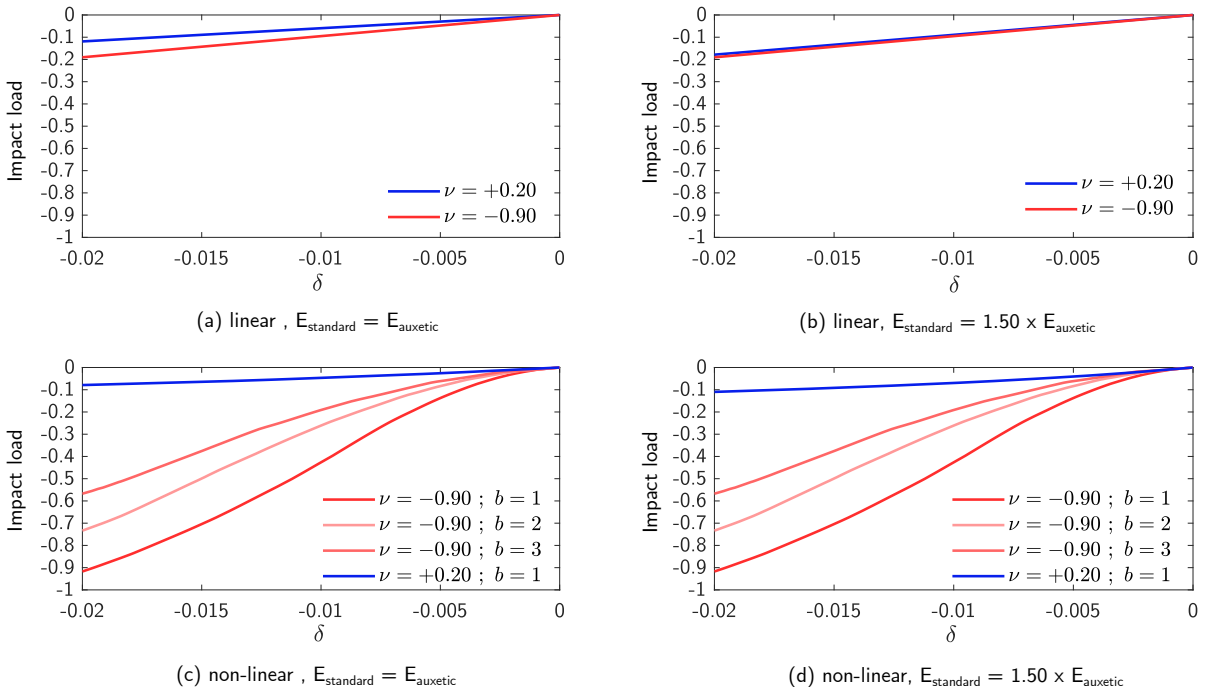


Figure 4: Indentation Force-displacement curve. Adopted yielding strain of $\varepsilon_y = 5 \times 10^{-3}$.

displacement. The map of vertical displacements of Figure 5 shows a local indentation when $\nu = +0.20$, while the response is quite different when $\nu = -0.90$, for which the maximum vertical displacements is five times lower. The effect of the coupled-stress stiffness term $2Gd^2$ in Eq.(4), addressed in benchmark 1 (sub-section 3.1), plays a key role in propagating the damage to areas that are far in respect to the vicinity of the impact region.

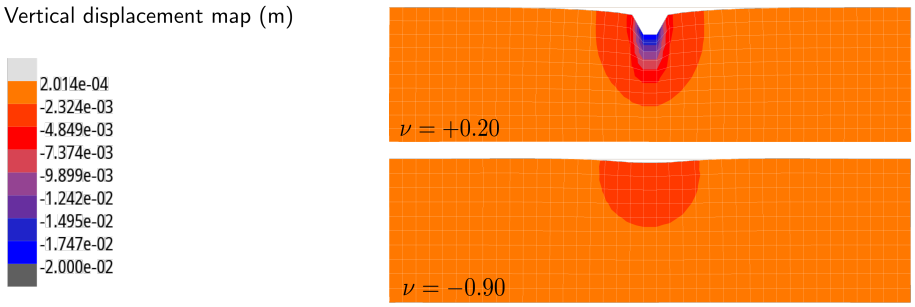


Figure 5: Map of vertical displacement for an impact load of 0.1 kN. Adopted yielding strain of $\varepsilon_y = 5 \times 10^{-3}$ and a parameter $b = 1.0$.

4 FINAL REMARKS

A micropolar molecular model, which stems from a Rigid-Body-Spring Model (RBSM), is applied as a framework for the design of different microstructures that can either have a standard or a negative Poisson's ratio. The unit-cell, i.e. the heuristic molecule, consists of shaped atoms connected by spring-based bonds. The stiffness of these bonds is derived within an objective framework that relates the stiffness to the macroscopic elastic properties of the targeted isotropic micropolar material. This study addressed first how the mechanical response of microstructures designed with the micropolar heuristic molecular approach differs from that

of materials modelled according to a Cauchy-based continuum. This was demonstrated by modelling 2D beams with different slenderness ratios and boundary conditions and made of an auxetic or standard (positive) Poisson's ratio. Despite sharing the same Young's modulus, the shear deformation and micropolar effects play a critical role depending either on the slenderness ratio and boundary conditions. The investigation was then further extended to study a planar domain under a concentrated impact load. Linear and non-linear material response have been considered. It is shown that despite the response is comparable in the linear elastic field, the non-linear response is significantly different. The auxetic microstructure proved to resist a significant larger load. Damage is lower, but it propagated around the impact zone such that the indentation displacements tend to reduce significantly. The onset of contact between the rigid elements of the internal structure when in compression, together with the auxetic nature that allows a significant increase of the shear stiffness and in the related local bending stiffness from coupled-stress, play a critical role.

5 ACKNOWLEDGEMENT

This work has been developed with the financial support of the Italian Ministry of Scientific Research MUR (Ministero dell'Università e della Ricerca nell'ambito del Bando relativo allo scorrimento delle graduatorie finali del bando PRIN 2022: Progetti di Ricerca di Rilevante Interesse Nazionale) titled' *An integrated and fully discrete approach for the optimal topology design and the testing of meta-materials considering the non-linear geometric and elastic response*', Finanziato dall'Unione europea- Next Generation EU, with Prot. *2022FLY8N7*.

REFERENCES

[1] Casolo, S.: Modelling in-plane micro-structure of masonry walls by rigid elements. International Journal of Solids and Structures **41**(13), 3625–3641 (2004). https://doi.org/https://doi.org/10.1016/j.ijsolstr.2004.02.002

[2] Casolo, S.: A linear-elastic heuristic-molecular modelling for plane isotropic micropolar and auxetic materials. International Journal of Solids and Structures **224**(111042) (2021). https://doi.org/10.1016/j.ijsolstr.2021.111042

[3] da Silva, L.C., Grillanda, N., Casolo, S.: Heuristic molecular modelling of quasi-isotropic auxetic metamaterials under large deformations. International Journal of Mechanical Sciences **251**, 108316 (2023). https://doi.org/https://doi.org/10.1016/j.ijmecsci.2023.108316

[4] Dell'Isola, F., Seppecher, P., Spagnuolo, M., Barchiesi, E., Hild, F., Lekszycki, T., Giorgio, I., Placidi, L., Andreaus, U., Cuomo, M., Eugster, S.R., Pfaff, A., Hoschke, K., Langkemper, R., Turco, E., Sarikaya, R., Misra, A., De Angelo, M., D'Annibale, F., Bouterf, A., Pinelli, X., Misra, A., Desmorat, B., Pawlikowski, M., Dupuy, C., Scerrato, D., Peyre, P., Laudato, M., Manzari, L., Göransson, P., Hesch, C., Hesch, S., Franciosi, P., Dirrenberger, J., Maurin, F., Vangelatos, Z., Grigoropoulos, C., Melissinaki, V., Farsari, M., Muller, W., Abali, B.E., Liebold, C., Ganzosch, G., Harrison, P., Drobnicki, R., Igumnov, L., Alzahrani, F., Hayat, T.: Advances in pantographic structures: design, manufacturing, models, experiments and image analyses. Continuum Mechanics and Thermodynamics **31**(4), 1231–1282 (2019). https://doi.org/10.1007/s00161-019-00806-x

[5] Desmorat, B., Spagnuolo, M., Turco, E.: Stiffness optimization in nonlinear pantographic structures. Mathematics and Mechanics of Solids **25**(12), 2252–2262 (2020). https://doi.org/10.1177/1081286520935503

[6] Matlack, K.H., Serra-Garcia, M., Palermo, A., Huber, S.D., Daraio, C.: Designing perturbative metamaterials from discrete models. Nature Materials **17**(4), 323–328 (2018). https://doi.org/10.1038/s41563-017-0003-3

[7] Noll, W.: A Frame-Free Formulation of Elasticity (2006). https://doi.org/10.1007/s10659-005-9046-9, https://doi.org/10.1007/s10659-005-9046-9

[8] Wang, K., Chen, Y., Kadic, M., Wang, C., Wegener, M.: Nonlocal interaction engineering of 2D roton-like dispersion relations in acoustic and mechanical metamaterials. Communications Materials **3**(1), 35 (2022). https://doi.org/10.1038/s43246-022-00257-z

[9] Zou, Q., Luo, G.: Geometric modeling for microstructure design and manufacturing: A review of representations and modeling algorithms. Computer-Aided Design **180**, 103834 (2025). https://doi.org/10.1016/j.cad.2024.103834