Advances in Nano Research, *Vol. 13, No.3 (2022) 247-257*
https://doi.org/10.12989/anr.2022.13.3.247

Effect of nano-composite materials on repair of ligament injury in sports detoxification

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(*Received January 4, 2022, Revised May 9, 2022, Accepted May 11, 2022*)

Abstract. Extraordinary properties of nanocomposites make them a primary replacement for many conventional materials. Anterior cruciate ligament (ACL) reconstruction, which is a frequent surgery in sport activities, is one of the fields in which nanocomposites could be utilized. In the present study, the mechanical properties of different porous scaffolds made from graphene nano-composites are presented ad load bearing capacity of these materials is calculated using finite element method. The numerical results are further compared with experimental published data. In addition, several geometrical and material parameters are analyzed to find the best configuration of nanocomposite scaffolds in reconstruction of ACL. Moreover, coating of detoxification chemicals are extremely easier on the nano-structured materials than conventional one. Detoxification potential of nano-composites in the injured body are also discussed in detail. The results indicated that nano-composite could be successfully used in place of auto- and allografts and also instead of conventional metallic screws in reconstruction of ACL.

Keywords: artificial intelligence; cancer; ligament injury; nanoparticles; pediatric patients

1. Introduction

Drug abuse has become one of the global public health problems, seriously affecting human life and security (Yan *et al.* 2020, Lai 2021, Ning *et al.* 2021, Obireddy and Lai 2021, Sheng *et al.* 2021, Tang *et al.* 2021). Drug abuse causes personal and social problems in youths. This problem is a worldwide concern and every country wants to prevent drug abuse and rehabilitate youth addicts by different medical and physical intervention methods. One of the main physical intervention is the exercise intervention (Adamian *et al.* 2020, Al-Furjan *et al.* 2020a, b, Li *et al.* 2020b, Liu *et al.* 2020b, 2021b, Zare *et al.* 2020, Dai *et al.* 2021b, Habibi *et al.* 2021a, He *et al.* 2021, Huang *et al.* 2021a, Zhang *et al.* 2021). Exercise has attracted much attention as a green and healthy intervention method, which can reduce the use of drugs in drug-dependent people, and may play a role as an alternative non-drug enhancer. Several studies showed the effectiveness of exercise in treatment and prevention of drug addiction. Long-term moderate-intensity aerobic exercise can reduce withdrawal symptoms, reduce drug cravings, and increase withdrawal rates (Liu *et al.* 2020a, Wang *et al.* 2020, Zhou *et al.* 2020, Dai *et al.* 2021a, Guo *et al.* 2021a, Shao *et al.* 2021, Wu and Habibi 2021). As we all know, long-term drug abuse leads to the loss of endogenous calcium and urinary calcium, accelerates the negative calcium balance, and increases the body's demand for calcium, so it is prone to osteoporosis. Animal studies have found that the collagen content of the anterior cruciate ligament in the osteoporosis animal model is lower than that of the control group, indicating that under the same exercise intensity, the osteoporosis population is more prone to ligament damage (Ma *et al.* 2022, Zhao *et al.* 2022, Hou *et al.* 2021, Huang *et al.* 2021b, c, Jiao *et al.* 2021, Liu *et al.* 2021c, Moradi *et al.* 2021, Xu *et al.* 2021, Dong *et al.* 2022, Luo *et al.* 2022, Yang *et al.* 2022, Yu *et al.* 2022).

Anterior cruciate ligament (ACL) injury and rapture are common injuries in athletes. Ligament repair procedure is a well-established and usually successful surgery. However, fixing of the new ligament graft using solid metallic or biodegradable screws in some cases complicated the problem due to lack of bone filling and graft injury. On the other hand, metallic screws are not suitable for examinations using MRI. Therefore, a novel type of porous biodegradable fixations screws are devised to overcome the problems of graft injury during fixation, magnetic properties and bone filling (Shariati *et al.* 2012, 2016a, b, 2019, 2020d, e, f, g, h, i, j, 2021a, b).

In this porous biodegradable scaffolds, the bone easily grows through the porous channels and later surgery is not required to remove the scaffold and it permits full filling of the bone (Parry *et al.* 2017). Parry *et al.* (2017) experimentally examined the load endured by wedge scaffolds with different porosity and compared results with solid wedge and native ACL. The results indicate that all of the reconstruction method had a significantly lower load capacity in comparison to the native ACL. However, the load capacity of porous wedge with 20% porosity was the same as solid wedge. In addition to introducing porosity, some chemical coatings were also added to the scaffold to increase bone regeneration. Liu *et al.* (2016) utilized 3D desktop printers to produce porous scaffolds for internal fixation of grafts in ACL reconstruction in rabbits. Both in vitro and in vivo tests demonstrated high efficiency of the

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http://www.techno-press.org/?journal=journal=anr&subpage=5

ISSN: 2287-237X (Print), 2287-2388 (Online)

porous scaffolds in terms of bone growth and graft attachment. Silva *et al.* (2021) used graphene nanoplatelets in nanocomposite material with poly(L-lactic acid) (PLA) matrix to produce porous scaffold capable of tolerate large loads. They compared the load capacity of this type of composite with two other devised nano-composites. Alongside to the 3D printed scaffolds, textile-engineered were also produced for the aim of efficacy comparison. Biodegradable screws showed promising load capacity in ACL reconstruction as demonstrated experimentally by Herrera *et al.* (2010). They used a screw-like wedge to fix grafts in bone and several experiments including tensile and pull-out tests were conducted on the assembly. It was concluded that wider and longer screws (28mm) provide sufficient graft fixations.

In the field of tissue engineering, there several studies dedicated to utilization of superior properties of nano-composites in design and fabrication of grafts in reconstructions of ligaments (Doulabi *et al.* 2014, Santoro *et al.* 2016, Purohit *et al.* 2019). In a review article, Silva *et al.* (2020) listed studies on polymer based nanocomposite which used in place of tendons and ligaments. Chung *et al.* (2017) examined a tri-component nanocomposite in an in vivo study to observe their functionality in rabbits. These nanocomposites, with tensile properties close to ACL ligaments, showed a satisfying interlocking with bone and tissue ingrowth after 6 weeks. They concluded that nano-composites had a promising potential to be used instead of auto- and allografts. Correia Pinto *et al.* (2017) evaluated biocompatibility of graphene platelet and functionalized carbon nanotube based nano-composites in their studies. These composite were used for the purpose of ligament reconstruction. They observed that there is no significant cytotoxic, physiological and inflammatory responses in the animals under study.

The graphene nano-composites have been the subject of many studies to evaluate their mechanical properties. Habibi *et al.* (2021b) investigated the static and dynamics of graphene based nanocomposites. They revealed that these nanocomposites have extraordinary mechanical responses under static and dynamic loads. Thermal instability of graphene nanocomposites were considered in an article by Al-Furjan *et al.* (2020p). The results of this theoretical study indicated that under certain thermal conditions, nanocomposites demonstrate instability in their dynamical behavior. Pourjabari *et al.* (2019) investigated the porosity effects on the dynamic responses of nanocomposite structure which is of interest in the field of ligament reconstruction. There are also several other studies using theoretical, semi-numerical and finite element methods considering behaviors of nanocomposite structures under different static, dynamic and thermal loadings. Interested readers are referred to following references for more information of these class of composites.

Measurement of forces on the ligaments in a body is barely feasible. Therefore, in silico simulations aid scientists to extract modes of loads on the ligaments. Among computer simulations, finite element method (FEM) (Massoumi *et al.* 2018, Amelirad and Assempour 2019, 2021) is the most suitable approach to analyze loads and stresses in the bones and ligaments and to apply versatile boundary condition on the models. In doing so, Limbert *et al.* (2004) analyzed stress distribution in the ACL ligament using 3D-FEM simulations. They utilized a hyperelastic constitutive equations to observe the critical loading mode in the ACL. Forces exerted on reconstructed ACL in different pre-tension and flexion angles was investigated by Peña *et al.* (2005) using FEM. They concluded a pre-tension of 60N gave close functionality of reconstructed ACL to native ACL. However, they recommended 40N pre-tension due to undesirable consequences of high pre-tension loads. Vairis *et al.* (2016) constructed knee joint models and employed FEM to evaluate responses of three types of ACLs, i.e. Intact ACL, ACL-deficient and reconstruct ACL. The numerical simulations indicated that kinematic behavior of reconstructed ACL is highly similar to the native ACL under different static and dynamic loading conditions. A wide range of loading conditions were applied in FE analysis in a study by Kiapour *et al.* (2013) and the results compared to experimental measurements for ACL and medial collateral ligament (MCL). This comprehensive study shows the power of well-established FE models. Thus, FEM could be used to apprehend the conditions lead to rapture of ACL. There could be found several other studies on the application of FEM in force analyses in ligaments showing the capability of this numerical method in design and utilization of material, geometry and reconstruction of raptured ligaments (Park *et al.* 2010, Tampere *et al.* 2019, Bartolin *et al.* 2021).

In the present study, the mechanical properties of different porous scaffolds made from graphene nano-composites are presented ad load bearing capacity of these materials is calculated using finite element method. The numerical results are further compared with experimental published data. In addition, several geometrical and material parameters are analyzed to find the best configuration of nanocomposite scaffolds in reconstruction of ACL. Moreover, coating of detoxification chemicals are extremely easier on the nano-structured materials than conventional one. Detoxification potential of nano-composites in the injured body are also discussed in detail.

2. Materials and methods

2.1 Graphene platelet nano-composites

Graphene platelets has some extraordinary mechanical, electrical and chemical properties which distinguish it from other nanostructures (Dai and Safarpour 2021, Forsat *et al.* 2021, Ghamkhar *et al.* 2021, Khadimallah *et al.* 2021a, b, Kumar *et al.* 2021, Madenci 2021, Tlidji *et al.* 2021). Applications of graphene platelets are widespread from super-capacitors to polymeric composites. The production methods, properties and applications are listed in the Refs (Habibi *et al.* 2016, 2018a, b, 2019a, b, d, e, Esmailpoor Hajilak *et al.* 2019, Pourjabari *et al.* 2019, Safarpour *et al.* 2019a). Graphene platelet (GPL) nanocomposites are made from dispersed single layer Graphene in a polymer matrix (Habibi *et al.* 2017, 2019a, c, Safarpour *et al.* 2018, 2019b,

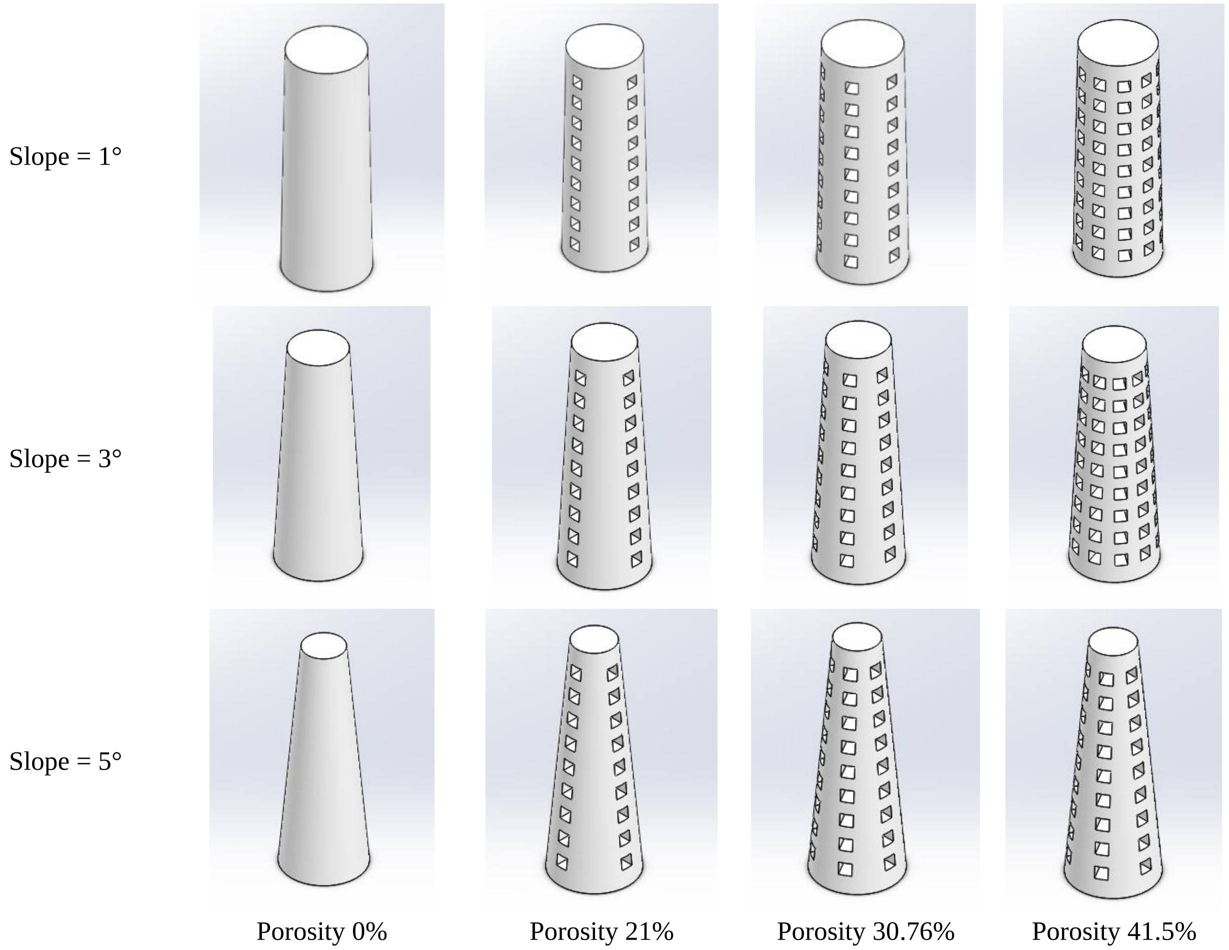

Fig. 1 Porous nano-composite wedges with diameter $d = 7mm,\ h = 20mm$ and different slopes and porosity values

2020, Alipour *et al*. 2020, Ebrahimi *et al*. 2020a, Ghazanfari *et al*. 2020, Chen *et al*. 2022). In some cases, microscale carbon fibers are also added to the polymeric matric to produce high efficacy composites. The mechanical properties of the GPL-reinforced composites (GPLRC) have proven to be superior to other conventional composites with an extra application in the micro-scale devises (Ebrahimi *et al*. 2019b, c, Hashemi *et al*. 2019, Moayedi *et al*. 2019, 2020a, b, Mohammadgholiha *et al*. 2019, Mohammadi *et al*. 2019, Ebrahimi *et al*. 2020b, Habibi *et al*. 2020, Shariati *et al*. 2020a, b, Oyarhossein *et al*. 2020, Shokrgozar *et al*. 2020). In some MEMS and NEMS devises conventional composites with fibers in scale of mm or micron cannot be regarded as a continuum structure with homogenous properties and nano scale reinforcement should be utilized in such scales (Hashemi *et al*. 2019, Al-Furjan *et al*. 2020c, j, k, m, Bai *et al*. 2020, Cheshmeh *et al*. 2020, Li *et al*. 2020a, Lori *et al*. 2020, Najaafi *et al*. 2020, Shariati *et al*. 2020c, Zhang *et al*. 2020, Guo *et al*. 2021b, Liu *et al*. 2021a).

In the present study, GPLRC is selected for the numerical simulations to observe the comparative responses under different loading conditions. The selected material is adopted from (Silva *et al*. 2021) with various reinforcement material percentage from 0.5% to 2%wt. In addition to the scaffold modeled to be used as graft, porous wedges are also modeled according to (Parry *et al*. 2017). Different wedge slope, diameter and porosity are examined to find optimum values of pull-out forces.

2.2 Finite element simulations

The present study is devoted to assess the force-displacement curve in pull-out testing of composite force bearing capacity of each model. In doing so, a wide range of porous wedges with different diameters from 7 to 9, height of 20mm, 25mm and 30mm, angle of 1°, 3° and 5° and different porosity of 0%, 21%, 30.76% and 41.5% is prepared using SolidWorks 2018 (BIOVIA, San Diego: Dassault Systèmes 2018) as shown in Fig. 1 for the case of $d = 7mm$. Moreover, a graft model from GPLRC material is prepared for different hole diameters in accordance with each porous wedge diameters.

The model of the femur bone is acquired from open source models in GrabCAD website (). The model was further modified and cut to be suitable for the aim of the present study. The bone model is shown in Fig. 2.

The assembly of the model is prepared in SolidWorks and imported in Ansys Workbench 2021 for stress analysis. The contact between all three parts are defined with a friction constant 0.2 and maximum shear 10MPa. The boundary condition are selected similar to Ref. (Herrera *et*

Fig. 2 Femur bone cut and the position of screw and graft is drilled

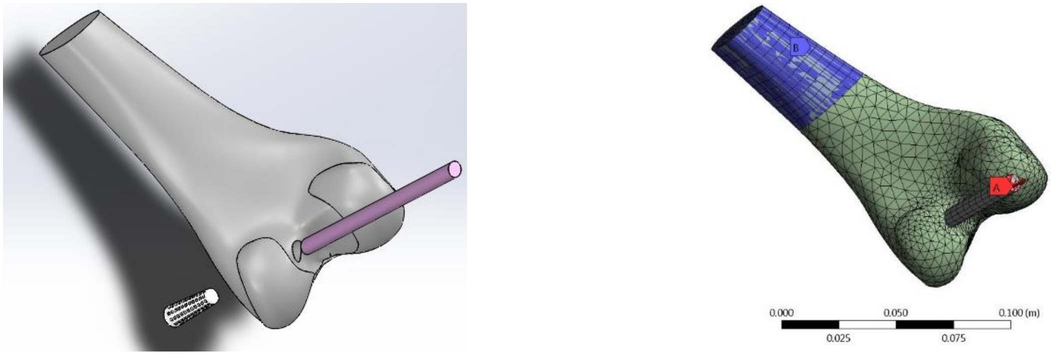

Fig. 3 Femur bone, porous GPLRC wedge and nanocomposite graft as assembled in SolidWorks and mesh generated in Ansys workbench

al. 2010). Fig. 3 demonstrated a sample of assembly and boundary/loading conditions along with meshed model. The total number of elements is 30723 and quadratic element types are used.

2.3 Material properties

All the materials under consideration is elastic materials and permanent change in their shape will not occur during loading process. However, in bone and screw, the displacement remains small and a linear elastic property is enough to define material characteristics. On the other hand, The graft experiences extremely large elastic deformation and a hyper elastic nonlinear model is adopted to define the material properties. The following are formulations for hyper elastic material

$$\mathbf{S} = \frac{\partial \psi}{\partial \mathbf{E}} \tag{1}$$

in which $\mathbf{S}$ is second Piola-Kirchhoff stress tensor and $\mathbf{E}$ is Green strain tensor. Free energy of the body is represented by ψ and the below form is adopted in this analysis:

$$\psi = \frac{\lambda}{2}[(\mathrm{tr}\,\mathbf{E})^2 + \mu \mathrm{tr}(\mathbf{E})^2] \tag{2}$$

where λ and μ are Lame constants having the following relations with Young's modulus E and Poisson's ratio ν:

$$\mu = \frac{E}{2(1+\nu)}, \lambda = \frac{\nu E}{(1+\nu)(1-2\nu)} \tag{3}$$

Table 1 Elastic constants of bone, GPL and polymer matrix

	$E\ [GPa]$	ν	$\rho\ [kg/m^3]$
Bone	13.4	0.3	1900
GPL	1010	0.186	1060
Polymer epoxy	2.85	0.34	1200

Moreover, the dispersion of GPL in the composite structure are random, all materials regarded as isotropic and two parameters are enough for defining elastic properties: equivalent elasticity module and equivalent Poisson's ratio. The bone properties is adopted form Ref. (Massoumi *et al.* 2018) and equivalent composite constant calculated using Halpin-Tsai formulations which is comprehensively provided in Refs. (Al-Furjan *et al.* 2020d, e, f, g, h, i, l, n, o). All the material properties are presented in Table 1.

3. Result

The central focus of this study is to evaluate pull-out forces in different material and geometrical condition. In doing so, all geometries in term of diameter, wedge slope, porosity and height of the wedge scaffolds are models and numerically analyzed for an axial pulling displacement. When the forces needed to pull out the graft reaches a maximum the analyses halted. The maximum force is regarded as pull-out force for each condition. Distribution of von Mises stress in both bone and graft are shown in Fig. 4. As mentioned above, we focus on the force responses of the structure.

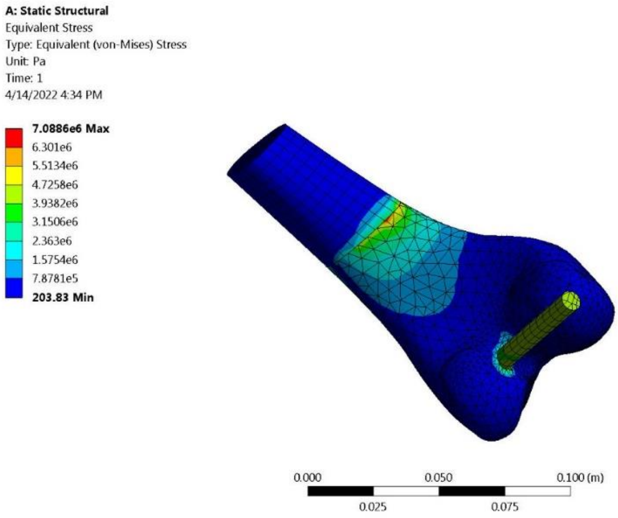

Fig. 4 Femur bone, porous GPLRC wedge and nanocomposite graft as assembled in SolidWorks and mesh generated in Ansys workbench

Pull-out forces are measured in a comprehensive FEM analysis and the results are shown in Figure 5. The effect of porosity which is important in bone filling is demonstrated in all graphs. In general increase in porosity from 0% to 20% does not significantly change the pull-out force. However, from 30.36% to 41.5% porosity abrupt drop in pull-out forces are observed which necessitate cautions on the porosity of wedges. Increasing in porosity cause softer behavior of wedges and less resistance against pulling forces. Thus, it is recommended to limit porosity up to 30% in designed wedges.

Slope angles of wedges have some interesting results. It is seen that the best results, in terms of maximizing pull-out forces is obtained for slope angle $\alpha = 3°$. In lower angle, the wedge is pulled easily into the bone hole and this slip is not favorable in graft fixation. On the other hand, higher angles do not fully touch the wall of the bone and cause lower forces even less that angle 1°. Thus, it is recommended in the design of the wedges to keep the angles around 3°.

Wedge diameter has a slight effect on the pulling forces as depicted in Figure 5. However, the wedges with $d = 8mm$ demonstrate higher pull-out forces. The reason is laid in the fact that elastic properties of graft do not allow high curvature and it tends to push the wedge out of the hole in reverse direction. The wedge with $d = 9mm$ shows similar values as $d = 8mm$ except for high values of porosity. In high porosity, larger diameters show softer behaviors. Consequently, the diameter should be kept close to 8mm.

As expected, longer wedges demonstrated better functionality as larger contact area between wedge and graft is possible. Therefore, wedges with height of 30mm is suggested for design in the case they not exceeded bone thickness. Finally, effects of GPL content shown in Figure 5, indicates that 2%wt of GPL in polymer nanocomposite have superior results. Higher GPL content results in stiffer grafts which cannot be bent and contact area is limited in this case. Lower content of GPL results in lower equivalent module of elasticity and under pulling forces they are easily narrowed and pulled out from the bone hole.

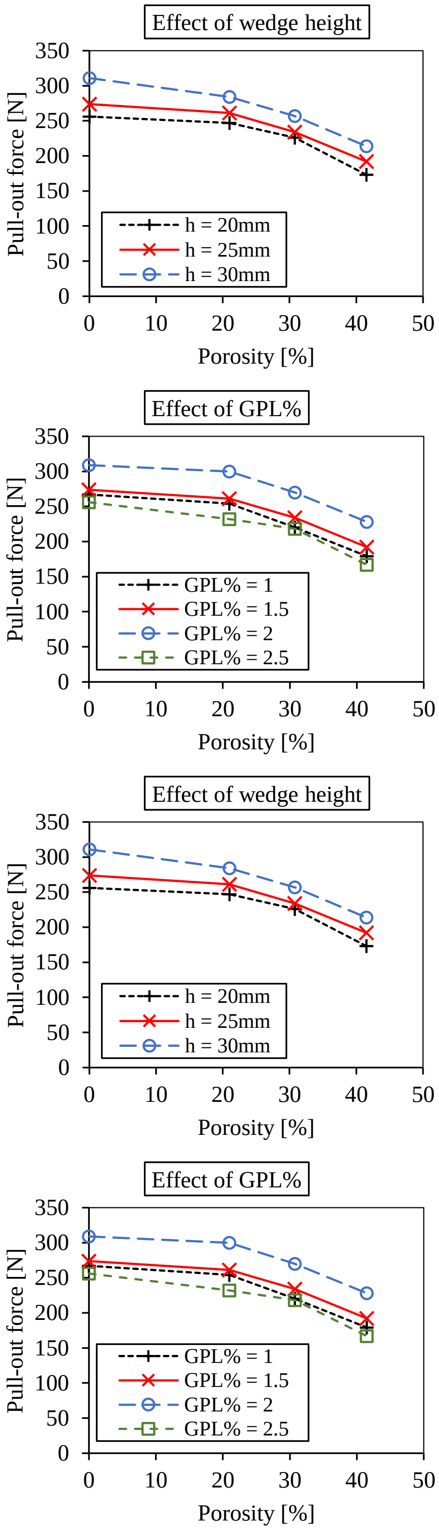

Fig. 5 Effect of porosity on the pull-out force for different geometrical parameters of the wedge and GPL weight fraction

The above results are a preliminary assessment of functionality and efficacy of nano-composites in ligament reconstruction in ACL. However, for other ligament injuries similar results could be obtained using procedure presented in current study. From this numerical study, the best wedge and GPL content could be deduced for the first phase design of such structures.

4. Conclusions

In the present study, the mechanical properties of different porous scaffolds made from graphene nanocomposites are presented ad load bearing capacity of these materials is calculated using finite element method. The numerical results are further compared with experimental published data. In addition, several geometrical and material parameters are analyzed to find the best configuration of nanocomposite scaffolds in reconstruction of ACL. Moreover, coating of detoxification chemicals are extremely easier on the nano-structured materials than conventional one. Detoxification potential of nanocomposites in the injured body are also discussed in detail. The main concluded results are listed below:

- Increasing in porosity cause softer behavior of wedges and less resistance against pulling forces. Thus, it is recommended to limit porosity up to 30% in designed wedges.
- The best results, in terms of maximizing pull-out forces is obtained for slope angle $\alpha = 3°$.
- The wedges with $d = 8mm$ demonstrate higher pull-out forces.
- Longer wedges have better functionality than short ones.
- The results indicate that 2%wt of GPL in polymer nanocomposite have superior pulling forces.
- Detoxification is feasible in nano-composite due to their functionalized surface properties.

Acknowledgment

This work was supported by Philosophy and Social Science Project of Hunan Province (21YBA046)

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