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Relative Characteristics of Various Nano-Cement Composite

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Abstract

A comparative study between two nano cementitious materials, i.e., Graphene Nanoplatelet (GNP) and Montmorillonite Nano Clay (MNC) cement matrix are considered in this paper. Nanofibers are introduced as an alternative to macro reinforcement to enhance the mechanical property and reduce the crack growth in the cement matrix at the nanoscale. Various analytical simulation has been carried out by ANSYS 15.0 to know the optimum percentage of water. A 3D Represent Volume Element (RVE) is used to simulate nano cementitious material as the material sizes differ. RVE is the minimum volume upon which a measurement can make, yielding an expected value of the entire. The GNPs and MNCs are added to the cement matrix with various percentages (0.02%, 0.08%, 0.1%, 0.15%, 0.17%, 0.22%, and 0.3%) by the weight of cement. After simulating the pullout models with proper boundary conditions, the behavior of nano-cementitious material is observed. A comparative study of all percentage variations revealed that the mechanical property increases up to 0.17% and 0.22% for GNPs and MNCs. It also observed that GNPs cementitious material performs better than MNCs cement matrix.

Keywords: *Nano Cementitious Material, Represent Volume Element (RVE), Simulation, The Mechanical Property*

1.0 Introduction

Nanotechnology has been very popular among researchers for the last few decades. Recently, carbon nanofiber has been used in building construction as a micro reinforcement to enhance the property of the building material. As graphene is used as a macroreinforcement in the structural member, the researcher also used graphene nanofiber as a micro reinforcement. This paper uses the Graphene Nanoplatelet (GNP) and Montmorillonite Nano Clay (MNC) as micro reinforcement to observe the behavior of nanocomposite cementitious material. Mouras *et al.* 1987 first introduced a crystal lattice of sp2 bond with carbon in a single layer. As the crystal is bonded with carbon, graphene's strength capacity is much higher[1]. Andre Geim and Konstantin Novolesov achieved the Nobel prize for a revolutionary experiment to extract the monolithic layer of graphene[2]. Novoselov *et al.*, in 2004 and 2005 find out the property, *i.e.*, young modulus, intrinsic strength, etc, from nanoindentationatomic force microscopy[3-4]. These values were used in my paper at the time of modeling. A monolayer sheet of graphene was examined by Lee *et al.*, in 2008 and categorized as the toughest material. Graphene Nano Platelet (GNPs) and Montmorillonite Nano Clay (MNC) will be very popular for their excellent mechanical properties and unique morphology[5].Besides the mechanical, chemical, electrical, electromagnetic field, and polymeric conditions, nanofiber also gave a better result. Graphite flakes are also used as a cementitious material to enhance strength.

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Many researchers describe functionalized graphene platelets' or montmorillonite nano clay behavior, but fixing the performance of the GNP/MNC cementitious material is necessary. So in this article, the behavior and mechanical properties of nano cementitious material are found. This article also finds the optimum percentage of nanofiber that gives the maximum strength of nano cementitious material.

2.0 Methodology

This study considered Graphene Nanoplatelet (GNP) and Montmorillonite Nano Clay (MNC) cementitious composites. The property of the two materials is taken from Sigma-Aldrich, given in Table 1. This property is introduced to simulate these composite materials in ANSYS-15.0. There are various methods described by Chen, Liu, and Qian to find out the mechanical behavior of RVE models[6-8]. Among these methods, the 3-D elastic theory method is the best for the RVE model, and this method is adopted in this paper[9].

Table 1. Geometric and material parameter a) GNPs b) MNCs

(a)

Property	Range
Length	10 µm
weight	2.01 g/mol
Sheet Resistance	< 22
No of layers(atomic layers)	5-7

(b)

Property	Range
Length(**µm**)	10
Hardness	1.5-2
Density(kg/m^3)	1300-1370
Specific surface area(m^2/g)	220-270
pH	3-4
Electrical Conductivity (MV)	25
Moisture (%)	1-2

Mainly three types of RVE models are described, *i.e.,* hexagonal RVE, square RVE, and cylindrical RVE, as shown in Figure 1. As per Liu and Chen, an array of the nanofiber marked the RVE model, *i.e.,* for the hexagonal array, hexagonal RVE, and for the square display, square RVE was introduced. The cylindrical RVE decreases the simulation work time under any loading type. In this paper square RVE model is adopted, and after analyzing the model, stress and load behavior of nano cementitious material was observed.

Table 2. Types of RVE model

Sl No	Number of CNF	Concentration of CNF/ GNP by weight of cement (%)
1	0	0.00
2	1	0.02
3	4	0.08
4	6	0.1
5	8	0.15
6	9	0.17
7	12	0.22
8	16	0.3

After observation of both the materials, a comparative study was made, and the optimum nanofiber percentage was focused on. Figure 2 represents the RVE in cement composites. This paper will first employ the square RVE to estimate Young's moduli and Poisson's ratios of the GNPs, and MNCs-based compounds. The following section will establish the actual analytical results from the results. This study prepares seven consecutive models for each nanocomposite using Finite element simulation (ANSYS – R15.0) as per Table 2. The 1st model is constructed with cementitious material only, other model is built with one

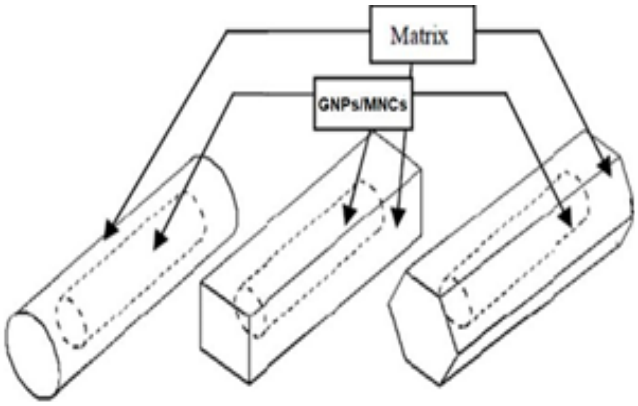


Figure 1. Types of RVE model.

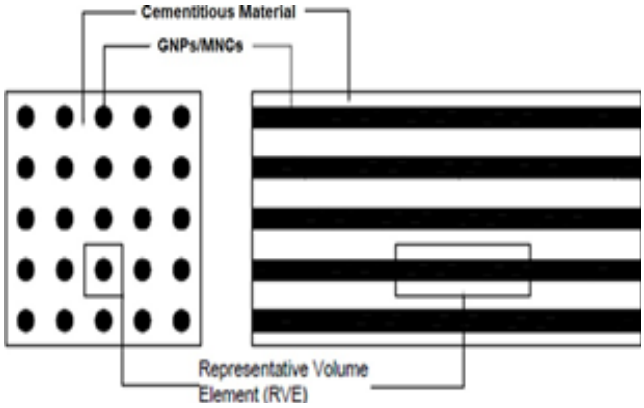


Figure 2. Representation of RVE in cement composites.

nano reinforcement in the center of the model, as per Figure 3. The other model is done by creating four GNPs/MNCs in the middleof the beam with some offsets[10]. The third model is done by creating nine GNPs/MNCs inside the beam with a specificoffset. Here, the size of the RVE model was considered 850nm x 850nm. The length of the RVE model is 5 μm as per Table 3. Theproperties of GNPs/MNCs are taken from Sigma Aldrich. Different models having the exact dimensions giving the various percentages of GNPs/MNCs by weight of cement have been established. It is presumed that the GNPs/MNCs is uniformly distributed over the entire cementitious model[11-14].

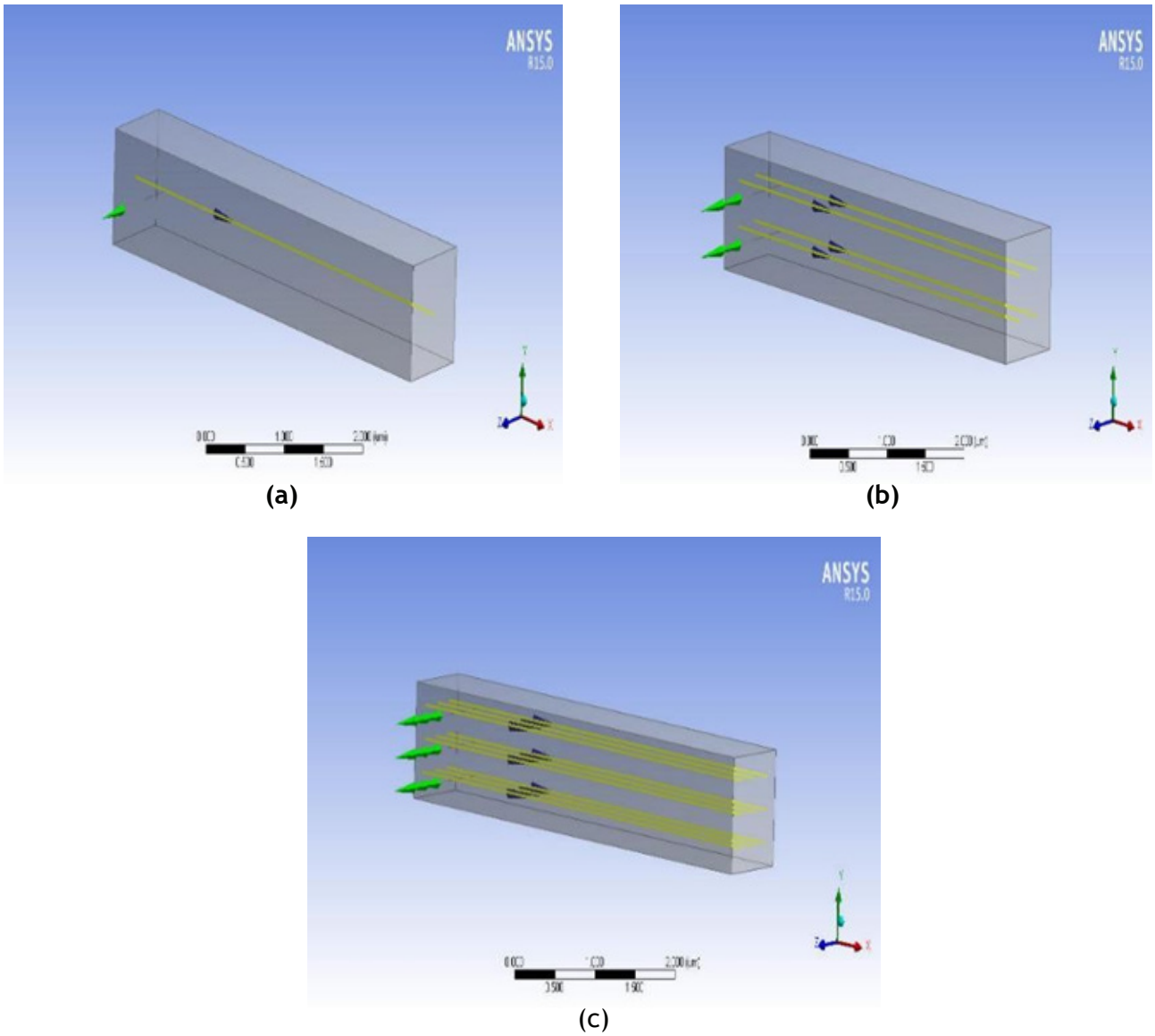


Figure 3. RVE Pull-out Models (cement with a) 0.02 b) 0.08 (c) 0.17 percentages of nanofiber.

Table 3. Size of RVE model

Property	Range
Width and Height of the cement matrix, a	850nm
Length of the matrix, L	10 μm
The outer diameter of GNPs/MNCs	130nm
The thickness of GNPs/MNCs	60 nm
The inner diameter of GNPs/MNCs	70 nm

The boundary condition is taken on one side fixed, and on the other face, loads are acting. Here this model is endangered to an axial distance ΔL at the loading end. Both GNPs/MNCs and cement are displayed using 3-D solid elements in ANSYS workbench. Fluorides also synthesis the graphite intercalation compounds[15,16]. The property of GNPs/MNCs was obtained from sigma-aldarich.com. Some nonlinear analysis was done as cementitious material is poor in tension and crushed in compression. At the time of modeling, an eight-noded element with proper boundary conditions was considered.

The assumptions of this element are as follows:

- The material is supposed to be primarily isotropic
- At each amalgamation point, cracking is allowed in three orthogonal directions
- If any type of cracking occurs at an amalgamation point, it is simulated through an alteration of material properties. These discrete cracks are treated as a tarnished band of cracks.

3.0 Results and Discussion

After meshing, appropriate boundary conditions, and the proper manual contact with GNPs/MNCs and cement matrix, the results for three models with various percentages of GNPs/MNCs are shown below.

The RVE model, along the longitudinal direction, shows incremental flexural pressure. From that, a load-displacement curve is plotted for varying percentages of GNPs/MNCs by weight of cement. From that, the peak load and peak displacement are found in Figure (4,5). Figure 4 represents the peak loads of various percentages of nanofibres, and it is observed that with the increase of a

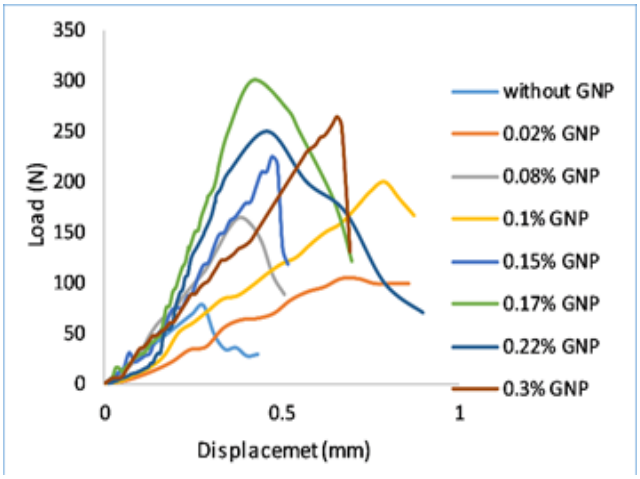


Figure 4. Peak load of the various percentage of GNPs used in cement composites.

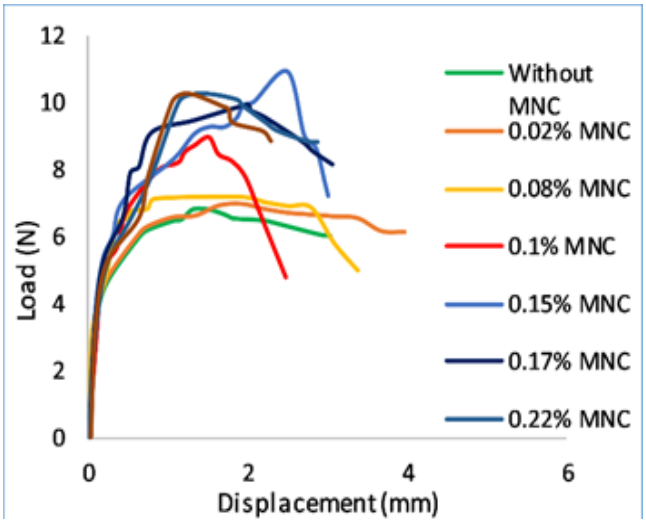


Figure 5. Peak load of the various percentage of MNCs used in cement composites.

percentage of nanofibres, the load resisting capacity is also increased. From Figure 5, it is also observed that GNPs have more resisting capacity than the same percentage of MNCs; Figure (6,7) also describes the elastic modulus and toughness of a variable proportion of nanofibers that are introduced to Enhance the strength of cement.

Young's modulus is tabulated with various nanofiber percentages using the strength of materials method. Figure 4 shows the elastic modulus obtained from the stress-strain graph of every sample. Figure 7 elaborates on the toughness of various typesof sample, which introduce

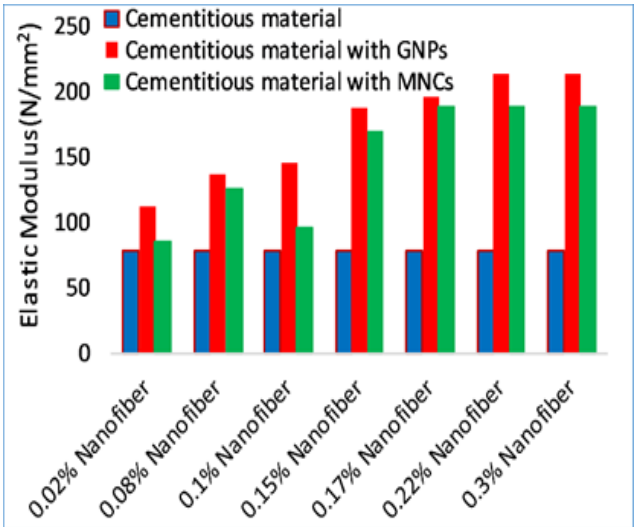


Figure 6. Elastic modulus of various percentages of nanofibres used in cement paste.

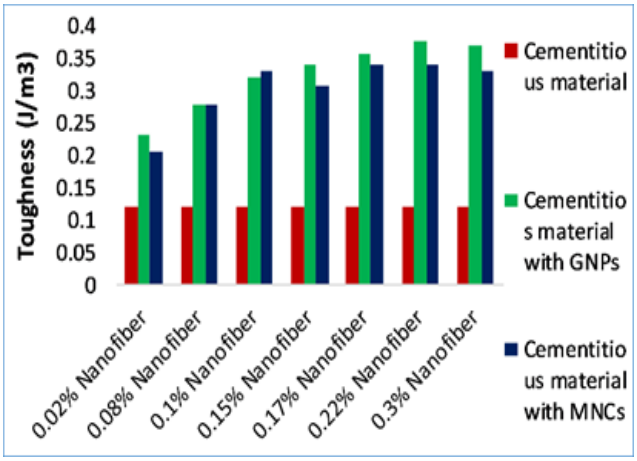


Figure 7. Toughness of various nanofibres used in cement paste.

that using Nanofibre, the mechanical properties of cement paste are increased.

4.0 Conclusion

This paper discusses an overview of different percentages of GNPs/MNCs mixed with cement paste and their mechanical properties. From Figure 4, it is observed that 0.17% of GNP nanofiber gives the maximum strength, and from Figure 5, 0.15% of MNC carries the maximum load. The simulation procedure of GNPs/MNCs cementitious material is also carried out to change the behavior of Young's modulus and the toughness. A load-displacement relationship of GNPs/MNCs cementitious material subjected to axial tension is carried out with different percentages of GNPs/MNCs incorporated into it. It is noticed that the rate of increase in the toughness of GNPs/MNCs cement matrix is increasing for both the material but instead of that GNP cementitious material gives much beteer result than MNC cementitious material.

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