Performance of Graphene Oxide nanosheets on the dispersion of nano SiO_2 and its effect on the mechanical properties of cement mortar

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ABSTRACT

In the present study was investigated the Sedimentation mechanism of SiO_2 nanoparticles (NS) on Graphene Oxide (GO) nanosheets by hydrolysis of Tetra Ortho Silicate (TEOS) in water/ethanol solution. In the first part, the possible interactions among nanoparticles by UV-Vis and Transmission electron microscopy (TEM), and in the second part, the mechanical properties of nanocomposite materials contain NS and GO (NS&GO) by molecular dynamic simulation (MDS) was discussed. Finally, the application of single and hybrid nano materials on 12 kinds of mixture of mortars containing natural pozzolan was compared with mechanical properties. the improvement of dispersion of NS on GO nanosheets was visible in TEM. Also, the results of MDS demonstrate 75% increase in tolerable stress and 250% increase in Young's modulus in nanocomposite compared with single nano-SiO_2. 28-day compressive and tensile strength mortars containing NS&GO increased by 31% and 100%, respectively and compared with the control. As a result, appropriate dispersion and distribution of nanoparticles, NS&GO through nucleation properties, and zeolite through pozzolanic properties improved the mechanical function of mortars.

KEYWORDS

Graphene Oxide, NanoSiO_2, Natural Pozzolans, Mechanical properties, Molecular dynamics simulations

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1. Introduction

concrete has been known as the second most widely used materials and today many of the research studies are about its improvement [1]. According to some researches more than 7% of world's carbon dioxide is formed by cement production process [2]. Iranian pozzolans like pumice and zeolite that are found completely naturally can be replaced by all or part of the cement and improve the durability and transition properties. Base on experimental results, they might decrease compressive and tensile strength as well. On the other hand, the nanomaterials can improve and make up these possible defects. The combination of graphene oxide and nano-SiO2 have demonstrated the acceptable results in improvement of some varied properties of mortars. For instance Junlin Lin [3] reported increase of 21.7% and 17.9% at 28days compared to the control cement paste in both compressive and tensile strength, respectively. Also, their observations show that the dispersion of Sio_2 nanoparticle is affected by GO nanosheets. As a new approach, the present study aims to evaluate the performance of mortars containing natural pozzolans, reinforced with graphene oxide and nanoSiO_2.

2. Experimental program

First, the optimum percentages for SiO_2 and GO were obtained by 3 and 7days compressive strength test. Accordingly, 1% of nanoSiO_2 and 0.02% of GO were selected as the optimal values for the single state. Also, the optimum percentage for GO and NS in preparing NS&GO were 0.02% and 0.5% NS&G. amount of Zeolite and Pumice were selected as a fix value of 15% by pervious researches. According to this 12 mixtures mortar were prepared, which has been shown in Table 2. The water/cement ratio and sand/cement ratio were 0.485 and 2.75 respectively. Cubic samples sized 50×50 were prepared for compressive strength test according to ASTM C109, and briquette samples for the tensile strength test according to ASTM C307.

For the second part, the dispersion of prepared solution of NS&GO was evaluated by TEM and Uv-Vis. For better comparison two approaches were considered for preparing hybrid solutions. In the first approach, graphene oxide and nanoSiO_2 and a little bit superplasticizer were separately dissolved in water. While the hybrid solution in second approach was obtained by hydrolysis of Tetra Ortho Silicate (TEOS) in the presence of GO.

Finally, the molecular scale properties of hybrid NS&GO were investigated by MDS (Molecular dynamics simulation). For this purpose, Lammps and Avito were used for simulation part and visual outputs respectively. The dimensions of the simulation box in the direction of X, Y and Z vectors are equal to about 40, 40 and 20 angstroms, respectively (figure. 1). Also, in order to create a bond between oxygen groups on the surface of graphene oxide, and to consider the possibility of bonding between these agents with silicon dioxide, all interatomic interactions of the system were modeled by Reaxff potential [4]. The steps of the simulation is assumed to be 0.5 fs and during the simulations, before mechanical testing, the whole system was relaxed by Nose-Hoover and Barostat [5, 6].

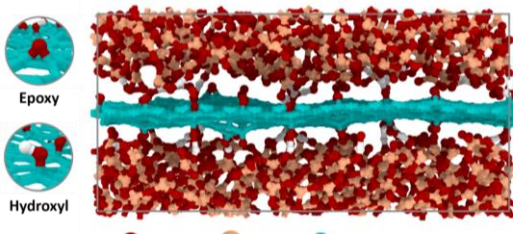

Figure 1. Simulation box of GO and nonoSiO_2 from the side

Table 1 . Mortars' mixture design (Kg/m^3)

Sample	Cement	Pumice	zeolite	GO	SiO_2
Ctrl	666.0	-	-	-	-
Z	566.0	-	100	-	-
P	566.0	100	-	-	-
GO	665.8	-	-	0.13	-
ZGO	565.8	-	100	0.13	-
PGO	565.8	100	-	0.13	-
NS	659.3	-	-	-	6.66
ZNS	559.3	-	100	-	6.66
PNS	559.3	100	-	-	6.66
NS&GO	662.5	-	-	0.13	6.66
ZNS&GO	562.5	-	100	0.13	6.66
PNS&GO	562.5	100	-	0.13	6.66

3. Results and Discussion

The most important part of the results, is related to the characteristics of NS&GO. The difference between both approaches is Comparable in figure. 2. According to TEM images of the suspension NS&GO based of which SiO2 nanoparticle isolated from TEOS have chemically reacted to GO nanosheets. Therefore, the quality of dispersion in NS&GO is more acceptable than NS+GO.

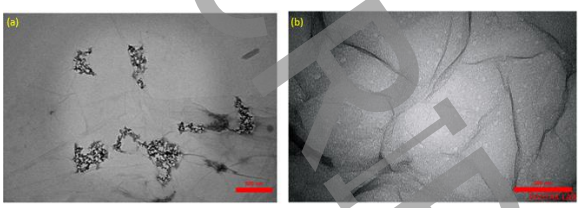

Figure 2. TEM images: (a) NS+GO, (b) NS&GO

According to the results in Molecular dynamics simulation part (Figure 3), the tolerable tensile stress in the GO-SiO_2 composition is increased by 65% compared with single SiO_2 nanoparticles. The Young's modulus has been also increased by approximately 250%, which is a significant amount. The GO nanosheets will absorb most of the tensile stresses just up to the breaking point. After the breaking point, the absorption of tensile stresses in the GO-SiO_2 is accompanied by large deformations.

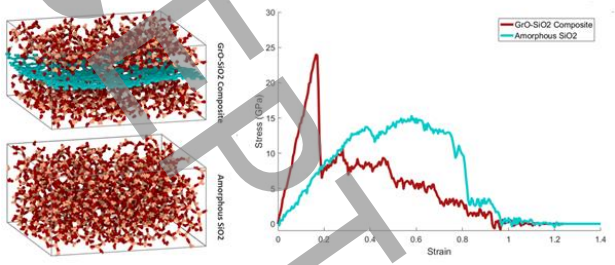

Figure 3.

In terms of binary mortars containing single nanomaterials, the assessment of the data collected in this section was done by comparing them with the control sample and the similar mortars regarding the content and type of the replaced nanomaterials which only differed in terms of the amount of zeolite and pumice. In this regard, compared with control sample, the 28day compressive strength of NS and GO samples increased by 28% and 18%, respectively. NS&GO mortar had the highest compressive strength at 7, 28, and 90 days of age with increases of 49%, 40%, and 38%, respectively. It shows the powerful effects of nanocomposite on improving mechanical properties. Addition zeolite and pumice to mortars containing composite nanomaterials have reduced the compressive strength. But this reduction in the case of ZNS&GO and PNS&GO mortar are almost negligible.

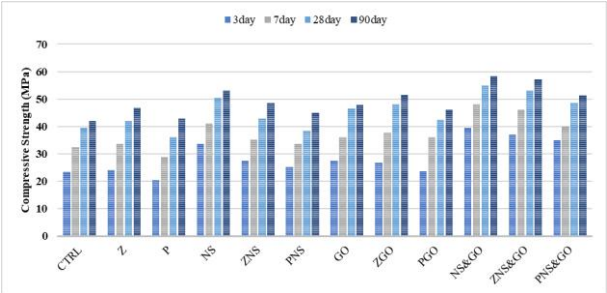

Figure 4. Compressive strength of mortar specimens

A similar function was observed when the tensile strength was done. In fact, the best performance of mortars is assigned to NS&GO by 69% and 100% increase at the ages of 28day and 90day, respectively. The most important difference between compressive and tensile strength is pumice. As an exception, pumice had a better function than zeolite in tensile strength compared with compressive strength. overall, results showed that the mechanical properties of mortar with NS&GO are much better than single nanomaterials.

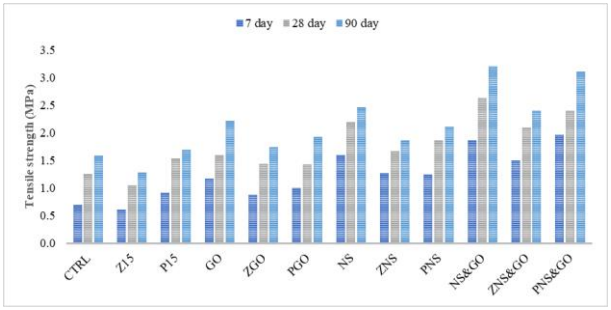

Figure 5. Tensile strength of mortar specimens

4. Conclusions

to conclude, addition of Nano-SiO2 and GO nanosheets in a single state to cementitious mortars improves the mechanical property as well as microstructure. However, in the present study, an effective composite of nanomaterials containing Nano-SiO2 and GO (NS&GO) was developed and obtained during a chemical process. Moreover, zeolite and pumice with a relatively high percentage of substitution were used to address the environmental and durability issues. the discoveries show dispersion and molecular properties of nano was improved by GO. Finally, ZNS&GO is introduced as an optimal design.

5. References

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