



Performance of Graphene Oxide nanosheets on the dispersion of nano SiO₂ and its effect on the mechanical properties of cement mortar

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ABSTRACT: In the present study, the sedimentation mechanism of SiO₂ nanoparticles (NS) on Graphene Oxide (GO) nanosheets by hydrolysis of Tetra Ortho Silicate (TEOS) in water/ethanol solution was investigated. 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) were discussed. Finally, the application of single and hybrid nano materials on 12 kinds of the 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-SiO₂. 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.

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1- Introduction

concrete has been known as the second most widely used material and today many research studies are about its improvement [1]. According to some research, more than 7% of the world's carbon dioxide is formed by the cement production process [2]. Iranian pozzolans like pumice and zeolite are found completely naturally and can be replaced by all or part of the cement and improve the durability and transition properties. Based 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 28 days compared to the control cement paste in both compressive and tensile strength, respectively. Also, their observations show that the dispersion of SiO₂ nanoparticles 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 nano SiO₂.

2- Experimental program

First, the optimum percentages for SiO₂ and GO were obtained by 3 and 7-day compressive strength test. Accordingly, 1% of nano SiO₂ 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 was selected as a fixed value of 15% by previous researches. According to this, 12 mixtures of mortar were prepared, which has been shown in Table 1. The water/cement ratio and sand/cement ratio were 0.485 and 2.75 respectively. Cubic samples sized 50×50 were prepared for the 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 the 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 nanoSiO₂ and a little bit of superplasticizer were separately dissolved in water. While the hybrid solution in the second approach was obtained by hydrolysis of Tetra Ortho Silicate (TEOS) in the presence of GO.

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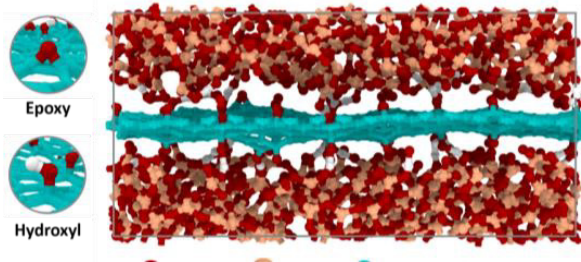


Fig. 1. Simulation box of GO and nanoSiO₂ from the side

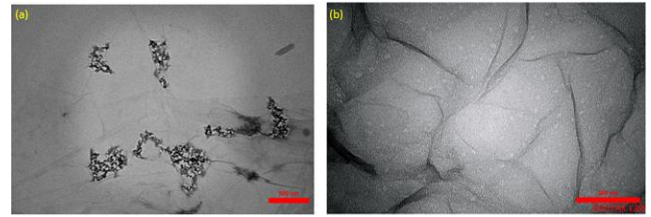


Fig. 2. TEM images (a) NS+GO, (b) NS&GO

Table 1. Mortars' mixture design (Kg/m³)

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

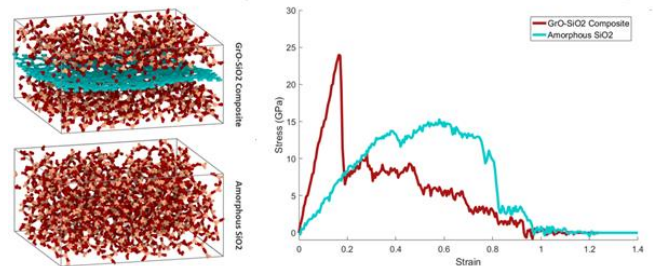


Fig. 3. Comparison of Stress-strain diagram of amorphous silica and GO-Silica B: the image of GO-Silica simulation box C: the image of silica simulation box

Finally, the molecular scale properties of hybrid NS&GO were investigated by MDS (Molecular dynamics simulation). For this purpose, Lammmps and Avito were used for the 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].

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.

According to the results in the molecular dynamics simulation part (Figure 3), the tolerable tensile stress in the GO-SiO₂ composition is increased by 65% compared with single SiO₂ nanoparticles. Young's modulus has 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-SiO₂ is accompanied by large deformations.

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 the control sample, the 28-day 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. The addition of zeolite and pumice to mortars containing composite nanomaterials has reduced compressive strength. But this reduction in the case of ZNS&GO and PNS&GO mortar is almost negligible.

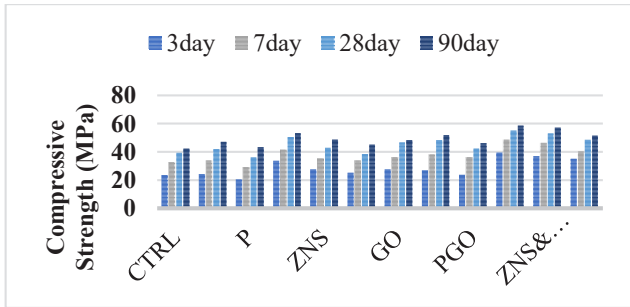


Fig. 4. Compressive strength of mortar specimens

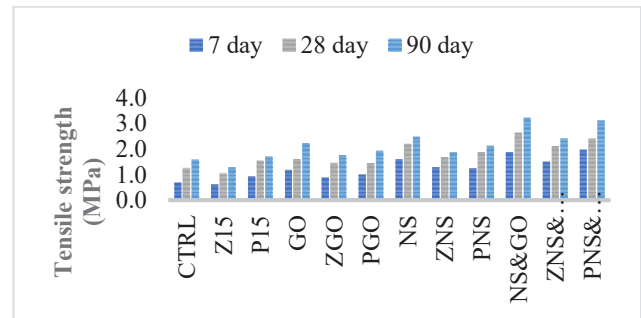


Fig. 5. Tensile strength of mortar specimens

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 28 days and 90 days, 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.

4- Conclusions

To conclude, the 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 were improved by GO. Finally, ZNS&GO is introduced as an optimal design.

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