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Experimental and theoretical studies of ordinary Portland cement composites contains nano LSCO perovskite with Fokker-Planck and chemical reaction equations

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HIGHLIGHTS

- Introduction of LSCO perovskite nanoparticles leads to a more condensed matrix.
- LSCO perovskite nanoparticles improved the microstructure of OPC.
- LSCO perovskite nanoparticles enhanced the flexural strength of OPC.
- The optimum amount of LSCO perovskite nanoparticles replaced with OPC is 2%.

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ABSTRACT

In this study, $LaSr_{0.5}Co_{0.5}O_3$ perovskite (LSCO), with 1, 2 and 4 wt% of LSCO nanoparticle inserted into the OPC (Ordinary Portland Cement) matrix via the sol-gel route. The sample nanocrystallite characteristics, surface topography, flexural strength, the influence of crystallite's size, chemical interaction, and the correlation between carrier diffusion; surface roughness were studied using some related techniques and Master and Fokker-Planck approaches. The obtained results from LSCO/cement discrete cell structure show that the sample cement mortar containing 2 wt% LSCO nanocrystallites has a more stable mechanical structure and higher flexural strength due to the its permanent electric dipole, more occupation of the trap sites into the cement, and diffusion of particles (crystallites) through the cell boundary and inside the cells.

For this purpose, microscopic parameters such as the trap and escaping rate in the LSCO+ cement discrete cells have been introduced and discussed with considering Master nonlinear Fokker–Planck and chemical reaction equations based on non-fluctuations of the LSCO particle position explored in the cells (which strongly correlated with random sequence). The results indicate an inhomogeneous nano structures characteristic, which is beyond the equilibrium stationary state with Gaussian fluctuations for the particle position.

1. Introduction

Today, considerable usage of different types of concrete in construction industry led to conducting many researches [1–8] in this regards. Obviously, modification of cement characteristic, as one of the main basic components of concrete, has direct relationship with enhancement of concrete properties. Moreover, the mechanical property of the material highly depends on its mix design properties [9,10]. The performed researches [11–17] show that a number of nanoparticles are able to enhance some properties of materials.

Some undesirable, noxious gases and unburnt hydrocarbons such as Co produced from cementitious materials are released into the surrounding environment and can damage our life. To get rid of unwanted emissions of these gases, the bond and correlation between them should be broken. It leads to understanding how additive nanoparticles behave in the cement matrix. Although previous investigations have found [18–22] that cement-based materials with nanocrystallites are tailored from elongated cement

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discrete cells or aggregated/cluster crystallites, cement properties and nanostructural characteristics heavily change with features, surface topography, and the diffusion phenomenon into the cement discrete cell.

Researchers previously studied the effect of nanoparticles such as TiO_2 [20,21], CNT [23–26], montmorillonite [27–29], and SiC [30,31] on cement and found that these nanoparticles can effectively influence the mechanical nanostructure of the cement matrix. It is worth mentioning that the mechanical properties of cement-based materials are recognized as the most essential factors in their quality assurance purposes [32,33]. As a result, in this study, perovskite–type oxides, $LaSr_{0.5}Co_{0.5}O_3$ (LSCO), due to their potential to fulfill requirements such as high activity and mechanical stability [34,35] have been studied. In one glance, these various properties arise from the crystal symmetry adopted by these materials. For this purpose, for finding the influence of additive nanoparticles of LSCO (synthesized with sol-gel processes) on the cement cluster or matrix, topography variation of cement compounds were investigated using energy dispersive X-ray spectroscopy (EDS), Fourier transform infrared spectroscopy (FTIR), atomic force microscopy (AFM), and DE- SPM techniques.

Depending on the amount of LSCO nanocrystallites in the cement materials, different mechanical and durability properties can be seen in these materials. The crystallite's phases and surface topography, compressive and flexural strength of the cement matrix with 0, 1, 2, and 4 wt% of LSCO nanoparticle's additives, labeled CS, SN-1, SN-2 and SN-4, respectively, along with the influence of particle size and other phenomena were experimentally and theoretically discussed by considering Master nonlinear Fokker–Planck equation, chemical reaction, and diffusion through the discrete cells.

2. Material and methods

In this research, tap water and natural sand for all mixtures according to ASTM C778 [36] standard were used. Ordinary Portland Cement (OPC), ASTM type I [37], produced by Bojnourd Cement Co., with chemical (Table 1) and physical (Table 2) properties was used in mortar mixtures (Table 3). A superplasticizer was used in order to keep the flow ability constant at about 15 mm. To measure the flexural strength of the present samples, ASTM C348 [38] was used. After 24 h, mortar samples were extracted from the mold and cured in a storage tank of water until they were tested.

LSCO samples with La:Sr:Co; 2:1:1 M ratio were synthesized with the sol-gel method. Indeed, in the present study, after heating the samples to 50 °C (in the atmospheric media) in a hotplate containing a magnet piece, they (LSCO:Cement) were turned into powder (T = 80 °C in this case). In the end, different weights of crystallites in the cement matrix (1, 2, and 4 wt% LSCO/Cement), labeled SN-1, SN-2, and SN-4, respectively, were synthesized using the sol-gel processes. Cement paste containing 0, 1, 2, and 4 wt% LSCO nanoparticles' structural characteristics were thus evaluated using FTIR and AFM techniques.

3. Results and discussion

3.1. Flexural strength

Fig. 1 shows the results of the flexural strength of cement mortar specimens processed at different times (3, 7, and 28 days). In general, the cement mortar flexural strength of perovskite samples SN-1 and SN-2 is increased up to 2% weight of Portland cement compared to the control sample (CS) by adding nanoparticles. It is clear that the largest increase in flexural strength can be observed in the sample containing 2 wt% nano-perovskite particles, whereas the flexural strength reduced in other samples (SN-4), due to the agglomeration of LSCO nanoparticles on the samples. The increasing in flexural strength can be related to enhancement of nanostructure of the cement matrix, indeed, this result is in favor of previous studies [19,22,24,27,29,30,39,40].

3.2. Energy-dispersive X-ray spectroscopy (EDS) analysis

The LSCO additive effects in the cement compound and sample surface topography were investigated using an EDS analyzer (SAMx Company, France) operating at an accelerating voltage of 5 kV, Fourier transform infrared spectroscopy (FTIR), atomic force microscopy (AFM), and DE-SPM techniques.

The EDS (Fig. 2) as an example, and Tables 4–6), FTIR (Figs. 3–5, Table 6) spectra, and AFM images (Figs. 6–8) reveal that the cement structure and mechanical characteristics, which naturally contain efficient catalysts including (Fe_2O_3) and sensible supporting materials ($CaCO_3$, CaO, SiO_2, MgO, and Al_2O_3), are affected by the LSCO nanoparticle additive.

3.3. Fourier transform infrared (FTIR) spectroscopy analysis

To study single- and double-bonds with different vibrations and characterizing their related functional group of OPC, FTIR analysis, reported on a Bruker-Tensor 27 spectrometer was applied. The FTIR spectrum in Fig. 3 shows that LSCO is consistent with 1500, 1860, and 2540 cm^{-1} peaks of perovskite $La_{0.5}Sr_{0.5}CoO_3$ phases, labeled P_1, P_2 and P_3. In the prepared gel, the 3200 cm^{-1} band has to be attributed to hydroxyl groups and to the OH from water and ethanol.

Fig. 4 shows the FTIR spectra of cement powder according to which the peak located at the wave numbers of 3447 cm^{-1} is related to the moisture in cement powder which may have been adsorbed during sample preparation for the FTIR analysis. The characterization and related functional groups of OPC are presented in Fig. 4 and Table 7. The FTIR spectra of cement sample containing 2 wt% of LSCO nanoparticles is presented in Fig. 5 as well.

Figs. 4 and 5 reveal that the amount of two main bands of CO_3^{-2} (v_3) and Si—O (tetrahedron) increased as compared to the reference sample (OPC in Fig. 4). These two bands assigned to asymmetric stretching vibrations (v_3) of CO_3^{-2} and stretching vibrations have also some other out-of-plane bending vibrations v_2 of CO_3^{-2} and bending vibrations of O—H bands. It is because the density of particles and/or carriers can be changes and make an electrostatic potential to bend the pointed bands. The results show an improvement of nano structural and mechanical properties of LSCO/cement samples due to higher transmittance peak of Si—O.

There is the stretching vibration mode of functional group of CO_3 at 1429 cm^{-1}. It could be due to Co in LSCO which is relatively consumed (or reduced the intensity of transmittance of v_3 of CO_3^{-2} peak in Fig. 5) by the reaction of LSCO nano particles with cement matrix. Moreover, it could be due to cubic closed – packed arrangement of CO and O ions with La (or Sr) ions and filling ratio of octahedral interstitial sites.

Table 1
The amount of material in the chemical composition of cement (wt%).

Items	SiO_2	Al_2O_3	Fe_2O_3	CaO	MgO	Na_2O	K_2O	SO_3	L.O.I
OPC	20.40	4.56	3.40	64.12	1.93	0.32	0.70	2.30	2.20