Simulations of Electrical Conductivity of Composite Materials and Optimization of Artificial Neural Networks

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INTRODUCTION

Structural health monitoring (SHM) has become an established field of engineering in the past few decades. SHM aims to give a diagnosis on the condition of materials, elements, and of the whole structure at every moment of the structure's lifespan. Design dictates the structure's nominal behavior and SHM allows keeping it in that nominal domain. Thanks to the time-dimension of monitoring, which builds a full historical database of the structure, it is possible to determine damage progression and residual life of the observed structure.

When it comes to concrete, i.e. cementitious materials, the lack of two main properties - electrical conductivity and piezoresistivity, hinders them from simultaneously becoming both structures and sensors. The application of nanotechnology can significantly improve the performance of traditional concrete, giving it novel abilities and improving overall mechanical properties [1]. Self-sensing materials used in SHM drastically change the maintenance planning process by minimizing human involvement and human errors and by aiming to replace scheduled and periodic maintenance inspections or at least to reduce the current maintenance labor, thus improving safety and reliability.

THE CONCEPT

Richard P. Feynman's idea (1959) of controlling matter at the nanoscale remained only a concept for several decades until the technology was developed enough and observations at a quantum level were possible. Since Iijima and Ichihashi published their discovery of "*single-shell tubules*" in 1993, there have been many discoveries regarding the properties and possible applications of single-walled carbon nanotubes (SWCNTs). Comparing to conventional materials, carbon nanomaterials possess some unusual size-/surface-dependent (e.g., morphological, electrical, optical, and mechanical) properties. They can exist in numerous forms, differing in structure, size, chemistry, and mechanical properties. The most represented and investigated materials are nanocarbons (C60, carbon black, carbon nanotubes (CNTs), graphene) because of their superior mechanical properties and conductive capabilities. Single-walled CNTs have been regarded as one of the most promising material, opening the door for multi-functional, cementitious composite applications. Concrete is an electrically nonconductive material, however, the addition of CNTs (Figure 1) provides it with piezoresistivity which makes it an excellent choice for a sensor while preserving the role of a structure at the same time.

The most recent developments in SHM are connected to different types of nanosensors such as transducers, electrochemical and optical sensors, as well as techniques of environmental pollutants' detection via nanomaterials. While the development of nanoscale devices and nanoelectromechanical systems (NEMS) is an evolving area of nanotechnology, there is also considerable interest in making macroscopic engineered materials that can exploit these properties.

Self-sensing CNT/concrete composites possess piezoresistivity, giving the ability to monitor strain by using the change in the electrical resistance i.e. self-sensing capability of large-scale structures [2]. CNT networks are highly valuable in SHM for strain mapping, damage detection, identification of crack initiation and propagation, and more.

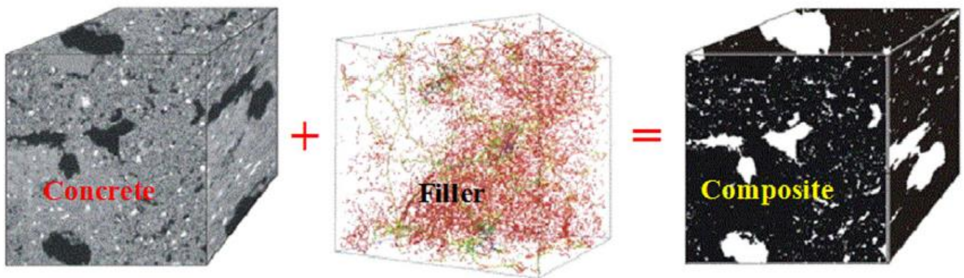

Figure 1. Structure of self-sensing concrete [2]

The neural network approach is a way of modeling data based on computer learning in order to perform complex functions. The application of machine learning represents a new direction in the evolution of monitoring concrete structures. Artificial neural networks (ANNs) have been developed as an interconnected group of nodes inspired by a simplified representation of neurons in the brain. Although the original idea of ANN was to solve problems in the same way as a human brain would, over time it deviated from biology towards solving some specific tasks (pattern recognition, identification, classification, vision and control systems, cancer predictions, etc). Recently, machine learning became an attractive tool to reduce model complexity and so ANNs have been successfully used for a variety of applications, some including structural analysis and material science, ranging from studies of atomic properties to the mechanical properties of concretes or an individual carbon nanotube [3]. The choice of ANNs to model so many different systems is, in part, due to their flexibility and adaptability as well as their easy application in software and hardware devices and materials [4].

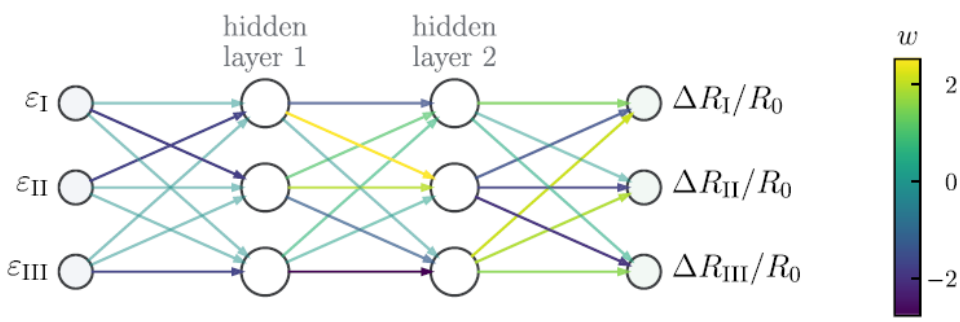

Figure 2. Schematics of the optimized ANN and of respective weights [4]

THE METHODOLOGY

Basic units of the neural network are artificial neurons, which represent the processing elements. Their connections typically have assumed weights that are adjusting as the learning proceeds based on the back-propagation rule. The architecture of the ANN is formed by the input and the output layer and a series of hidden layers, each of which is formed by a determined number of neurons (Figure 2). Building of the artificial neural network starts with building its data library. Data library contains the data sets divided into 3 subsets: training, selecting and testing set. Data collection comprehends experimental data including laboratory investigations as well as numerical simulations of the mechanical properties of the composites. Data collected from Konsta-Gdoutos et al. [5], shown in Table 1, as an example of the information which may be used as training data and also as testing data, after supplementing it with the results of the measured sensitivity of the sensing ability (e.g. ΔR/R [%]).

Table 1. Mechanical properties of cement with 0.1%vol. and 0.5%vol. of CNT and 0.1%vol. of CNF, collected from [5]

Material	Fiber count	Age (days)	Compressive strength [MPa]	Young's modulus - bending test [GPa]	Young's modulus - compressive test [GPa]	Resistance [kΩ]	Resistivity [kΩ*cm]
Plain cement	\	3	19.8	9.2±0.96	9.5±0.97	12.6	8.4
		7	25.6	10.8±0.87	11.5±0.83		
		28	31.7	14.1±0.71	13.9±0.7		
0,1% CNT	3.61E+11	3	22.6	16±0.44	15.4±0.49	9.2	6.1
		7	26.5	18.1±0.13	18.3±0.15		
		28	33.8	27.4±0.09	27.9±0.12		
0,5% CNT	1.08E+12	3	22.7	9.9±0.93	10.2±0.94	10.6	7.1
		7	27.6	12.2±0.74	12.3±0.62		
		28	35.3	20.1±0.67	20.9±0.59		
0,1% CNF	1.69E+11	3	22.5	11.7±0.78	12.0±0.73	10.8	7.2
		7	25.2	16.9±0.32	16.7±0.46		
		28	33.7	27.6±0.11	27.4±0.14		

Among various modeling techniques, multiscale modeling (MM) showed to be the most efficient method that can model the mechanical behavior of the CNT and its composites accurately. The following scales are distinguished: quantum scale, nanoscale, microscale, macroscale, and continuum scale. The MM method entails solving physical problems that have important features at multiple scales. It is aimed at calculating material properties or system behavior at one scale using information from different scales, and at each scale, particular approaches describe each system. Garcıa-Macıas et al. [6] have presented a 3D generalization of the micromechanics models of the overall conductivity and uniaxial piezoresistivity of CNT-reinforced composite materials subjected to arbitrary strain states. The authors [6] have proposed an approach shown to be capable of determining the piezoresistivity coefficients. The presented technique showed to be able to reliably model the complex electromechanical behavior of the CNT/concrete composite materials.

This research work assumes testing of the mechanical properties and electrical conductivity of cementitious composite materials and further use of the results to train and test the ANN model. The numerical simulations include finite element models made using ANSYS software and the ANN model developed using MATLAB script. The training and selecting phase of the neural network will be conducted until the desired output and the network output don't relatively match, when the testing phase may be conducted. The architecture of the ANN model predicting the optimal mixture for self-sensing concrete is configured as follows. The input layer for the training of the ANN consists of 5 neurons: (1) water/cement ratio, (2) final weight of cement per $1m^3$ of concrete, (3) final weight of fine aggregate per $1m^3$ of concrete, (4) weight fraction of the functional filler, (5) conductivity of the functional filler. Output data include (i) electrical resistance of the composite material [Ω*cm], (ii) sensitivity of the sensing ability ($\Delta R/R_0$ [%]), (iii) compressive strength of the composite [MPa], (iv) flexural strength of the composite [MPa]. The output neurons can be represented by (v) stress sensitivity coefficient, (vi) gage factor and (vii) Young's modulus.

CONCLUSIONS

A novel approach to manufacturing self-sensing materials for SHM is now possible, implying concepts of determining mixtures and conductivity of specific self-sensing composites using artificial neural networks. The idea of a self-sensing structure is to mimic a biological system through sensing, actuation, adaptability, self-repair, etc. and the ultimate form of intelligent structures are the ones that have the additional ability to learn in contrast to the pre-programmed response. This learning feature is realized by employing ANNs. Real-time effective and cost-efficient monitoring of structures is possible to obtain by developing a conductive composite with a predetermined mixture predicted by a trained neural network. The application of machine learning implies a very low computational cost and can be immediately used by relatively inexperienced users [3].

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