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HDPE 기반의 나노다이아몬드 복합소재의 물성 예측을 위한 인공신경망 연구

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Artificial Neural Network for Prediction of Mechanical Properties of HDPE Based Nanodiamond Nanocomposite

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Abstract: The mechanical performance of the nanocomposite depends on the processing conditions of the samples. Therefore a predictive model is essential to proceed the combination of processing conditions into account, for accurately predicting the mechanical properties is a critical requirement in manufacturing industries. The current investigation explores the prediction of mechanical properties of high-density polyethylene (HDPE)-based nano-diamond nanocomposite (i.e., HDPE/0.1 ND) using an artificial neural network (ANN) model under various processing conditions of temperature and pressure. A 2-10-2 (2 input, 10 hidden and 2 output layer) neural network model with Levenberg–Marquardt algorithm is developed to predict Young's modulus and Hardness of HDPE/0.1 ND nanocomposite. The model accurately predicted Young's modulus and hardness with a correlation coefficient of more than 0.99. The root means square error (r.m.s) of experimental *vs*. predicted value is minimal, confirming the proposed ANN model's high reliability and accuracy.

Keywords: artificial neural network, mechanical properties, nanodiamond, polymer matrix nanocomposite.

Introduction

Over the decade, attention to thermoplastic material has increased substantially due to its exceptional properties such as short processing time, ease of production, superior mechanical properties, and corrosion-free material. High-density polyethylene (HDPE) is classified under thermoplastic material as the best choice owing to its low weight, higher tensile strength, exceptional impact strength, higher tribological, excellent thermal properties, and chemically stable. The above advantages made the adoption of HDPE suitable material in industries like automotive, aeronautical, naval, biomedical, and piping industries. However, compared to virgin HDPE, with the addition of nanofillers into the matrix of HDPE, named HDPE nanocomposite, the mechanical,[1] thermal,[2] tribological,[3] and rheological[4] properties are enormously enhanced. The followings are some significant pieces of literature in the context of the topic discussed.

Obeid *et al.*[5] studied the effect of nano-sized WO_3 particles on the mechanical properties of HDPE composite. The WO_3 particle concentration varied from 10 to 35 wt% and there is a significant improvement of Hardness, and Young's modulus values are noted up to 25 wt% of WO_3 particles. Konakar *et al.*[6] observed an enhancement of mechanical properties with the addition of graphite nono-platelets (GNP) nanoparticles from 0 to 10 wt% in the HDPE matrix. Moreover, the mechanical properties were influenced by the coating of nanoparticles. Olesik *et al.*[7] compared the mechanical properties of HDPE composite filled with either glassy carbon (GC), carbon nanotube (CNT), graphene (Gr), or GNP nanoparticles. It was noted that the GC nanoparticles showed the optimum mechanical properties, i.e., Hardness and Young's modulus, compared to other samples. Khan *et al.*[8] demonstrated the mechanical properties of walnut shell powder filled in HDPE composite. The wt% of walnut shell powder varied from 0 to 20 wt% for the above study. The enhancement of mechanical properties was

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noted with the increase in % of walnut shell powder. Morimune-Moriya *et al.*[9] evaluated the mechanical properties of polyethylene (PE)/nano-diamond (ND) nanocomposite with the addition of 0.5 to 5 wt% of ND nanoparticles into low-density polyethylene matrix. It is observed that there is a significant improvement of mechanical properties up to 1 wt% ND nanoparticle, and then there is a drop due to agglomeration of ND particles. Badgayan *et al.*[10] reported the mechanical behavior of HDPE/MWCNT/h-BNNP nanocomposite and hybrids. The best mechanical properties were exhibited by 0.25/0.15 wt% of MWCNT/h-BNNP hybrid nanocomposite among all the samples. Sahu *et al.*[11] investigated the mechanical properties HDPE based composite reinforced with 0.1 wt% of ND, CNT, and GNP nanoparticles. It was noted that the addition of 0.1 wt% ND nanoparticle showed the highest Young's modulus and hardness value, which increased by 18.5% and 45.3% compared to pure HDPE. This was explained due to the morphology of ND nanoparticles and the uniform dispersion inside the HDPE matrix. Several research reported on improvement in mechanical properties with the addition of CNT,[12-14] GNP,[15-17] graphene,[18-20] and very few on addition ND[21] in to polymer matrix.

The literature review concluded that by adding nanoparticles, exclusively ND nanoparticles into the HDPE matrix, the mechanical properties were significantly enhanced. The current investigation is on evaluating the mechanical properties of 0.1 wt% of ND nanoparticles at various processing conditions. The choice of ND particle is due to its extraordinary Hardness and greater tensile strength.[22,23] The author is profound to explore the mechanical properties of the addition of 0.1 wt% ND nanoparticle into HDPE matrix. The novelty of the current study is that, an artificial neural network (ANN) model is employed to predict the mechanical properties (e.g., Young's modulus and hardness value) of polymer nanocomposite. ANN is a mathematical tool that mimics the work of nerve cells in the human system.[24] Very few works are available in the context of predicting the mechanical properties of polymer nanocomposite using ANN.[25-27]

Experimental

Materials. High-density polyethylene (HDPE) pallets were purchased from IOCL, India, with specifications as follows: size 5 to 8 mm; MFI of 0.7 g/10 min; density more than 0.940 g/cm^3; tensile strength at yield more than 20 MPa; tensile strength at break more than 30 MPa; elongation at break more than 900%; melting point of 125-135 ºC. The filler chosen was nano-diamond (ND) supplied by Reinste Nano Venture, India. The morphology of nanodiamonds as dot-like structures is confirmed by Transmission electron microscopy (TEM), as shown in Figure 1.[1]

Fabrication of Composite. The composite sample is fab-

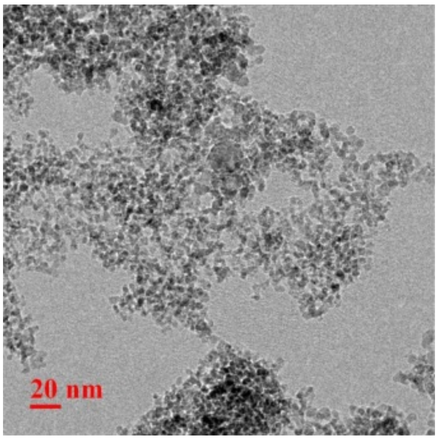

Figure 1. TEM morphology of ND nanoparticle.[1]

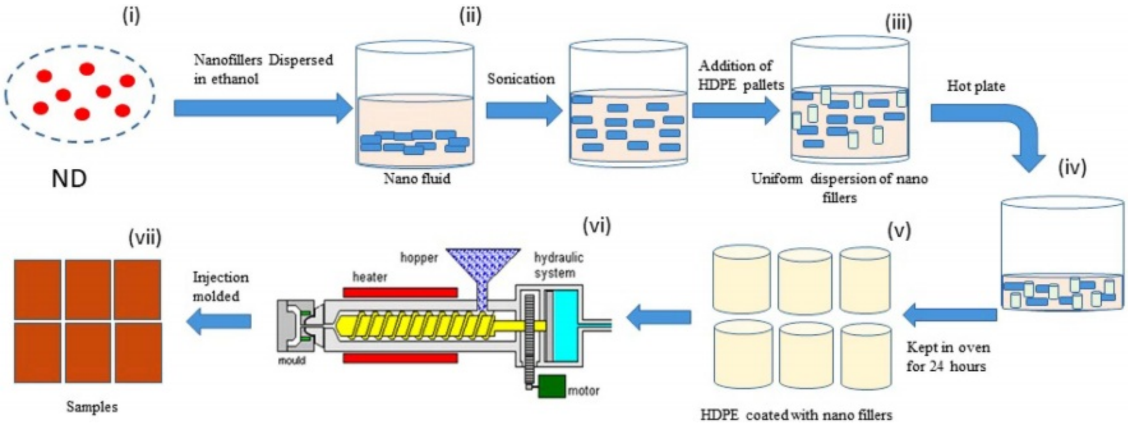

Figure 2. Fabrication process of ND composite.

ricated with an HDPE matrix filled with 0.1 wt% of ND nanofillers. The fabrication route is illustrated in Figure 2 from (i) to (vii). Initially, the ND nanoparticles are chemically modified, as explained in the literature by Sahu *et al.*[21] Then the 0.1 wt% of ND nanoparticles were taken in a beaker followed by mixing with ethanol at a 1:0.5 ratio. The solution was then magnetically stirred on a sonicator to achieve uniform dispersion. The nanofluid solution thus prepared is mixed with HDPE pallets and kept on a hot plate till all the ethanol is evaporated. Then to remove any strain of moisture, the mixture is kept in an oven for 24 hours. The HDPE now coated with ND nanofillers is fed to an injection molding machine for nanocomposite fabrication, i.e., HDPE/0.1 nanocomposite. The injection molding process parameters like temperature and pressure are varied and different samples of HDPE/0.1 nanocomposite are obtained for further investigation discussed in the next section.

Experimental Tests. The tensile test was carried out to find Young's modulus of the samples as per ASTM D1708. The Instron 8801 UTM is employed with a dynamic load capacity of ±100 kN at a load cell accuracy of 0.005%. The crosshead speed for the test is 1 mm/min and is maintained. The Hv-1000Z Vickers indenter equipment is used to evaluate Hardness, which has a diamond pyramid indenter. There were five tests repeated in each test to confirm the accuracy.

Results and Discussion

The ANN is performed using MATLAB R2021a software. The training is conducted to determine the best fit for the adopted ANN model. The temperature and pressure are the two injection molding parameters used as input for ANN. The corresponding target values are Young's modulus and Hardness. The Young's modulus and Hardness is noted from the experiment and illustrated in Table 1 and detail steps are shown in Figure 3. The architecture consists of three layers (2-10-2), i.e., two input layers, one hidden layer, and two output layers, as shown in Figure 4. The hidden layer has ten neurons. The hidden layers' transfer function is tangent or sigmoid, and the algorithm was Levenberg–Marquardt (LM) used to train the network. Once the training was completed, the model was collected at the output layer. Figure 5(a-d) shows the regression plot during three stages, i.e., training, validation, and testing of Young's modulus results. The additional plot denotes the overall regression results. It is noted that at all three stages, the regression value is more than 0.99, indicating that the net-

Table 1. Processing Conditions of Composite and Corresponding Experimental Young's Modulus and Hardness

Runs	Temperature (°C)	Pressure (MPa)	Young's modulus (GPa)	Hardness (GPa)
1	160	28.3	1.281	7.215
2	151.5	30	1.252	7.232
3	146.2	27.5	1.264	7.143
4	132.4	17.5	1.252	6.921
5	135.5	21	1.256	6.934
6	148.2	25.3	1.275	7.121
7	148	31.2	1.264	6.932
8	127.3	24	1.213	6.824
9	132	26.4	1.224	6.934
10	145.4	18	1.245	7.221
11	152.3	22.5	1.265	7.314
12	156.4	23	1.272	7.323
13	160	30	1.274	7.412

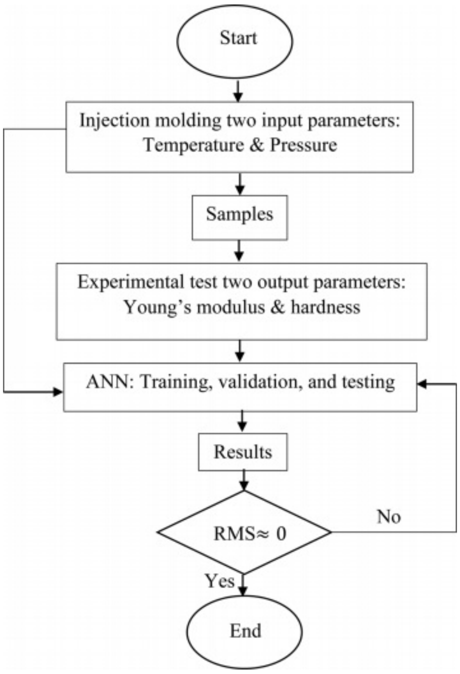

Figure 3. Steps followed for prediction of mechanical properties.

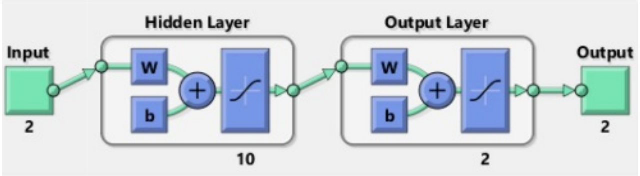

Figure 4. Adopted ANN model (w: weight, b: bias).

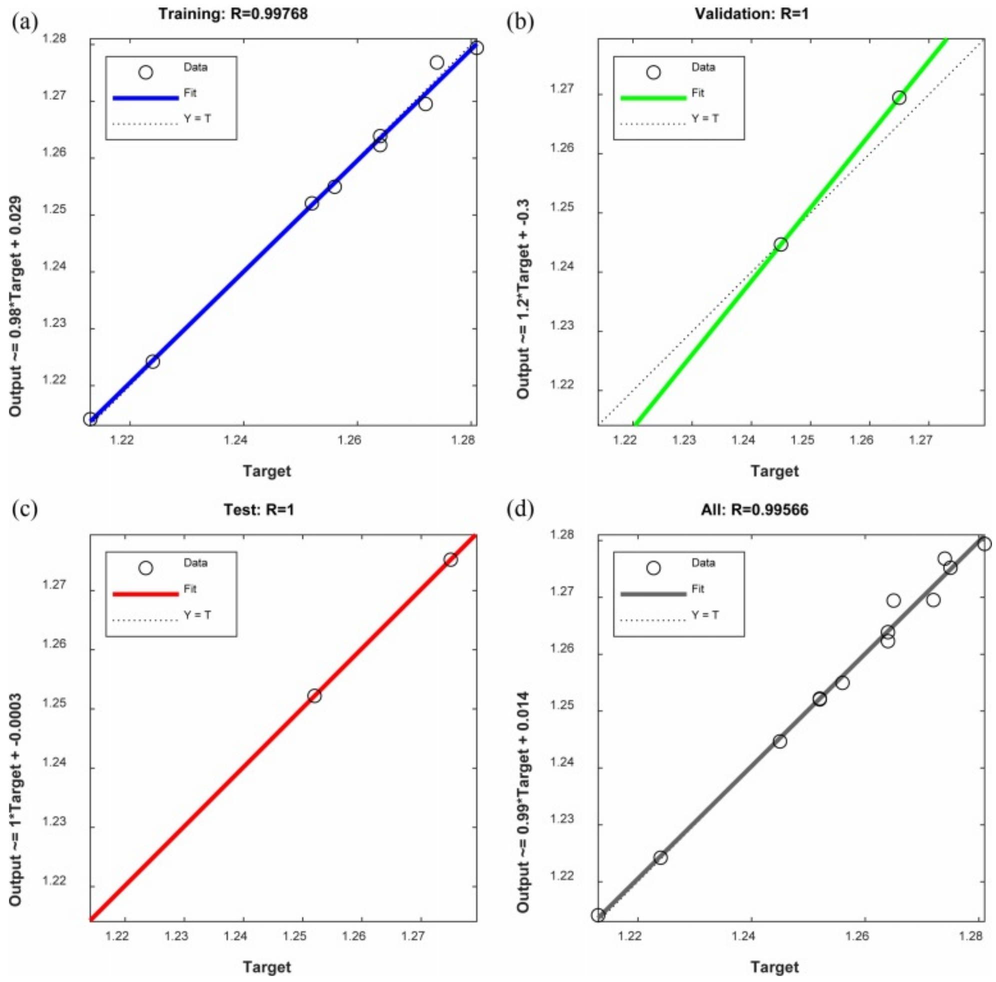

Figure 5. Regression plot for Young's modulus prediction (a) training; (b) validation; (c) test; (d) overall.

work's performance is optimal. Similar results were observed during the regression plot of hardness value with a regression value of more than 0.99, as shown in Figure 6(a-d). The predicted line equation for Young's modulus and hardness properties is represented in eqs. (1) and (2).

$$Y = (0.99)T + 0.014 \tag{1}$$

$$Y = (0.97)T + 0.22 \tag{2}$$

The obtained results from the experimental test and the ANN predicted responses are expressed in Table 2.

The actual root-mean-square value ($A_{\mathrm{R.M.S}}$) is expressed as eq. (3)

$$A_{\mathrm{R.M.S}} = \sqrt{\frac{\Sigma_{\mathrm{i=1}}^{\mathrm{i=n}}(Actual)^2}{n}} \tag{3}$$

The root-mean-square error ($E_{\mathrm{R.M.S}}$) is given by eq. (4)

$$E_{\mathrm{R.M.S}} = \sqrt{\frac{\Sigma_{\mathrm{i=1}}^{\mathrm{i=n}}(Actual-Predicted)^2}{n}} \tag{4}$$

The ratio of root-mean-square error ($E_{\mathrm{R.M.S}}$) to root-mean-square value ($A_{\mathrm{R.M.S}}$), which expresses the degree of agreement and is represented in eq. (5),

$$E_{\mathrm{c}} = \frac{E_{\mathrm{R.M.S}}}{A_{\mathrm{R.M.S}}} \tag{5}$$

From the calculation, the R.M.S value of Young's modulus noted was 1.256839, and the corresponding R.M.S error was 0.001781. The degree of agreement was found as 0.001417. Similarly, the R.M.S value of hardness was observed as 7.119697, and the related R.M.S error was 0.016636. The degree of agreement was noted as 0.002337 for Hardness. This is evidenced by the magnitude of the r.m.s value for Young's modulus (0.001781) and the hardness (0.016636).

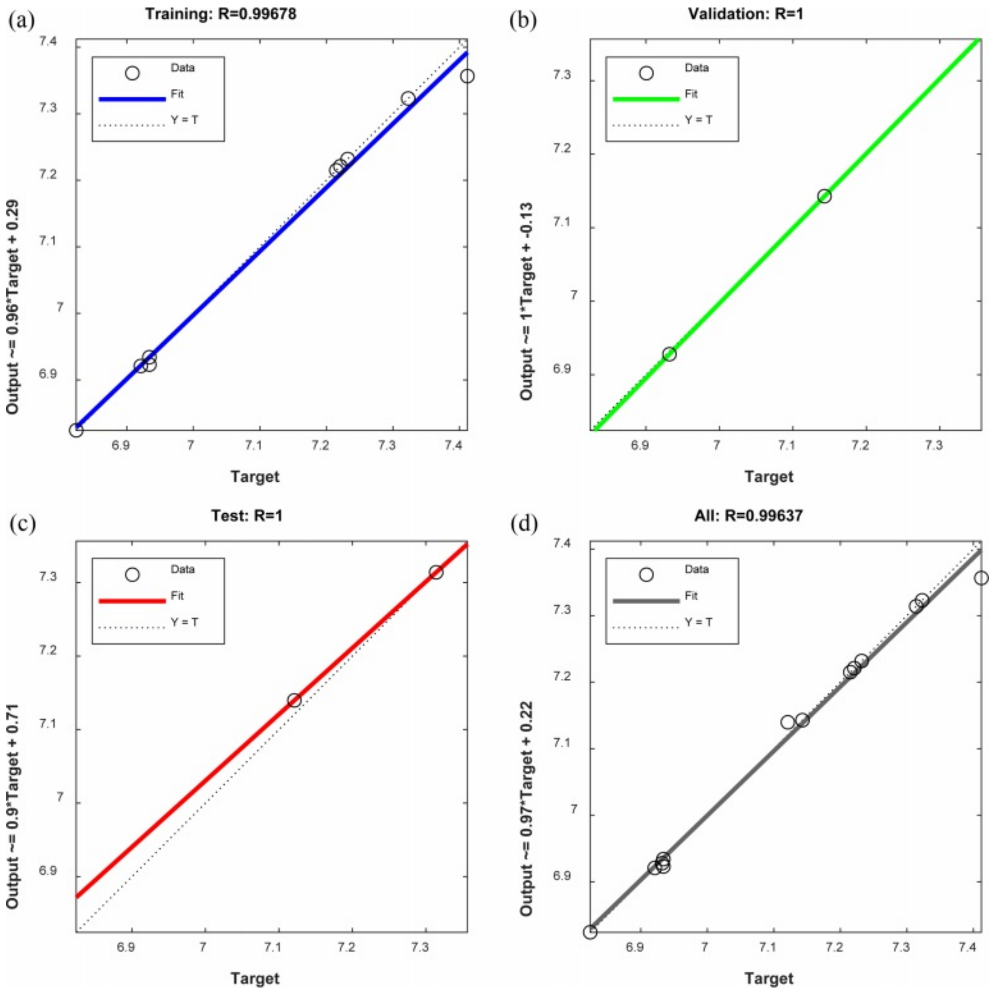

Figure 6. Regression plot for hardness prediction (a) training; (b) validation; (c) test; (d) overall.

Table 2. Experimental and ANN Predicted Values of Young's Modulus and Hardness (unit : GPa)

	Experimental values		ANN predicted values	
Runs	Young's modulus	Hardness	Young's modulus	Hardness
1	1.281	7.215	1.279	7.215
2	1.252	7.232	1.252	7.232
3	1.264	7.143	1.262	7.142
4	1.252	6.921	1.252	6.921
5	1.256	6.934	1.255	6.923
6	1.275	7.121	1.275	7.139
7	1.264	6.932	1.264	6.928
8	1.213	6.824	1.214	6.824
9	1.224	6.934	1.224	6.934
10	1.245	7.221	1.245	7.221
11	1.265	7.314	1.269	7.314
12	1.272	7.323	1.2695	7.323
13	1.274	7.412	1.277	7.356

The error is minimal, and the developed model accurately predicted Young's modulus and hardness values. The actual *vs*. predicted value is represented in Figure 7(a) and (b) for Young's modulus and Hardness, respectively.

Conclusions

HDPE/0.1 ND nanocomposite was fabricated using the injection molding route with varying process parameters like temperature and pressure was investigated. The mechanical properties such as Young's modulus and Hardness were experimentally obtained for the above process condition. The ANN technique is adopted to predict the mechanical properties of HDPE/0.1 ND nanocomposite with a 2-10-2 (two input, ten hidden layers, and two output) neural network model using the LM technique to train the model. The model accurately predicted Young's modulus and Hardness with a correlation coef-

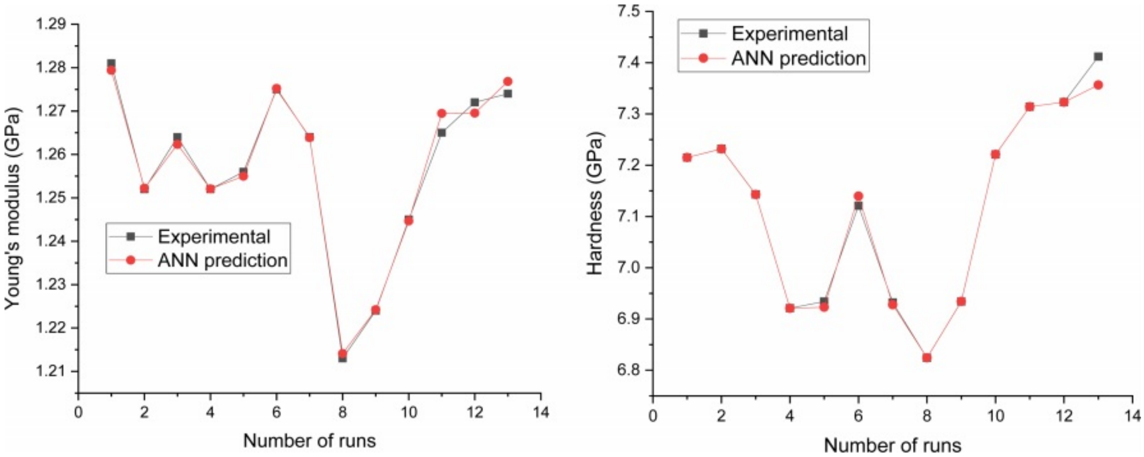

Figure 7. (a) Actual *vs.* predicted values of Young's modulus; (b) actual *vs.* predicted values of hardness *vs.* number of runs.

ficient of more than 0.99 during training, testing, and validation of test samples. In addition, the r.m.s value of experimental *vs.* predicted value is minimal, which confirms the high reliability and accuracy of the proposed ANN model.

Conflict of Interest: The authors declare that there is no conflict of interest.

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