Detection of the Electronic Attributes of the Nanostructured Materials with Fuzzy Logic

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Abstract- **This is a study, in which a trial was done to estimate the energy band gap (E_g) of single-walled carbon nanotubes (SWCNTs) by using a fuzzy logic algorithm that uses five inputs (strain value, fermi energy level, average energy, repulsive potential and electronic band structure energy).**

Keywords- SWCNTs, fuzzy logic, strain value, energy band gap, prediction

I. Introduction

Single-walled carbon nanotubes (SWCNTs) are a hollow cylindrical structure of carbon atoms with a diameter that ranges from 1 to 10 nm and have a length longer than this diameter. Nanoparticles are used or evaluated for use in many fields. It is one of nanomaterials which are used most. It is used in a lot of fields like electronics, computer science, medicine, aviation and environmental science [1].

For this reason, a lot of experiments are being done about SWCNTs nowadays. Purpose of these experiments is to produce the materials that can be used to provide these fields that are mentioned before to develop. But an experiment on nanomaterials can be very costly.

With this work, it was aimed to open a road for these high costs to be decreased. To do this, fuzzy logic was used as a prediction tool. A tool, which can predict the experiment result with a high percent, means the result is obtained without any experiment.

In this study, prediction of the energy band gap (*Eg*), that is an electronic attribute of SWCNTs was done. So, this value was used as an output. Five inputs were used to predict that. These are fermi energy level, average energy, strain value, repulsive potential and electronic band structure energy.

II. Review of Previous Works

S. Ahadian and Y. Kawazoe worked on a topic about using an adaptive-network-based fuzzy inference system (ANFIS) for carbon nanotubes (CNTs) in 2009. With this algorithm (ANFIS), they aimed to model and predict the water flow in CNTs [2].

M. H. Esfe, S. Saedodin, N. Sina, M. Afrand and S. Rostami, conducted a study that predicts thermal conductivity and dynamic viscosity of ferromagnetic nanofluids in 2015. In this study, they used an artificial neural network (ANN) [3].

C. S. Johanyak, in his work in 2013, served a low-complexity fuzzy model. This model identifies the relationship between percentage amount of multi-walled carbon nanotube (MWCNT), polycarbonate (PC), acrylonitrile-butadiene-styrene (ABS) and melt volume-flow rate(MVR) of the generated composite [4].

M. Shanbedi, S. Z. Heris, A. Amiri, S. Adyani, M. Alizadeh and M. Baniadam, conducted a study in 2014. At first, they synthesized pristine and functionalized multi-walled carbon nanotubes with silver/water nanofluids. They used the synthesis of human algorithm interaction (HAI), and fuzzy logic rules to research thermal performance of two-phase closed thermosiphon [5].

R. Leghrib and E. Llobet, in 2011, conducted a study to detect traces of benzene by using a quantitative fuzzy adaptive resonant theory network (ART) and an array of plasma-treated metal-decorated carbon nanotubes [6].

S. Prabhu, M. Uma and B. K. Vinagayam, did an experiment to predict the surface roughness, where the mixture of CNT and nanofluids is dielectric by using Taguchi technique, fuzzy logic and neural network algorithm in 2014 [7].

M. Shanbedi, A. Amiri, S. Rashidi, S. Z. Heris and M. Baniadam used ANFIS and predicted thermal efficiency and thermal resistance of a two-phase closed thermosyphon in 2015 [8].

M. Mehrabi, M. Sharifpur, and J. P. Meyer utilized a model that consists of fuzzy C-means clustering (FCM) and ANFIS to estimate the viscosity of nanofluids in 2013 [9].

S. Ata and K. Dinçer, calculated inferentially the performance of polymer electrolyte membrane (PEM) fuel cell whose anode side was covered with CNT by employing fuzzy logic algorithm in 2015 [10].

In this paper, we designed a fuzzy expert system to detect of the electronic attributes of the nanostructured materials.

III. Method and Materials

There are a lot of factors to affect the energy band gap of an SWCNT. Here are some factors below [1]:

- (n, m) values (these values constitute the symmetry axis and structure of CNT)
- Fermi Energy Level *(E_f (eV))*
- Diameter *(d_t)*

- Atom Number
- Strain Value (%)
- Average Energy (eV/atom)
- Electronic Band Structure Energy *(E_{bs})*
- Repulsive Potential *(U_{rep})*
- Temperature (K)

To make a healthy calculation, the factors, which aren't dependent on each other with an equation, were chosen as inputs. And it was considered that these factors are the ones that affect the energy band gap directly. As a result, the chosen inputs and output were given in Table 1 and Table 2.

TABLE 1
INPUTS AND THEIR RANGES

Inputs	**Small (Low)**	**Average (Average)**	**Large (High)**
Strain value(%)	[-6, -1]	[-4, +3]	[1, 6]
Fermi energy level (eV)	[3.7, 3.71475]	[3.71445, 3.71898]	[3.71668, 3.73]
Average energy (eV/atom)	[-8.29, -8.27229]	[-8.28227, -8.23621]	[-8.25744, -8.185]
U_{rep} (eV)	[22, 24.023]	[23.229, 25.866]	[25.163, 26.495]
E_{bs} (eV)	[-35, -33.828]	[-34.162, -31.938]	[-32,344, -30]

TABLE 2
OUTPUT AND ITS RANGES

Output(s)	
Membership Grades	**Energy Band Gap (eV)**
Very Narrow	[0, 0.05]
Narrow	[0.03, 0.1]
Average	[0.08, 0.2]
Wide	[0.16, 0.29]
Very Wide	[0.22, 0.5]

Besides, temperature value was chosen as 300 K and (n, m) values were chosen as (18, 0) respectively. According to inputs and output, the structure of the generated system is in Figure 1.

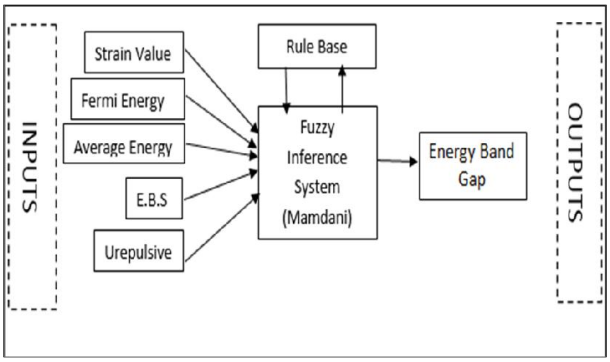

Figure 1. Structure of the Fuzzy System Calculating the Energy Band Gap of a SWCNT

In this work, one of the five inputs and one output were used. The input which is used is strain value. There are three membership functions for strain value: Small, Average and Large. For strain value, membership graphics are given in Figure 2.

For strain value, the formulas of the membership grades were given by the numbers from 3.1 to 3.3.

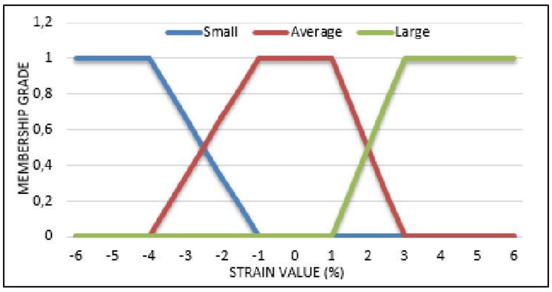

Figure 2. Strain value membership graphics

$$\mu small(x) = \begin{cases} 1, \ if \quad x < -4 \\ (-1-x)/3, \ if -4 \le x \le -1 \\ 0, \ if \quad x > -1 \end{cases} \qquad (3.1)$$

$$\mu average(x) = \begin{cases} 0, \ if \quad x < -4 \\ (x+4)/3, \ if \quad -4 \le x \le -1 \\ 1, \ if \quad -1 < x < 1 \\ (3-x)/2, \ if \quad 1 \le x \le 3 \\ 0, \ if \quad x > 3 \end{cases} \qquad (3.2)$$

$$\mu large(x) = \begin{cases} 0, \ if \quad x < 1 \\ (x-1)/2, \ if \quad 1 \le x \le 3 \\ 1, \ if \quad x > 3 \end{cases} \qquad (3.3)$$

Their fuzzy set representation as follows:

μ_{small}={ 1/(-6) + 1/(-5.5) + 1/(-5) + 1/(-4.5) + 1/(-4) + 0.833/(-3.5) + 0.666/(-3) + 0.5/(-2.5) + 0.333/(-2) + 0.166/(-1.5) + 0/(-1) + 0/(-0.5) }

$\mu_{average}$={ 0/(-4) + 0.166/(-3.5) + 0.333/(-3) + 0.5/(-2.5) + 0.666/(-2) + 0.833/(-1.5) + 1/(-1) + 1/(-0.5) + 1/0 + 1/0.5 + 1/1 + 0.75/1.5 + 0.5/2 + 0.25/2.5 + 0/3 + 0/3.5 }

μ_{large}={ 0/1 + 0.25/1.5 + 0.5/2 + 0.75/2.5 + 1/3 + 1/3.5 + 1/4 + 1/4.5 + 1/5 + 1/5.5 + 1/6 }

In the fuzzy inference system, there is only one output and it is energy band gap. There are three membership functions for energy band gap: Very narrow, narrow, average, wide and very wide. For energy band gap, membership graphics are given in Figure 3.

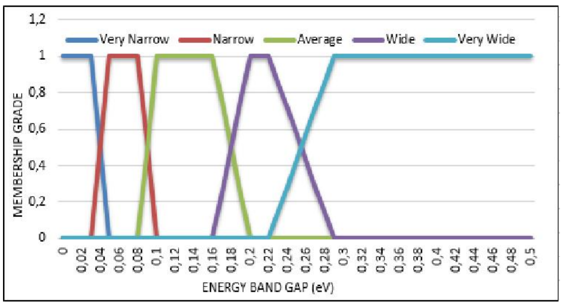

Figure 3. Energy band gap membership graphics

For energy band gap, the formulas of the membership grades were given by the numbers from 3.4 to 3.8.

$$\mu VeryNarrow(x) = \begin{cases} 1, & if \quad x < 0.03 \\ (0.05 - x)/0.02, & if \ 0.03 \leq x \leq 0.05 \\ 0, & if \quad x > 0.05 \end{cases} \quad (3.4)$$

$$\mu Narrow(x) = \begin{cases} 0, \ if & x < 0.03 \\ (x - 0.03)/0.02, \ if & 0.03 \leq x \leq 0.05 \\ 1, \ if & 0.05 < x < 0.08 \\ (0.1 - x)/0.02, \ if & 0.08 \leq x \leq 0.1 \\ 0, \ if & x > 0.1 \end{cases} \quad (3.5)$$

$$\mu Average(x) = \begin{cases} 0, \ if & x < 0.08 \\ (x - 0.08)/0.02, \ if & 0.08 \leq x \leq 0.1 \\ 1, \ if & 0.1 < x < 0.16 \\ (0.2 - x)/0.04, \ if & 0.16 \leq x \leq 0.2 \\ 0, \ if & x > 0.2 \end{cases} \quad (3.6)$$

$$\mu Wide(x) = \begin{cases} 0, \ if & x < 0.16 \\ (x - 0.16)/0.04, \ if & 0.16 \leq x \leq 0.2 \\ 1, \ if & 0.2 < x < 0.22 \\ (0.29 - x)/0.07, \ if & 0.22 \leq x \leq 0.29 \\ 0, \ if & x > 0.29 \end{cases} \quad (3.7)$$

$$\mu VeryWide(x) = \begin{cases} 0, \ if \ x < 0.22 \\ (x - 0.22)/0.07, if \ 0.22 \leq x \leq 0.29 \\ 1, \ if \ x > 0.29 \end{cases} \quad (3.8)$$

Their fuzzy set representation is as follows:

$\mu_{Very\ Narrow}$= {1/0 + 1/0.01 + 1/0.02 + 1/0.03 + 0.5/0.04 + 0/0.05 + 0/0.06}

μ_{Narrow}={ 0/0.03 + 0.5/0.04 + 1/0.05 + 1/0.06 + 1/0.07 + 1/0.08 + 0.5/0.09 + 0/0.1 + 0/0.11 }

$\mu_{Average}$={ 0/0.08 + 0.5/0.09 + 1/0.1 + 1/0.11 + 1/0.12 + 1/0.13 + 1/0.14 + 1/0.15 + 1/0.16 + 0.75/0.17 + 0.5/0.18 + 0.25/0.19 + 0/0.2 + 0/0.21 }

μ_{Wide}={ 0/0.16 + 0.25/0.17 + 0.5/0.18 + 0.75/0.19 + 1/0.2 + 1/0.21 + 1/0.22 + 0.857/0.23 + 0.714/0.24 + 0.571/0.25 + 0.428/0.26 + 0.285/0.27 + 0.142/0.28 + 0/0.29 + 0/0.3 }

$\mu_{Very\ Wide}$={ 0/0.22 + 0.142/0.23 + 0.285/0.24 + 0.428/0.25 + 0.571/0.26 + 0.714/0.27 + 0.857/0.28 + 1/0.29 + 1/0.3 + 1/0.31 + 1/0.32 + 1/0.33 + 1/0.34 + 1/0.35 + 1/0.36 + 1/0.37 + 1/0.38 + 1/0.39 + 1/0.4 + 1/0.41 + 1/0.42 + 1/0.43 + 1/0.44 + 1/0.45 + 1/0.46 + 1/0.47 + 1/0.48 + 1/0.49 + 1/0.5 }

The rule base of the fuzzy inference system was specified by a nanotechnology expert. For each input, there are three membership grades. So, there are 243(3^5) rules in the rule base. Some examples of them were given in Table 3.

TABLE 3.
RULE BASE OF THE FUZZY STRUCTURE

#	Strain Value	Fermi En. Lvl	Average Energy	U_{rep}	E_{bs}	E_{gap}
1	Small	Low	Low	Small	Small	VNrw
40	Small	Avg	Avg	Avg	Small	Nrw
67	Small	High	Avg	Avg	Small	Avg
159	Avg	High	High	Avg	Large	Wide
243	Large	High	High	Large	Large	VWd

As it was mentioned before, Fuzzy Logic Toolbox of MATLAB R2015a was used to get the output results. The interface of the designed FIS which were prepared with the program was given in Figure 4. There are some examples here:

Example 1: Strain value: 1%, Fermi Energy Level: 3.71387 eV, Average Energy: -8.28227 eV/atom, U_{rep}: 24.02347 eV, E_{bs}: -32.34451 eV

According to the data in this example, four rules are fired from the fuzzy inference system. And the result is obtained as 0.0191 eV. The resulting image of the example was given in Figure 5. In the examples of this work, Mamdani fuzzy model was used as a fuzzification tool, and the centroid of area method was used as a defuzzification tool.

Example 2: Strain value: -6%, Fermi Energy Level: 3.72119 eV, Average Energy: -8.20914 eV/atom, U_{rep}: 26.494 eV, E_{bs}: -34.74192 eV

For the data in the example, one rule is fired from the fuzzy inference system. And the result is obtained as 0.219 eV. The resulting image of the example was given in Figure 6.

IV. CONCLUSION

This article shows how to predict energy band gap of SWCNTs. These terms are important to get efficient results:

1. There must be a direct relationship (like an equation) between inputs and outputs.
2. There must not be a direct relationship between inputs.
3. The right algorithm must be chosen for prediction. Here, the fuzzy logic algorithm was chosen as an artificial intelligence algorithm and Mamdani fuzzy model was chosen as a fuzzy inference system. Centroid of area method was chosen for defuzzification.
4. The original data must be used for prediction.

According to these terms, five inputs and one output which were mentioned before were chosen. To obtain a sharp result, output membership grade number was specified as five. And true results were gotten with minimum error and maximum proximity.

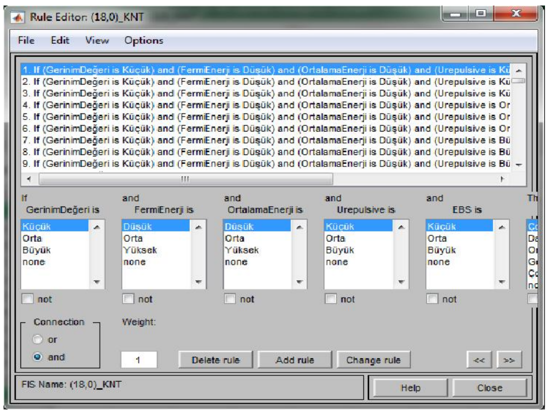

Figure 4. The interface of the designed FIS for the prediction of energy band gap

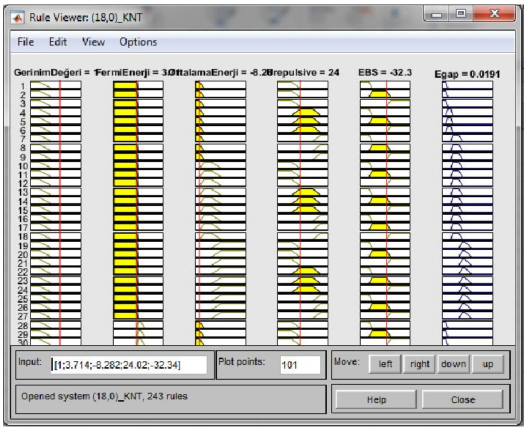

Figure 5. The resulting image of Example 1

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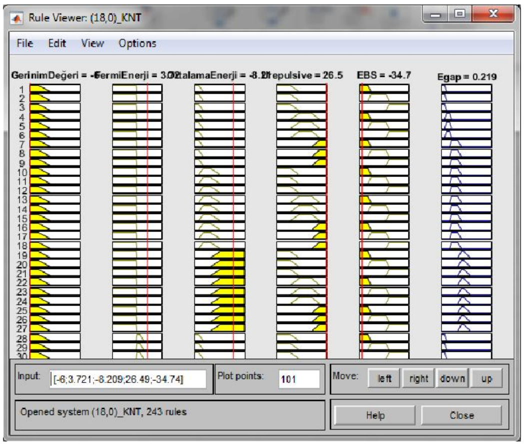

Figure 6. The resulting image of Example 1

REFERENCES

[1] Necati Vardar, *"Farklı Simetrik Yapılardaki Karbon Nanotüplerin Durum Yoğunluklarının Simülasyonu,"* MSc. Thesis, Yıldız Teknik Üniversitesi Fen Bilimleri Enstitüsü, İstanbul, 2006.

[2] S. Ahadian and Y. Kawazoe, *"An Artificial Intelligence Approach for Modeling and Prediction of Water Diffusion Inside a Carbon Nanotube,"*Nanoscale Research Letters, vol. 4, no. 9, pp. 1054–1058, Apr. 2009.

[3] M. H. Esfe, S. Saedodin, N. Sina, M. Afrand, and S. Rostami, *"Designing an artificial neural network to predict thermal conductivity and dynamic viscosity of ferromagnetic nanofluid,"* International Communications in Heat and Mass Transfer, vol. 68, pp. 50–57, 2015.

[4] Z. C. Johanyak, *"Fuzzy Modeling of Thermoplastic Composites' Melt Volume Rate,"* Computing and Informatics, vol. 32, pp. 845–857, 2013.

[5] M. Shanbedi, S. Z. Heris, A. Amiri, S. Adyani, M. Alizadeh, and M. Baniadam, *"Optimization of the thermal efficiency of a two-phase closed thermosiphon using active learning on the human algorithm interaction,"* Numer. Heat Transf. Part A Appl., vol. 66, no. 8, pp. 947–962, 2014.

[6] R. Leghrib and E. Llobet, *"Quantitative trace analysis of benzene using an array of plasma-treated metal-decorated carbon nanotubes and fuzzy adaptive resonant theory techniques,"* Analy. Chim. Acta, vol. 708, no. 1–2, pp. 19–27, 2011.

[7] S. Prabhu, M. Uma, and B. K. Vinayagam, *"Surface roughness prediction using Taguchi-fuzzy logic-neural network analysis for CNT nanofluids based grinding process,"* Neural Comput. Appl., vol. 26, no. 1, pp. 41–55, 2014.

[8] M. Shanbedi, A. Amiri, S. Rashidi, S. Z. Heris, and M. Baniadam, *"Thermal performance prediction of two-phase closed thermosiphon using adaptive neuro-fuzzy inference system,"* Heat Transf. Eng., vol. 36, no. 3, pp. 315–324, 2015.

[9] M. Mehrabi, M. Sharifpur, and J. P. Meyer, *"Viscosity of nanofluids based on an artificial intelligence model,"* Int. Commun. Heat Mass Transf., vol. 43, no. October 2017, pp. 16–21, 2013.

[10] S. Ata and K. Dinçer, *"Anot Tarafi Karbon Nanotüp ile Kaplanmış Pem Yakıt Hücresi Performansının Bulanık Mantık Yöntemiyle Modellenmesi",* UHTEK-2015 Ulusal Hidrojen Teknolojileri Kongresi, İstanbul, 1-7, (2015).