Diamond-Like Carbon (DLC) chemical vapor deposition technology: Characterization of DLC nano-layers and Artificial Neural Networks for process modelling

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Diamond-like carbon (DLC) is obtained cooling or quenching high energy precursive carbons on relatively cold surfaces. This deposition process can be performed by several methods as, for instance, by pulsed laser ablation, cathodic arc, ion beam or plasma enhanced chemical vapour deposition (PECVD). The speed of the deposition process does not allow the material to grow in the cubic crystalline geometry form as for the synthetic diamond production process. Therefore, the resulting DLC film has no long-range crystalline order. This characteristic allows obtaining flexible coatings with mechanical properties similar to that of diamond. The DLC-coating technology is nowadays widely used in medicine (brachytherapy, coating of blood-contacting surfaces etc.) [1,2,3], informatics (as protective material for hard-drives), tribology to prevent wear, solar cells technology [4] and in industry [5].
The properties of the final coating can be modified by doping DLC with elements such as nitrogen, silicon and oxygen, fluorine or metal atoms [6, 7]. Nitrogen incorporation has been used to improve field emission properties of DLC films [8]. One particular class of modified DLC coatings is that of diamond-like nano-composite films consisting of two amorphous interpenetrating networks, a diamond-like network and a silicon-oxide like network. nano-composite DLC films with SiO_x content exhibit enhanced fracture toughness, high surface hardness, low compressive stress and high thermo mechanical stability [9, 10].

Several parameters affects the growth rate of thin films in low pressure r.f. discharges and the following three groups may be considered:

- parameters of the deposition/etching process (i.e. frequency, applied power, substrate bias voltage, total pressure, flow rates of gases in the gas mixture, substrate temperature)
- experimental arrangement (i.e. geometry of the deposition chamber, geometry of the electrodes and their distance, position and design of the gas supply)
- Material parameters of the electrodes and the substrates.

The influence of such parameters is very complex and not fully understood up to now. Moreover, the process includes many reactions with complex kinetics [11]. A possible alternative is to employ "soft" modelling approach to model the process. Artificial Neural Networks (ANNs) are nowadays widely used as "soft" modelling tools in science and technology. Recently, some of us (F.A., J.H.) demonstrated the ability of ANN to model even quite complicated kinetic processes in homogeneous phase [12].

- In this work the possible use of supervised ANN to model the process of DLC nano-layers deposition and predict the conditions in order to obtain films with required properties is evaluated.

Results and discussion

- Diamond-like carbon nano-layers were prepared from a mixture of CH_4, H_2 and $C_6H_{18}Si_2O$ (HMDSO) employing plasma produced by high frequency discharge (HDF). Up to 50 different layers were synthesized varying the following experimental conditions: (1) Applied power for cleaning, (2) Argon flow rate, (3) Methane flow rate, (4) HDMSO flow rate, (5) Applied power, (6) Negative self bias voltage, (7) Total pressure and (8) Deposition time. The deposited nano-layers were characterized by measuring thickness, deposition rate, hardness, elastic modulus, interfacial fracture toughness and mass spectrometry.
- ANNs belong to Artificial Intelligence (AI) methods. They are formal structures that emulate the human brain behaviour and are formed by a series of logic units (called "neurons") organized in layers. Each "neuron" of a layer is connected, by means of a weighed connection, to all the neurons in the subsequent layer. The experimental data *(input)* are submitted to the neurons of the first *(input)* layer. From the input layer, the information is processed mathematically and transferred to the following *(hidden)* layers (it is possible to create a network with more than one

hidden layer). Each neuron process the received information. At the end, the neurons of the last *(output)* layer transform the processed information in order to estimate the values of parameters that are chosen as *outputs*. The mathematical processing of the information through the network is called *learning*. For a given system studied, the optimal architecture for the ANN must be found, that is to optimize the number of hidden layers and the number of neurons therein.

- In the first step of ANN application the optimal architecture was searched for. In spite of the fact that the plasma processes to be modelled are very complex, the quite simple architecture shown in Fig. 1 was found as "*the best*" one.
- In the learning step the optimal network was trained using the experimental conditions as *input* and properties of DLC nano-layers as *output*. The network found was able to model successfully the data.
- Trained network was then used to predict of the chosen output values. An example of the correlation obtained between predicted and experimental values of the DLC nano-layer elastic modulus is given in Fig. 2.
- Concluding, ANNs enable successful modelling even if the processes occurring during the deposition of DLC nano-layers are not completely understood. The developed approach allows the prediction of the experimental conditions needed to obtain DLC nano-layers with required properties.
- The described ANN approach is general and might be applied for optimization in nano-technology and/or even for development of new materials.

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Figures

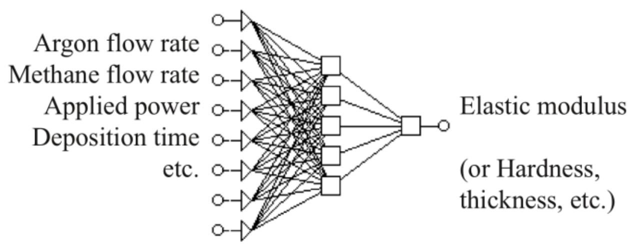

Fig. 1: *Optimal ANN architecture with one hidden layer to model DLC deposition.*

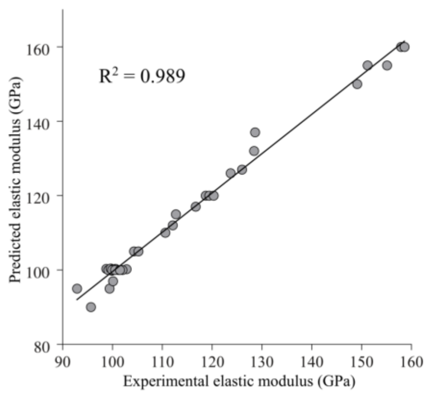

Fig. 2: *Correlation between predicted and experimental elastic modulus values.*