Available online at www.sciencedirect.com
SCIENCE DIRECT®
Wear 255 (2003) 708–713
WEAR
www.elsevier.com/locate/wear

Communication

Artificial neural network predictions on erosive wear of polymers

Z. Zhang*, N.-M. Barkoula, J. Karger-Kocsis, K. Friedrich

Institute for Composite Materials (IVW GmbH), University of Kaiserslautern, Erwin Schroedinger Str. 58, 67663 Kaiserslautern, Germany

Abstract

In the present paper, an artificial neural network (ANN) approach was applied to the erosive wear data of three polymers, i.e. polyethylene (PE), polyurethane (PUR), and an epoxy modified by hygrothermally decomposed polyurethane (EP-PUR). Three independent datasets of erosive wear measurements and characteristic properties of these polymers were used to train and test the neural networks. For the first two material examples, the impact angle of solid particle erosion and some characteristic properties were selected as ANN input variables. Whereas the third one, material compositions, i.e. epoxy and HD-PUR weight contents, were also involved as additional ANN input variables. In all these cases, the output parameter was the erosive wear rate. Acceptable ANN predictive qualities were reached, demonstrating that ca. 35–80% of the randomly selected test dataset had a coefficient of determination $B \geq 0.9$ for these three cases, respectively. Ranking of the importance of characteristic properties to erosive wear rate could offer some information about which property has a stronger relationship to wear in each polymer case. Even though the ANN approach is only a phenomenological method, a well-trained ANN is believed to be also of help for a mechanistic understanding of the problem considered.

Keywords: Artificial neural networks (ANN); Erosive wear; Polymer; Prediction

1. Introduction

The correlations between wear resistance and characteristic properties of polymers have been discussed in terms of various semi-empirical equations by some pioneers. These include, e.g. the Ratner–Lancaster equation [1,2], i.e. the relationship of the single pass abrasion rate with the reciprocal of the product of ultimate tensile stress and strain, or an equation used by Friedrich [3] to correlate the erosive wear rate of polymers with the quotient of their hardness to fracture energy. Although these equations are quite helpful to estimate the wear behavior of polymers in some special cases, wear normally is very complicated, and it therefore depends on many more mechanical and other parameters. This means that simple functions cannot always cover all the prevailing mechanisms under wear.

For predictive purposes, an artificial neural network (ANN) approach has, therefore, been introduced recently into the field of wear of polymers and composites by Velten et al. [4] and Zhang et al. [5]. An ANN is a computational system that simulates the microstructure (neurons) of biological nervous system. The most basic components of ANN are modeled after the structure of the brain. Inspired by these biological neurons, ANN is composed of simple elements operating in parallel. ANN is the simple clustering of the primitive artificial neurons. This clustering occurs by creating layers, which are then connected to one another. How these layers connect may also vary. Basically, all ANN have a similar structure of topology. Some of the neurons interface the real world to receive its input, and other neurons provide the real world with the network's output. All the rest of the neurons are hidden from view. As in nature, the network function is determined largely by the interconnections between neurons, which are not simple connections, but some non-linear functions. Each input to a neuron has a weight factor of the function that determines the strength of the interconnection and thus the contribution of that interconnection to the following neurons. ANN can be trained to perform a particular function by adjusting the values of these weight factors between the neurons, either from the information of outside the network or by the neurons themselves in response to the input. This is the key to the ability of ANN to achieve learning and memory.

The multi-layered neural network is the most widely applied neural network, which has been utilized in the most of the research works for materials science, reviewed by Zhang and Friedrich [6]. Backpropagation algorithm can be used to train these multi-layer feed-forward networks with differentiable transfer functions to perform function approximation, pattern association, and pattern classification. The

* Corresponding author. Tel.: +49-631-2017213; fax: +49-631-2017196.
E-mail address: zhang@ivw.uni.kl.de (Z. Zhang).

0043-1648/03/$ – see front matter © 2003 Elsevier Science B.V. All rights reserved.
doi:10.1016/S0043-1648(03)00149-2

term backpropagation refers to the process by which derivatives of network error, with respect to network weights and biases, can be computed. The training of an ANN by backpropagation involves three stages: (a) the feed-forward of the input training pattern, (b) the calculation and backpropagation of the associated error, and (c) the adjustment of the weights. This process can be used with a number of different optimization strategies.

In the present paper, three polymer examples were considered, i.e. polyethylene (PE), polyurethane (PUR), and an epoxy modified by hygrothermally decomposed polyurethane (EP-PUR). Independent datasets of erosive wear measurements and other characteristic properties of these polymers were used to train and test the designed neural networks. Acceptable ANN predictive qualities were reached, demonstrating that ca. 35–80% of the randomly selected test dataset had a coefficient of determination $B \geq 0.9$ for these three cases, respectively. Ranking of the importance of these characteristic properties to erosive wear rate could offer us some information about which property has a stronger relationship to wear in each case. Predictive results of erosive wear rate of EP-PUR as a function of polymer compositions and erosive test conditions were also presented, which is believed to be of help for a mechanistic understanding of the problem considered.

2. Evaluation

For materials research, a certain amount of experimental results is always required for developing a well-performing artificial neural network. In order to obtain an optimized neural network construction, a total dataset of measurement results:

$$D = \{(P^{(i)}, O^{(i)})|i = 1, \dots, N\} \tag{1}$$

is normally divided into a training dataset,

$$D_{\text{training}} = \{(P^{(i)}, O^{(i)})|i = 1, \dots, M\} \tag{2}$$

and a test dataset,

$$D_{\text{test}} = \{(P^{(i)}, O^{(i)})|i = M + 1, \dots, N\} \tag{3}$$

in which $P^{(i)}$ is the ith input variable selected, whereas $O^{(i)}$ is the ith output parameter for prediction. The total dataset with a number of N has been divided into a training dataset with M data, and, therefore, a test dataset with $N- M$ data. The training dataset is used to adjust the weights of all the connecting nodes until the desired error level is reached. Thereafter, the network performance is evaluated by using the test dataset.

The quality of the prediction can be normally characterized by the root mean square error (RMSE) of the predicted values to the real measured data of the test dataset. The smaller the RMSE of the test dataset is, the higher is the predictive quality.

As an improvement, the coefficient of determination B (also called R^2 coefficient in some literatures) has been introduced to the ANN quality evaluation, which is defined by

$$B = 1 - \frac{\sum_{i=1}^{M}(O(p^{(i)}) - O^{(i)})^2}{\sum_{i=1}^{M}(O^{(i)} - O)^2} \tag{4}$$

where $O(p^{(i)})$ is the ith predicted property characteristic, $O^{(i)}$ is the ith measured value, O is the mean value of $O^{(i)}$, and M is the number of test data. The coefficient B describes the fit of the ANNs output variable approximation curve with the actual test data output variable curve. Higher B coefficients indicate an ANN with better output approximation capabilities.

To avoid any artificial influence in selecting the test data, a random technique could be applied in the selection, and the entire process will be repeated independently for several times (e.g. 50 times). Afterwards the distribution of B values is recorded and the percentage of $B \geq 0.9$ is calculated, since this value is identified as a high predictive quality, i.e. less than 15% of the RMSE of the predicted values. It is clear that higher the percentage of $B \geq 0.9$ is, the better is the quality.

3. Dataset

3.1. Polyethylene (PE) [7]

The dataset of polyethylene contains 55 groups of data, i.e. 11 kinds of PE with various degrees of crystallinity, and impacted with solid erosive particles at five angles, i.e. 15, 30, 45, 60, and 90°. A type of corundum has been applied as the erodent (listed as case 1 in Table 1), and the erosive velocity was constant of 70 m/s and duration was 300 s. Five characteristic properties, i.e. Young's modulus, yield stress, yield strain and fracture energy, as well as the crystallinity (as a structural parameter) were selected as ANN input variables. The erosive rate was the ANN output for prediction.

3.2. Polyurethane (PUR) [7]

PUR database has 54 data with 18 kinds of thermosetting (crosslinked) or thermoplastic PUR, as well as three erosive impact angles, i.e. 15, 30, and 90°. The erodent was still the corundum, and the erosive velocity and duration were as the same as PE. Tensile stresses at $\varepsilon = 100$ or 300%, failure

Table 1
Summary of erodents and their erosive test conditions for EP-PUR [7]

S. no.	Erodent	Size (μm)	Mass flow rate (kg/s)	Velocity (m/s)
1	Corundum	60–120	0.015	70
2	Corundum	120–240	0.032	102
3	Steel grit	120–300	0.039	60
4	Glass beads	150–300	0.036	75

stress and strain, glass transition temperature (T_g), damping at T_g, hardness, density, as well as the thermal expansion coefficient were additional input variables for predicting the erosion rate, which is the ANN output parameter.

3.3. *Epoxy modified by hygrothermally decomposed polyurethane (EP-PUR) [7,8]*

Mechanical performances of epoxy resins can be varied in a very broad range by modifying with tough PUR. With various PUR amounts of EP-PUR system polymers, different properties can be reached between those of crosslinked thermosets and rubbers. In the present case, the weight content of epoxy (or PUR) as well as some mechanical and thermal parameters was considered as ANN input variables. The weight amount of PUR varies from 0, 20, 40, 60, to 80%. The characteristic properties considered include density, mean molecular mass between crosslinks, glass transition temperature (T_g), rubbery plateau modulus and onset temperature, crosslink density, and fracture energy. Four erosive impact angles, i.e. 30, 45, 60 and 90°, were applied, and four types of erodents were employed. Therefore, the whole dataset of EP-PUR contains 80 independent groups of data. The duration was 60 s for all the erosive measurements. Details of the erodents and their erosive conditions, i.e. mass flow rate and velocity, were summarized in Table 1.

4. Results and discussions

4.1. *Predictive quality*

In order to analyze the predictive quality, a similar ANN configuration was used for all three datasets mentioned above. The ANN configuration used for PE is of

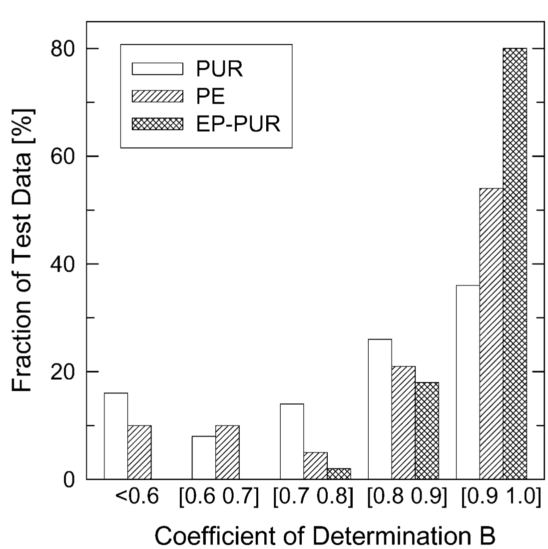

Fig. 1. Dependence of the percentage of test data on the B value of all three datasets.

Table 2
Ranking of importance of input variables to erosive wear of polyethylene (PE) predicted by ANN[a]

Ranking	Input variables [7]	Percentage of $B \geq 0.9$ (%)
1	Yield stress (MPa)	72
2	Young's modulus (MPa)	44
3	Crystallinity (%)	39
4	Yield strain (%)	12
4	Fracture energy (kJ/m^2)	12

[a] Erosive impact angle and one of the input variables in this table were applied as ANN input to predict the erosive wear rate using a 2-[25]-1 structured neural network, which contains 25 neurons in its hidden layer. The coefficient of determination was calculated according to Eq. (4), and the percentage of $B \geq 0.9$ was applied for ranking.

Table 3
Ranking of importance of input variables to erosive wear of polyurethane (PUR) predicted by ANN[a]

Ranking	Input variables [7]	Percentage of $B \geq 0.9$ (%)	Percentage of $B \geq 0.8$ (%)
1	Loss factor at T_g	23	43
2	Failure strain (%)	15	36
3	Failure stress (MPa)	13	34
4	Hardness (Shore A)	12	31
5	Stress σ at $\varepsilon = 300\%$ (MPa)	9	22
6	Density (g/cm^3)	7	28
7	Stress σ at $\varepsilon = 100\%$ (MPa)	7	28
8	Thermal expansion coefficient ($\times 10^{-1}$ K^{-1})	6	28
9	Glass transition temperature T_g (°C)	5	19

[a] Erosive impact angle and one of the input variables in this table were applied as ANN input to predict the erosive wear rate using a 2-[25]-1 structured neural network, which contains 25 neurons in its hidden layer. The coefficient of determination was calculated according to Eq. (4), and the percentage of $B \geq 0.9$ (additionally with $B \geq 0.8$) was applied for ranking.

Table 4
Ranking of importance of input variables to erosive wear of epoxy modified by hygrothermally decomposed polyurethane (EP-PUR) predicted by ANN[a]

Ranking	Input variables [7,8]	Percentage of $B \geq 0.9$ (%)
1	PUR content (wt.%)	84
2	Epoxy content (wt.%)	82
3	Density (g/cm^3)	77
4	Mean molecular mass between crosslinks (g/mol)	72
5	Fracture energy (kJ/m^2)	72
6	Rubbery plateau onset temperature (°C)	72
7	Glass transition temperature (°C)	60
8	Rubbery plateau modulus (MPa)	28
9	Crosslink density ($\times 10^{20}$ cm^{-3})	22

[a] Erosive conditions, i.e. impact angle, mass flow rate, and velocity of erodents, as well as one of the input variables in this table were applied as ANN input to predict the erosive wear rate using a 4-[25]-1 structured neural network, which contains 25 neurons in its hidden layer. The coefficient of determination was calculated according to Eq. (4), and the percentage of $B \geq 0.9$ was applied for ranking.

the form 6-[25]-1, in which all six parameters mentioned in Section 3.1 were applied as ANN input, and the erosive wear rate as the output. The ANN hidden layer possesses 25 neurons. Bayesian regularization (BR) [9] has been used as a neural network training algorithm, which is desirable to determine the optimal regularization parameters in an automated fashion. For PUR, five characteristic properties selected from the nine parameters given in Section 3.2 constituted its input dataset together with the erosive impact angle. In the case of EP-PUR, the input dataset was composed by the weight content of epoxy and PUR, as well as three erosive conditions, i.e. impact angle, mass flow rate and velocity of erodents.

Fig. 1 gives a bar chart for comparing predictive qualities of all the three datasets, in which about 15% of the data in each dataset has been used for testing. The *x*-coordinate of Fig. 1 refers to the *B* value distribution from the range less than 0.6 to that between 0.9 and 1.0. The *y*-coordinate represents the percentage of how many *B* values falling in this range in a 100 times randomly selection of test dataset. The higher the bar chart in the range of 0.9–1.0 is, the better is the predictive quality. Acceptable ANN predictive qualities were reached for all these three cases, demonstrating that ca. 35–80% of the randomly selected test dataset had a coefficient of determination $B \geq 0.9$, respectively. It is clear that the dataset of EP-PUR performs the best quality, which may be due to: (a) the largest number in the dataset, and (b) polymer compositions as input parameters which have a stronger correlation to the wear rate. A mixture of thermosetting and thermoplastic PUR in one dataset could be a reason that the worst predictive quality for PUR was observed.

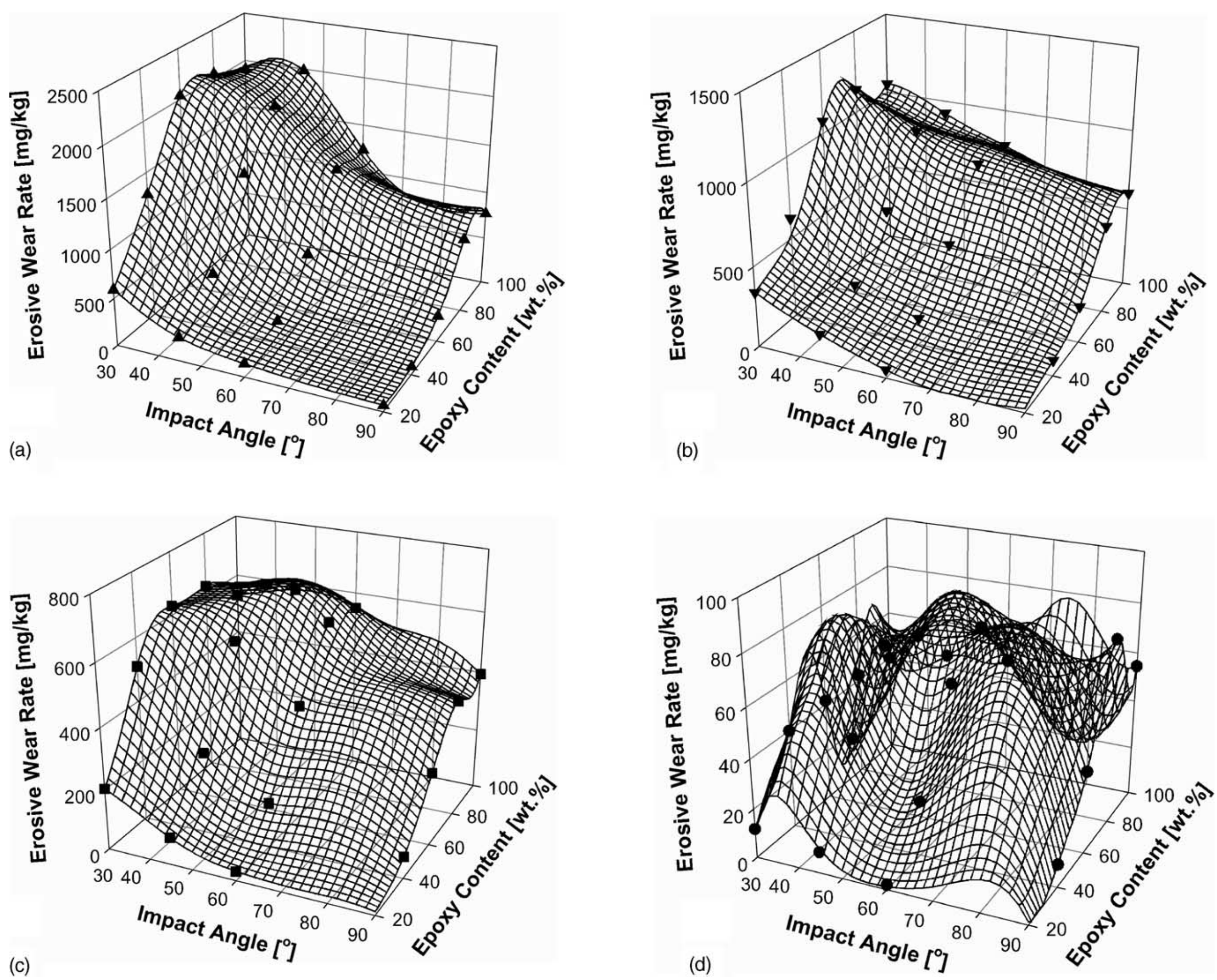

Fig. 2. Erosive wear rate of an epoxy modified by hygrothermally decomposed polyurethane (EP-PUR) as a function of epoxy weight content and impact angle of solid particle. Dots are experimental data, whereas the rest of the 3D-plane was calculated by an artificial neural network approach. (a) Erodent: corundum, size: 60–120 μm; (b) erodent: corundum, size: 120–240 μm; (c) erodent: steel grit, size: 120–300 μm; (d) erodent: glass beads, size: 150–300 μm.

4.2. Importance of input variables

In order to investigate the correlations between erosive wear rate and characteristic properties of these polymers, each characteristic property was used only with the necessary erosive conditions together as input variables for training the ANN. The qualities were analyzed by the percentage of $B \geq 0.9$, which were used to rank the importance of these characteristic properties to erosive wear as summarized in Tables 2–4 for various polymer examples.

In the case of PE, the yield stress displays a stronger dependence to erosive wear compared to other four properties in Table 2. A similar effect was also discussed by Friedrich [3]. Yield strain and fracture energy show weak influences to erosive wear of this polymer. For PUR, it was concluded by Barkoula [7] that a lack of correlation among PUR chemical, mechanical properties and erosive resistance was found. This result can be even confirmed by the low ANN predictive qualities in Table 3. Percentages of $B \geq 0.8$ were applied additionally for ranking. To combine the thermosetting and thermoplastic PUR data into one dataset may also reduce the predictive quality. Nevertheless, the high ranking of the mechanical loss factor suggests that the damping behavior may be the key aspect. In the case of EP-PUR, it is clear in Table 4 that material compositions, i.e. epoxy and PUR weight content, present the strongest correlation with wear performance, in which a similar effect was also found by Zhang et al. [5] for the ANN prediction of polymer composites. Density holds the second important position due to its strong relation to compositions. Mean molecular mass between crosslinks (M_c) and fracture energy (G_c) exhibit a similar quality, which may be explained by the linear dependence of G_c to $M_c^{1/2}$ [7,8]. The combinative effect of density and M_c may reduce the influence to erosive wear of rubbery plateau modulus and crosslink density.

Importance analysis by ANN attempts to investigate the possible correlations between some simple measured parameters (e.g. modulus, strength and failure strain) to more complex properties (e.g. wear), which will be of additional help to materials research for mechanistic understanding. The simple properties normally are easier to obtain than the complex ones, and therefore the success of prediction could be of benefit to reduce the number of more complex experiments.

4.3. Parameter studies

It is ideal when only material compositions and testing conditions serve as ANN input data in the case of EP-PUR. A well-trained ANN is expected to be very helpful to predict the material properties before manufacturing/testing the real materials. A look at the current situation in Fig. 2 shows that the predictive results exhibit an excellent match to the real measuring data. Fig. 2a-d exhibit as three-dimensional (3D)-planes the predictive results of the erosive rate as a function of epoxy weight content and impact angle of solid particle for four types of erodents, mass flow rates and velocities mentioned in Table 1, respectively. Compared to the real test results (dots in Fig. 2), the predictive results are very well acceptable. All these results predicted from one well-trained ANN, and various erodents were recognized by their mass flow rate and velocity. It is clear that once a well-trained ANN has been obtained, new data can be predicted without performing too many, long lasting experiments. For the first three erodents, presented in Fig. 2a-c, the lowest erosive wear rates are found with the lowest epoxy content and at erosive angle of 90° in each case. High erosive wear plateaus are found around 80 wt.% of epoxy. For the erodent of glass beads, the dependence of erosive wear is so complicated that an additional contour plot of Fig. 2d has to be given as Fig. 3, predicted by ANN as well. Even though the ANN approach is only a phenomenological method, a well-trained ANN is believed to be also of help for a mechanistic understanding of the problem considered.

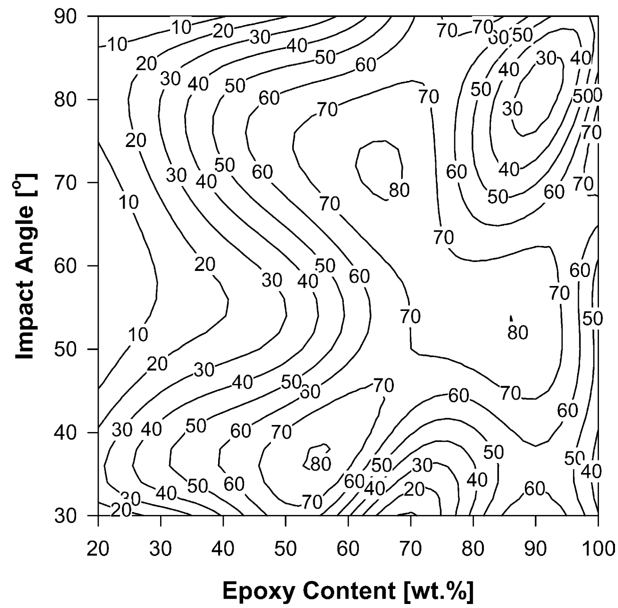

Fig. 3. Contour plot of erosive wear rate of EP-PUR predicted by ANN as a function of epoxy weight content and impact angle of solid particle. Erodent: glass beads, size: 150–300 μm.

5. Conclusions

Based on this work devoted to predicting the wear performance of the indicted polymeric systems by adopting the method of artificial neural networks, the following conclusions can be drawn:

- Ranking of the importance of characteristic properties to the erosive wear rate could offer some information about which property has a stronger relationship to wear of polymers.

- ANN is a helpful mathematical tool in the property analysis and prediction of polymers, being directly based on a limited number of measurement results.

Acknowledgements

The project was supported by the Alexander von Humboldt Sofja Kovalevskaja Award program, financed by the German Federal Ministry of Education and Research (BMBF) within the German Government's "ZIP" program for investment in the future.

References

[1] S.N. Ratner, I.I. Farberoua, O.V. Radyukeuich, E.G. Lure, Correlation between wear resistance of plastics and other mechanical properties, in: D.I. James (Ed.), Abrasion of Rubber, MacLaren, London, 1967, pp.145–154.
[2] J.K. Lancaster, Friction and wear, in: A.D. Jenkins (Ed.), Polymer Science and Material Science Handbook, North Holland, London, 1972 (Chapter 14).
[3] K. Friedrich, Erosive wear of polymer surfaces by steel ball blasting, J. Mater. Sci. 21 (1986) 3317–3332.
[4] K. Velten, R. Reinicke, K. Friedrich, Wear volume prediction with artificial neural networks, Tribol. Int. 33 (2000) 731–736.
[5] Z. Zhang, K. Friedrich, K. Velten, Prediction on tribological properties of short fiber composites using artificial neural networks, Wear 252 (2002) 668–675.
[6] Z. Zhang, K. Friedrich, Artificial neural network applied to polymer composites: a review, Comp. Sci. Technol., in press.
[7] N.-M. Barkoula, Solid particle erosion behavior of polymers and polymeric composites, in: M. Neitzel (Ed.), IVW Schriftenreihe Bd. 29, Institut für Verbundwerkstoffe GmbH, Kaiserslautern, Germany, 2002 (ISBN-3-934930-25-5).
[8] N.M. Barkoula, J. Gremmels, J. Karger-Kocsis, Dependence of solid particle erosion on the cross-link density in an epoxy resin modified by hygrothermally decomposed polyurethane, Wear 247 (2001) 100–108.
[9] H. Demuth, M. Beale, Neural Network Toolbox User's Guide—For Use with MATLAB, The MathWorks Inc., Version 4.0, September 2000.