Hierarchical Clustering Analyses of MTS Glow Curves

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Abstract

The aim of this research paper is to study the parameters which indicate changes in the TL materials' microstructure when exposed to irradiation. To this end we perform glow curve deconvolutions of the MTS dosimeters in the R programming language, using the OTOR model based on the Lambert W function. The obtained parameters of the activation energy and the ratio between retrapping and recombination probabilities are then used as input parameters for hierarchical clustering analyses from which unusual properties of the dosimeters have been observed.

Keywords: Glow curve analysis, OTOR model, hierarchical clustering analysis

1. Introduction

Thermoluminescence (TL) is a luminescence phenomenon of an insulator or semiconductor which can be observed when the solid is thermally stimulated, and there is a considerable literature which describes TL in detail [1,2]. TL is characterized as thermally stimulated emission of light following a previous absorption of energy from radiation. The necessities of one material for TL production can be perceived as follows. Firstly, the material must behave as an insulator or a semiconductor, as metals do not exhibit luminescent properties. Furthermore, the material must contain absorbed energy following a prior exposure to ionising radiation. Finally, the material should be capable to release its stored energy, absorbed from the exposure to ionising radiation, when exposed to heat.

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An explanation of the observed TL properties can be obtained from the energy band theory of solids. For further reading the reader is referred to [2]. The model in TL, which consists of two levels, i.e. the electron traps and recombination centre, is known as the One-Trap-One Recombination-Centre model (OTOR model). For a rather extensive description on this subject matter the reader is referred to [4]. A large variety of models enabled the investigation of different TL dosimeters and their parameters. Researchers developed dozens of approaches to monitor the changes of the dosimeters' parameters, and thus address the challenges brought forward by the obtained experimental data. Usually, however, the change of the parameters' values needed to understand changes within the microstructure of the materials, and primarily the TL phenomenon itself, cannot be captured by just applying these models, as most of the conclusions are based on assumptions rather than a correlation of the similarities and dependence of the changes with the materials properties. Therefore, much of the complexity in the analysis of the glow curves remains unexplained, and if it relies strictly on assumptions, it could never be fully explained, nor understood.

In this paper we perform deconvolution of TL glow curves according to the OTOR model in order to retrieve the activation energies and the ratios between retrapping and recombination probabilities (R values) for each peak of MTS100, MTS600 and MTS700 dosimeter disks. Afterwards, we perform hierarchical cluster analyses on the abovementioned parameters in order to examine the dependence of the measurement procedure and the dose with the changes in the material's microstructure and provide an outlook of the physical meaning corresponding to each change. Finally, we present an innovative approach in glow curve analysis in hope for a further application of different machine learning techniques for glow curve analysis.

2. Materials and methods

Glow curves from MTS standard TL dosimeter disks were obtained by using the Risø TL/OSL DA20 reader with BG9 filter. Then, glow curve deconvolution based on the semi-analytical expression derived from the OTOR model was performed [4]. The deconvolutions were obtained by using the “tgcd” package in R [6]. The activation energy was set in the range from 0.001 eV to 5 eV. The abovementioned model was formed on the assumption that there is a greater probability for recombination than retrapping, i.e. $A_n < A_m$. The quality of the fitting was measured using figure of merit (FOM).

The MTS100, MTS600 and MTS700 dosimeter disks were irradiated with 1 Gy and 50 Gy each and were measured with two procedures. In the first procedure the MTS dosimeters were annealed at 400 °C for 1 hour in nitrogen atmosphere followed by rapid cold, then 100 °C for 2 hours, then irradiated with Sr-90 beta source and eventually read out with a heating rate of 2 °C/s. The second procedure differs from the first one in one additional step: a preheat step, where following the irradiation process, the dosimeters were preheated at 100 °C for 10 minutes. The obtained FOM values for the glow curve deconvolutions were in the range from 0.3% to 0.92%. The deconvolutions are presented in Figures 1-3.

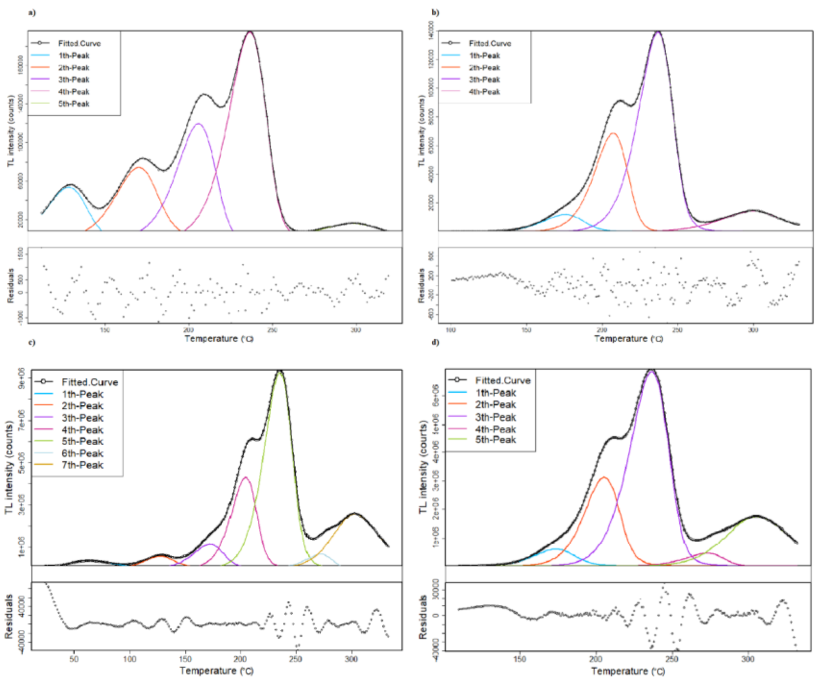

Fig. 1. Glow curve deconvolution of MTS100 treated with no preheat at 1 Gy (FOM: 0.52%) an9d 50 Gy (FOM: 0.52%) a), c) and MTS100 treated with preheat at 1 Gy (FOM: 0.63%) and 50 Gy (FOM: 0.63%) b), d) representatively.

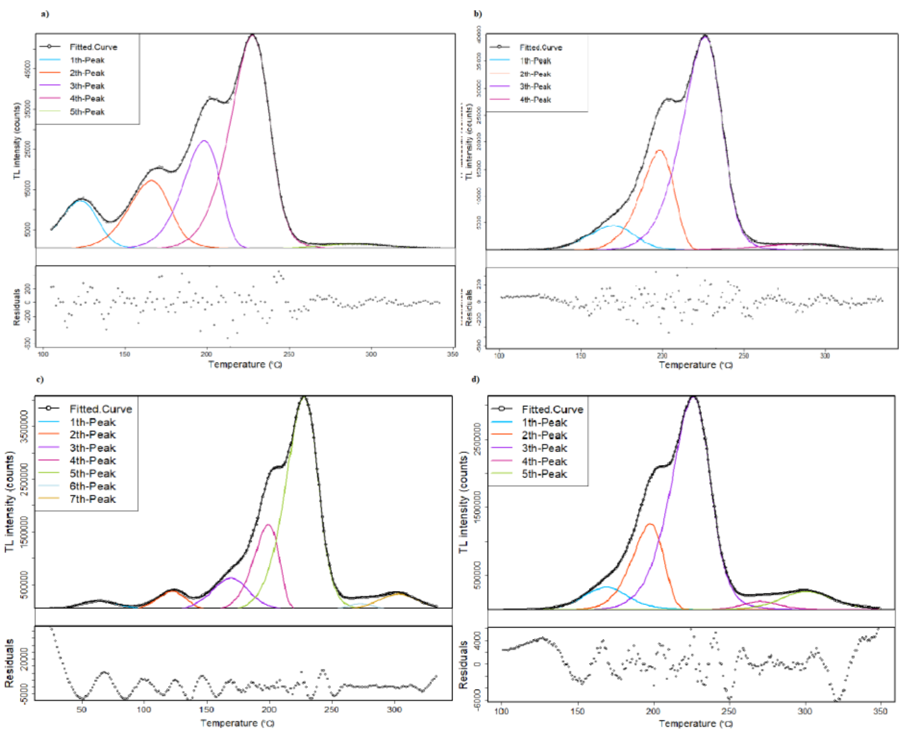

Fig. 2. Glow curve deconvolution of MTS600 treated with no preheat at 1 Gy (FOM: 0.72%) and 50 Gy (FOM: 0.55%) a), c) and MTS600 treated with preheat at 1 Gy (FOM: 0.83%) and 50 Gy (FOM: 0.30%) b), d) representatively.

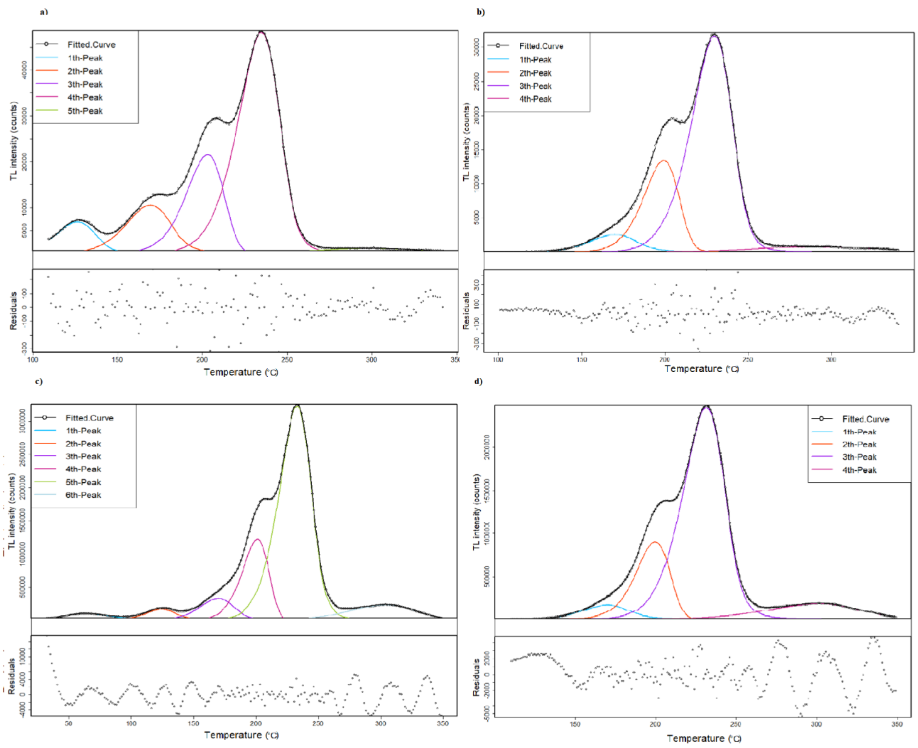

Fig. 3. Glow curve deconvolution of MTS700 treated with no preheat at 1 Gy (FOM: 0.65%) and 50 Gy (FOM: 0.35%) a), c) and MTS700 treated with preheat at 1 Gy (FOM: 0.92%) and 50 Gy (FOM: 0.30%) b), d) representatively.

3. Hierarchical cluster analyses of MTS dosimeters

Hierarchical clustering is an algorithm which groups objects into groups (called clusters) based on their similarity [7]. The result is a dendrogram, a tree showing the hierarchy of the set of clusters, where the objects in the same cluster are similar to each other, but dissimilar to objects in other clusters. In order to decide which clusters should be combined, a dissimilarity measure needs to be applied. For our data set, we use an agglomerative hierarchical clustering algorithm based on the Euclidian dissimilarity measure, defined as:

$$\|a-b\|_2 = \sqrt{\sum(a_i-b_i)^2},$$

where a and b represent the parameters of the materials, measured with a different procedure and/or irradiated with a different dose.

4. Results and discussion

The results of the hierarchical analysis clustering for the R value can be seen in Fig. 4. Unusual behaviour was observed for the MTS700 irradiated with different doses. Apparently, the R value for MTS700 at 1 Gy treated with both procedures did not have any similarity with the MTS700 at 50 Gy treated yet again with both procedures. The change of the dose drastically changed the R value for MTS700, which was not the case with the other tested dosimeters. Another unusual behaviour was observed for MTS600 treated with preheat at 1 Gy, which did not show similarities in the R value with the rest of the MTS600 tested dosimeters. This behaviour might be a result of the extremely low R values (in the range of 0.003 to 0.101). Identical behaviour was likewise observed for the MTS100 treated with preheat at 1 Gy, where the R values were in the range of 0.013 to 0.262. In conclusion, the preheat step influenced the trapping parameters for these dosimeters. The change of the preheat changed the defect concentration, hence changing the R value of the tested dosimeters. Moreover, the second peak of the other tested dosimeters was detected to have the lowest R value, i.e. $A_n < A_m$. The low R value most likely occurs from the competition among traps, probably arising from a hole trap. Similar conclusion for the fourth peak of MTS100 dosimeters, was also observed and reported [9].

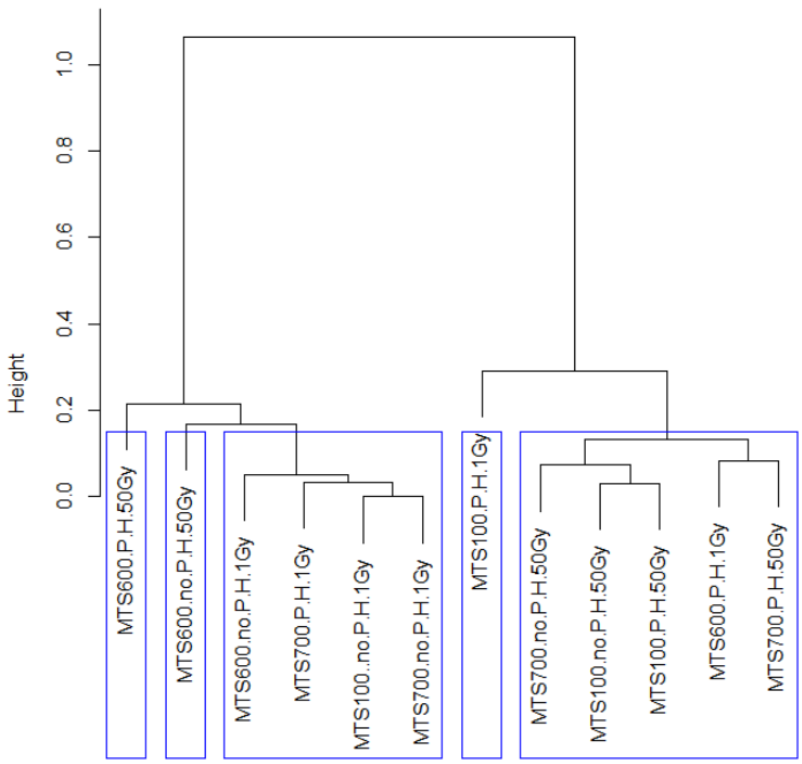

Fig. 1. Cluster dendrogram for the R values

As per the activation energy, the application of preheat in the measurment procedure for all of the MTS dosimeters treated with a dose of 50 Gy did not result in the change of the values of the activation energy, and therefore from the cluster analysis it could be concluded that the preheat step did not influence the binding energy of the trapped charges, and thus did not change the stability of the traps (Fig. 5.). On the contrary, the preheat step caused a significant change of the activation energy's values for all of the MTS dosimeters treated with a dose of 1 Gy. The preheat was initially used for removal of unstable peaks at low tempertures which have faster rates of loss of charge carriers and a greater possibility that the charge carriers would escape from their trapping centers at ambiental temperature, as well as a greater recombination possibility. Therefore, the preheat in our case changed the energy needed to release the electrons from traps to the conduction band. The hirearchical cluster analysis for the activation energy can be seen in Fig. 5.

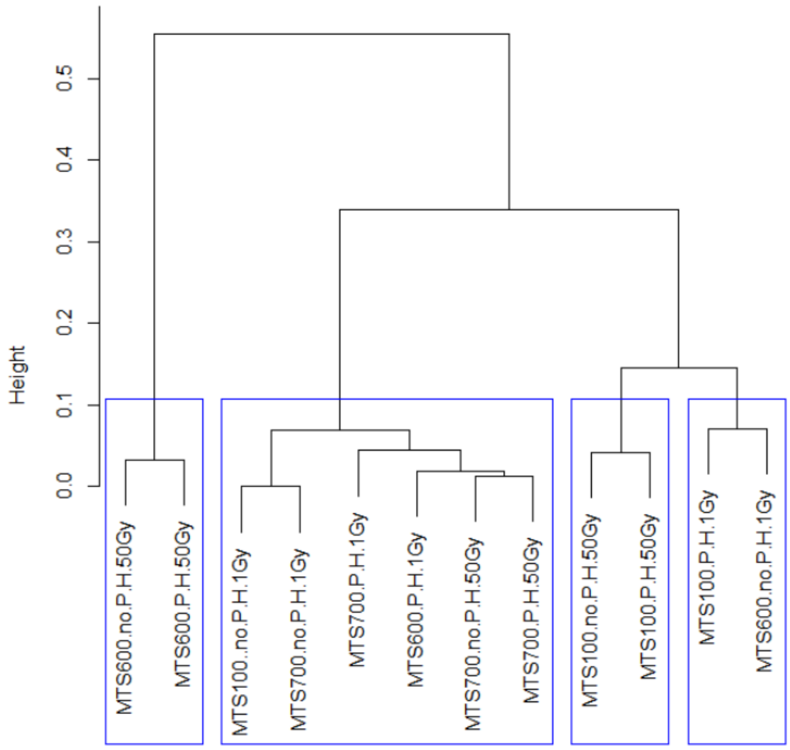

Fig. 2. Cluster dendrogram for the activation energy

5. Conclusion

There are great opportunities in using machine learning for glow curve analysis, as seen in our paper. Machine learning, per se, has already been implemented in many fields of research, such as biology, neuroscience, medicine, economy and others. However, when it comes to glow curve analysis, the application of machine learning is rather low. In particular, performing analyses based on assumptions or drag and drop software programs which do not allow any change in the parameters, not only limit the potential of discovery of new insights of glow curve analysis, but rather reduces the opportunities which may arise. In addition, as machine learning is currently a subject to many research projects, the need for implementation of it in the analysis of glow curves is essential. In this paper, we showed how the implementation of hierarchical clustering, a rather simple machine learning technique, could perform a powerful glow curve analysis. Furthermore, the hierarchical clustering analysis method did not only enable to ask new questions regarding the properties of LiF dosimeters, but showed its superiority in discovering and monitoring changes in the materials' crystal structure. Finally, the prime goal of this paper was to present a new approach in analyzing glow curves, which can hopefully lead to even greater analyses which could aid in understanding of the fundamental physics of MTS dosimeters.

Acknowledgements

The authors would like to thank Dr. Jun Peng for the contribution to this research paper.

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