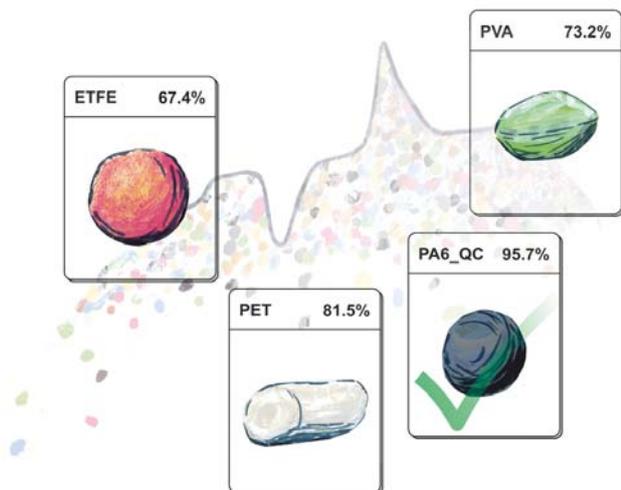


Identify

How this New DSC Curve Recognition System Simplifies Polymer Characterization

Dr. Alexander Schindler



interpretation of DSC curves is significantly simplified by *Identify*, the groundbreaking DSC curve recognition and database system.

With *Identify*, known database curves and literature data are used to recognize and identify unknown DSC curves, ultimately leading to interpretation of the DSC result. The process can be applied to a totally unknown sample or to routine quality control (QC), where *Identify* can show a sample's level of agreement with saved measurements for samples already deemed as acceptable. *Identify* is thus an extremely powerful tool for any day-to-day task such as material identification as well as for quality control and failure analysis. It also serves as an archiving system, since it allows direct access to the evaluated DSC curves stored in the database. And the best for last: *Identify* provides results with only a single click.

Introduction

The brand new NETZSCH DSC 214 *Polyma* makes DSC investigations easier and more comprehensive than ever before. It is comprised of a series of smart innovations which together addresses all aspects of a perfect DSC investigation (see figure 1): The totally new *Arena* furnace and *Corona* sensor in the instrument along with the novel *Concavus* sample pan allow for extremely fast and unique high-quality measurements.

A highlight of the new software is the *Smart-Mode* user interface which greatly facilitates operation. The unique *AutoEvaluation* even allows for completely autonomous evaluation of the measurement – reproducibly and reliably.

The final step in a complete DSC investigation is interpretation of the measurement results. Until now, interpreting DSC curves required both a certain level of experience and a certain expenditure of time – in order to conduct literature research, for example. Now for the first time in the history of thermal analysis,



1 All aspects (360° view) of a complete DSC investigation

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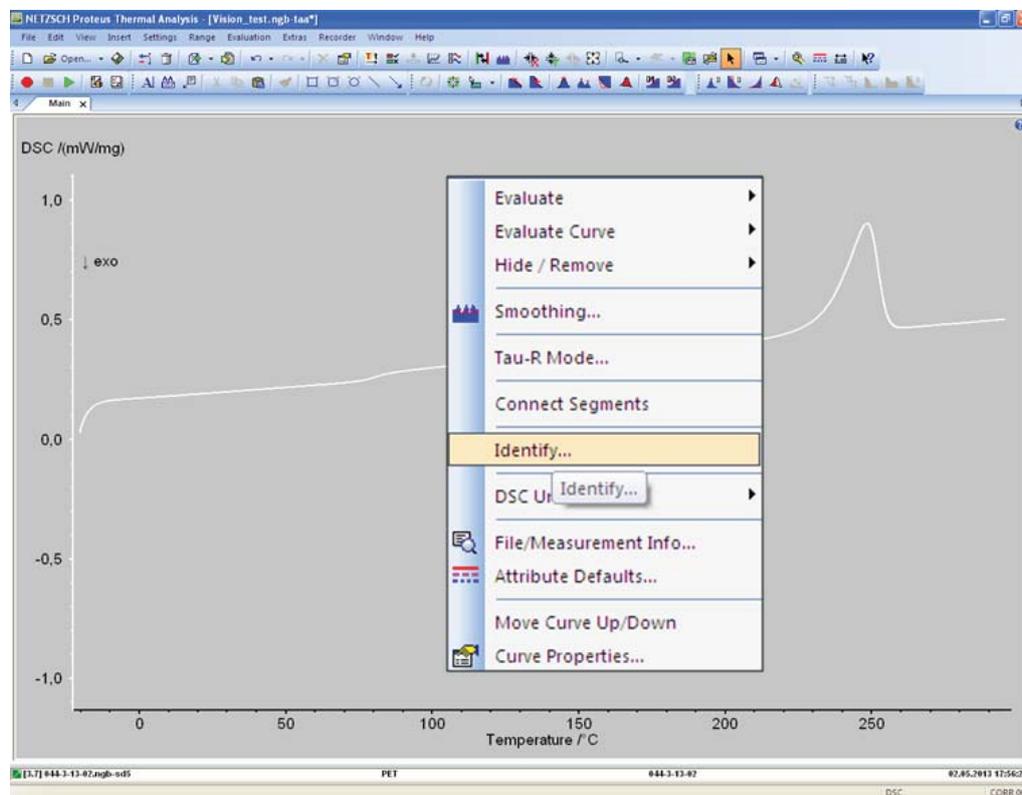
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As a basis for the database, libraries with measurements and literature data from the NETZSCH “Thermophysical Properties of Polymers” poster are supplied. Users can additionally create and manage libraries and classes of their own incorporating their own measurements and their knowledge, too.

Material Identification

Figure 2 illustrates how *Identify* is executed on a non-evaluated DSC curve. With a single click, the DSC curve

is autonomously evaluated by the NETZSCH *Proteus*® software using *AutoEvaluation*, and the *Identify* results are immediately displayed (see figure 3): The hit-list on the left shows measurements and literature data from the database sorted according to their similarity to the unknown DSC curve. On the right, a second hit-list indicates the similarity between the “unknown” and defined classes which are explained in detail below. In this example, the glass transition around 80°C and the melting peak around 250°C detected in the unknown DSC curve clearly allow the measured sample to be identified as PET.



2 Applying *Identify* to a non-evaluated DSC curve with a single click

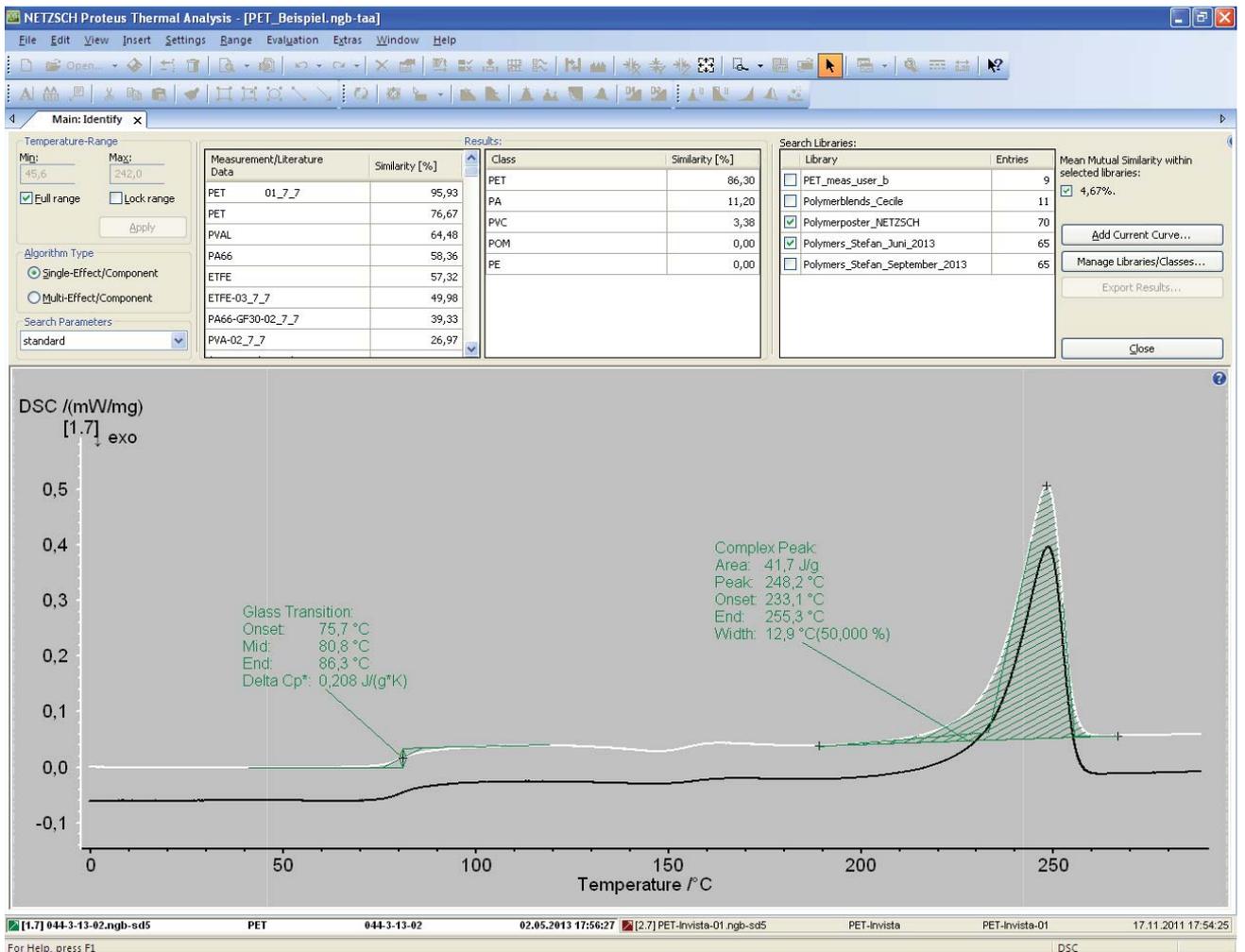
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Results:

Measurement/Literature Data	Similarity [%]
PET 01_7_7	95,93
PET	76,67
PVAL	64,48
PA66	58,36
ETFE	57,32
ETFE-03_7_7	49,98
PA66-GF30-02_7_7	39,33
PVA-02_7_7	26,97

Class	Similarity [%]
PET	86,30
PA	11,20
PVC	3,38
POM	0,00
PE	0,00



3 Identify results after only one click on a DSC curve; the white line represents the unknown curve, the black line the most similar database curve.

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How Does *Identify* Work?

Identify uses an approach very similar to that employed by modern image recognition software for identifying persons or objects (see figure 4). This approach can be divided into three main tasks:

1) Segmentation of the DSC Measurement Curve

Significant caloric effects like glass transitions or exothermic and endothermic effects must be identified and distinguished from irrelevant parts of the DSC curve. This extraordinarily challenging task is performed reliably for most of measurements by *AutoEvaluation* – without any user interaction required.

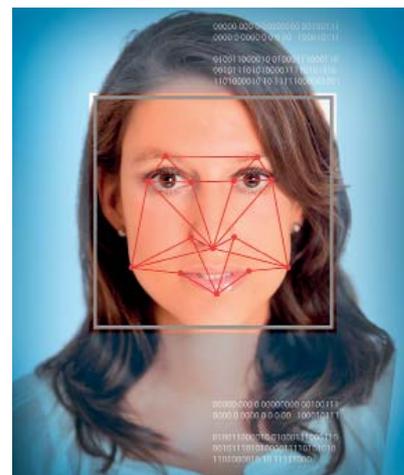
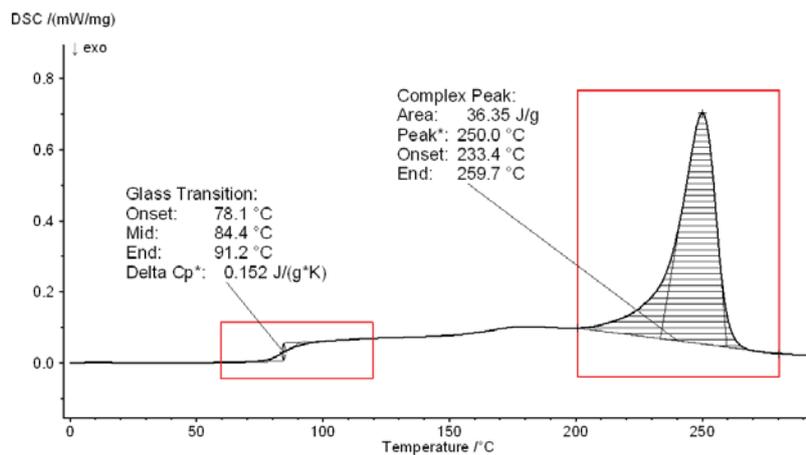
2) Extraction of the Properties of the Effects Found

Properties such as the extrapolated onset temperature or peak area are evaluated automatically using the classical features of the NETZSCH *Proteus*® software (according to known DIN or ASTM standards).

3) Recognition of the DSC Curve

The unknown DSC curve is compared not only to specific database measurements and literature data but also to classes of each. Similarity values are computed practically in-situ using advanced mathematical algorithms. The database “hits” are sorted by similarity (in decreasing order).

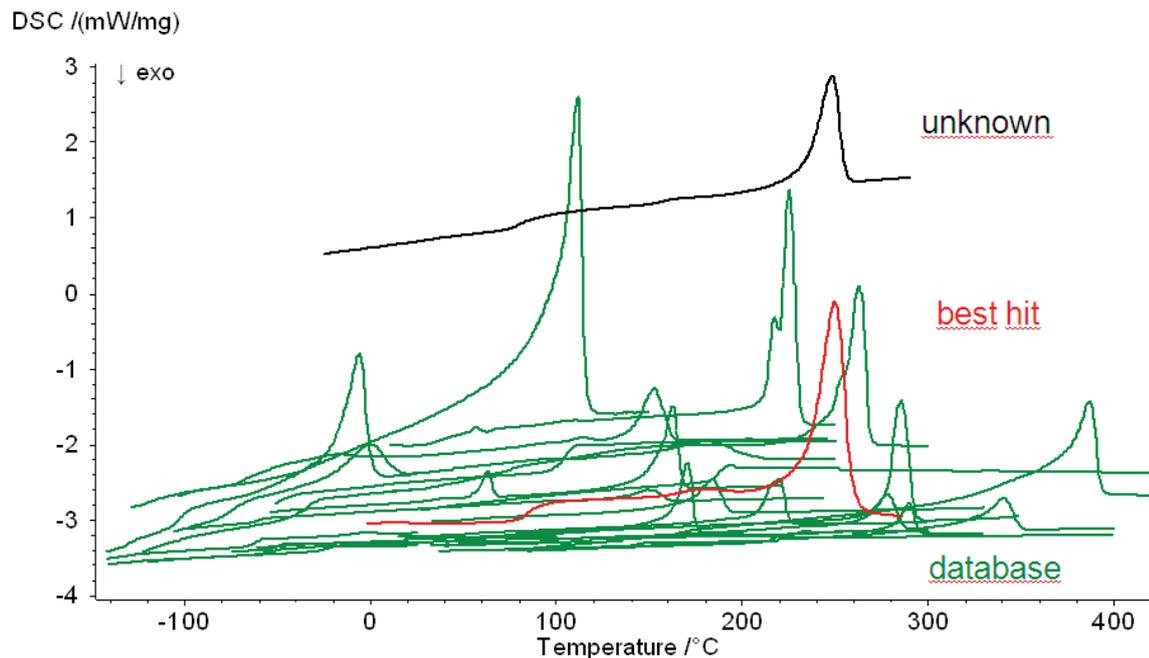
Of course, it is also possible to use manually evaluated DSC curves in *Identify* or to modify the results supplied by *AutoEvaluation*. Then, task 1) would be carried out at least in part by the user.



4 Approach used by *Identify* – based on image recognition.

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5 An unknown DSC measurement curve in comparison with some database curve examples. The most similar curve is labeled "best hit".

Thanks to this new curve recognition technology, *Identify* can search through hundreds of database entries and – within a single second – find the DSC measurement curves most similar to the unknown sample, as illustrated in figure 5. All it takes is just one click.

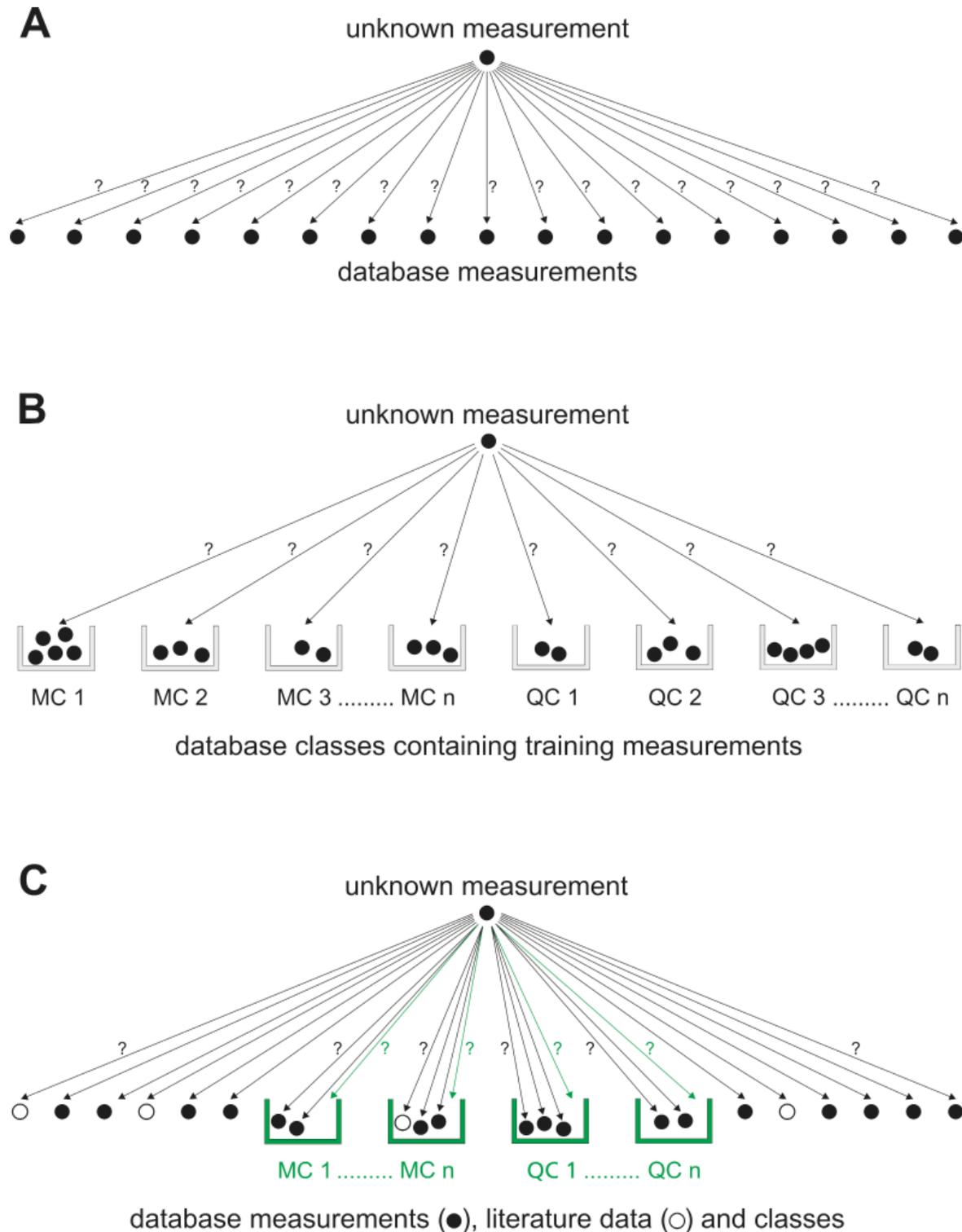
In addition – as already mentioned – effect-based algorithms allow *Identify* to work not only with true measurement results, but also with literature data as library entries.

Identify, however, is more powerful even than that. Different general approaches to database searches are displayed schematically in figures 6A and 6B. One approach is to use queries, which would compare the unknown curve to database measurements on a one-on-one basis (6A). Another is to apply classification, which would assign the unknown curve to a certain class which had been pre-defined by means of training measurements (6B).

Such classes might be material classes (MCs) containing, for example, all measurements obtained for any PA6 polymer samples. Quality classes (QCs) would contain, for instance, only those PA6 measurements stemming from "good" parts which successfully passed quality control. The solution used by *Identify*, illustrated in figure 6C, applies both queries and classifications where a single measurement might even belong to several classes at the same time. Some material classes such as PE or PET are already included in the software, but users can additionally create their own classes, which will "learn" as each new member is added. Such classes also incorporate user knowledge and expertise into *Identify*, whereas query results do not apply any such knowledge. Those depend – if *AutoEvaluation* was employed – only on the measurement result and in no way on the user, ensuring that the evaluations and interpretations so yielded are purely objective.

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6 Different approaches to a database search: Queries (A), classification (B) and the *Identify* solution (C), which applies both

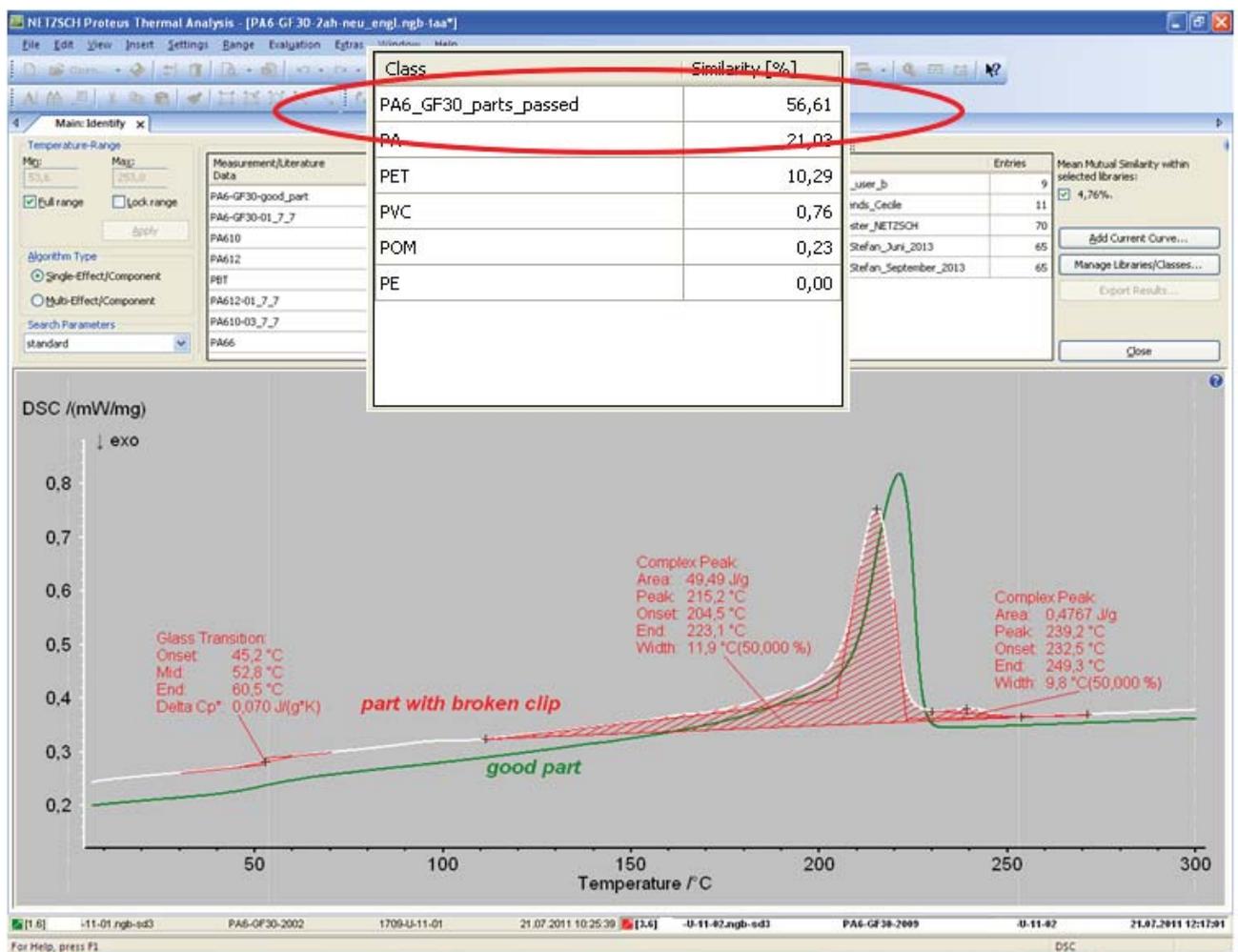
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Application in Quality Control

Identify is also highly beneficial in a quality control setting. Figure 7 depicts the use of a quality class within *Identify* to analyze a DSC measurement on a rejected PA6 part (with broken clip). The melting peak of the defective part is at a lower temperature than that of the good parts, and an additional small peak was detected at 239°C. The calculated similarity to the user class "PA6_GF30_parts_passed" was thus relatively low (only 56.61%).

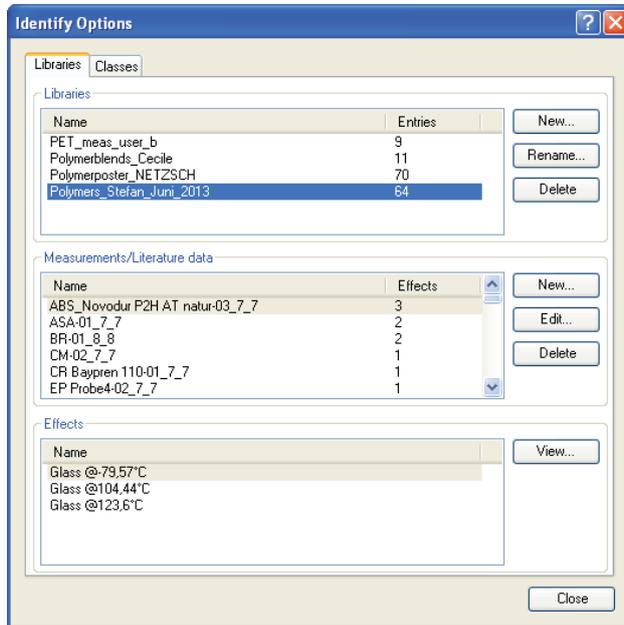
It can be concluded that the bad part is not pure PA6, but most probably a blend of different PA types such as PA6 and PA66. This particular case is a typical failure analysis, since the rejected part was already broken. It is clear, however, that routine quality control on both raw materials and final products using the DSC 214 *Polyma* with the *Identify* software as a standard tool can minimize product failures in the field.



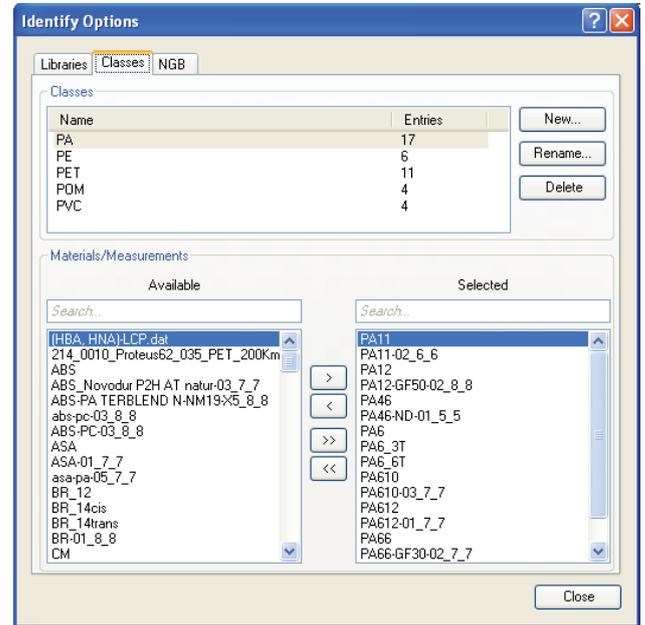
7 DSC measurement on a rejected PA6 part (with broken clip) analyzed by means of *Identify*

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8 Management of libraries, measurements and literature data under *Identify* options



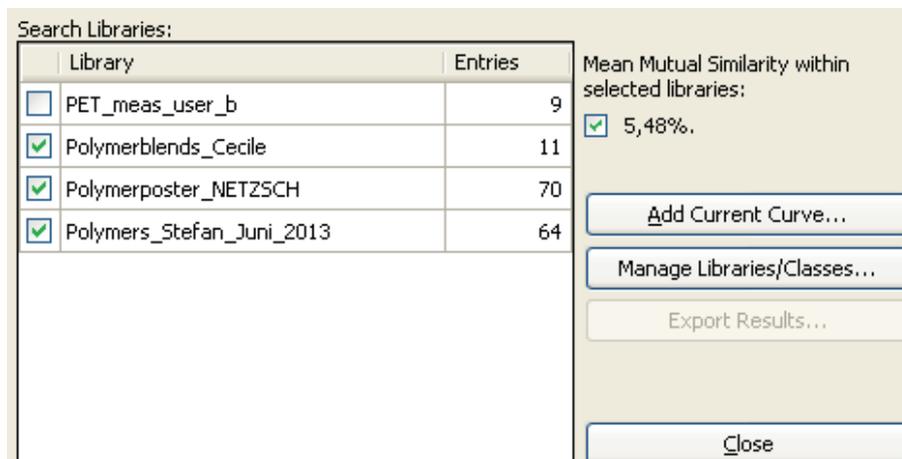
9 Management of classes under *Identify* options

Employment and Optional Settings in *Identify*

Although *Identify* is sophisticated and powerful, it is also very easy to use. Results appear after just one click and, with regard to the management of libraries (creation and extension) and their entries, everything is accessible at a glance, as can be seen in figure 8. It is also very comfortable to manage users' classes. Figure 9 displays how available measurements and literature data can easily be

added to or removed from a selected class, particularly when using the alphabetical search filters.

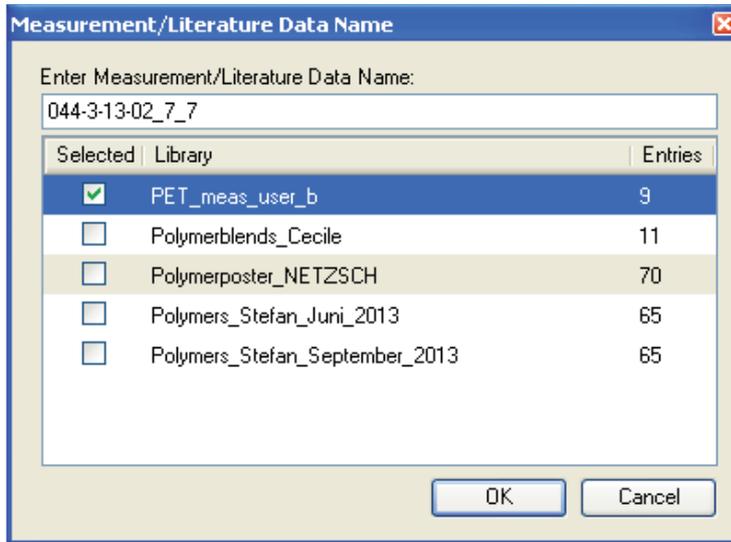
Existing libraries can be easily included or excluded from the search by means of a list with checkboxes (see figure 10) in the main view of *Identify*. Upon changing the choice of libraries, new similarity results are displayed immediately.



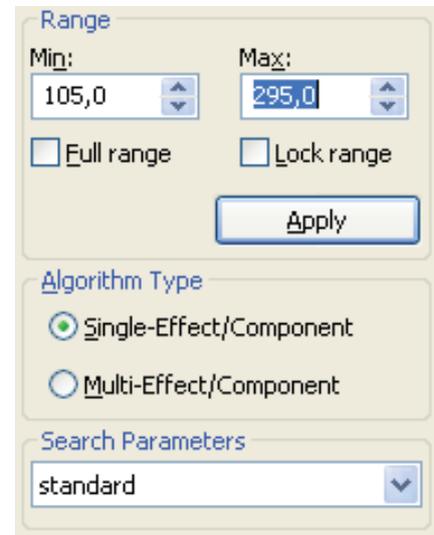
10 Selection of active libraries being included in a search

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11 Dialog after clicking on "Add Current Curve ..."



12 Settings accessible from the main view of *Identify*

Moreover, it is also easy to add a new DSC curve to existing libraries as depicted in figure 11. The program automatically suggests a default name for the library entry derived from the measurement name, which aids considerably in speeding up the process. All that needs to be done is to select the desired target libraries with a check-mark.

Furthermore, some optional settings for optimization of the search results are accessible from the main view of *Identify* as depicted in figure 12. Selection of the temperature range allows for restriction to only certain DSC effects or the disregard of certain parts of the measurement curve. This yields interpretation of individual effects and not only of the entire curve when using "full range". The algorithm types "Single" and "Multi" are used to distinguish between whether the DSC curve stems from a single- or a multi-component sample like a polymer blend. For the latter case, *Identify* assumes that the DSC measurement may actually be resulting from several components. Special parameter settings in addition to "standard", such as "qualitative", "amorphous" or "crystalline", would take into consideration any additional information on the

sample that the user may have. In general, default settings for the algorithm type and parameters are automatically selected – in consideration of the DSC curve.

Summary

In a nutshell, *Identify* ...

- ... is a unique DSC curve recognition and interpretation system providing results with a single click.
- ... is useful for material identification and quality control.
- ... is both easy to use and sophisticated.
- ... includes a database with NETZSCH libraries for polymers as a basis as well as libraries that can be created by the user.
- ... manages measurements, literature data and classes, incorporating the user's knowledge.

The Author

Dr. Alexander Schindler has worked in the fields of experimental physics, thermal analysis and thermophysical property measurements for over 15 years. He is a known expert in thermal characterization methods and their applications.