An Object-Oriented System for Engineering Polymer Information

Thesis

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An Object-Oriented System for Engineering Polymer Information

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Abstract

Issues arising from the development of a computer-based information system for engineering polymer data have been explored.

The system was designed with the aim of providing a user-independent representation of engineering polymers that would organise the data pertaining to them and be amenable to extension and evolution to allow for new materials and new properties.

A classification of engineering polymer materials was developed to provide the structure for the representation, and an existing computer information system was modified in order to accommodate it. The classification was designed to create and order classes of similar materials to enable easy access to their information. Criteria for grouping material grades into families and families into a hierarchy were assessed. Existing polymer classifications were analysed; several alternative approaches to the factoring process are described.

The final taxonomy was implemented within the object-oriented information system POISE, written in the language Smalltalk 80™ [1], [2]. Inherent in the system is a facility to support browsing of general class information. Other tools developed during the course of the project allow the addition and positioning of new classes, grades, properties and data and searching for grades by property value or name.

It was shown that a classification based on criteria of similar chemical structure is a prerequisite for extensibility. Also demonstrated was that no such classification will consistently group together grades that are similar in respect of all of their physical and engineering property data for the uses of engineering designers.

A detailed analysis of the properties used to describe grades of engineering polymer gave an insight into the above dichotomy. To accommodate the resulting conflict, the polymer

information system was enhanced to incorporate an orthogonal factoring at the grade level in addition to that already created by the final classification based on chemical families.

1. Introduction

1.1 Engineering design

Thomas Sheridan of Du Pont [3] identifies engineering design as that part of the design process which involves the selection and application of materials for specific functions according to established engineering principles. He states that:

"The possibilities of engineering design are limited only by (1) the physical property limits of the material, (2) the limitations of the manufacturing process in transforming a material into particular geometries, and (3) the imagination of the designer in combining form and function."

This illustrates how the design of an object is inextricably linked with the properties of its materials. Sheridan espouses the importance of design data: "One way that we, the material suppliers, can help design engineers is by providing engineering design data that characterises and positions our resins in a meaningful way."

The research described in this thesis is concerned with the engineering design information used to describe those materials termed engineering polymers, and the way in which it is presented and disseminated.

Engineering polymer property data are used in many contexts; a generally useful representation of this information is one that can interact with representations of other engineering design perspectives, such as process or geometry. The type of analysis of the information and its organisation offered in this study is essential if a successful interaction with these other perspectives is to be possible.

1.2 Polymers

A polymer is a high molecular mass compound built up from the repetition of small, simple chemical units known as monomers, usually found in the starting material from which the polymer is formed. In some cases the repetition is linear; in other cases the chains are branched or interconnected to form a three dimensional network. The chemical nature of the monomer and the way in which the monomers are joined to one another (the nature of the bonding) together with their spatial orientation all have significant influence on the chemical and physical properties of the resulting polymer. Other factors are also important in determining the properties of the final polymer substance, such as the nature of bonding within the monomer unit, the type of unit occuring at the end of the polymer chain, the degree of polymerisation or chain length, and the molecular mass distribution of the polymeric substance.

Polymer science divides polymers into two broad categories: the biological polymers, which form the foundation of life and occur naturally, and the non-biological polymers, which are produced synthetically. Polymers of the latter type occur in a number of different forms and have a variety of uses. A particular subset of those synthetic polymers that are solids at their use temperature, the engineering polymers, is the area under consideration for the purposes of this research.

1.3 Engineering polymers

The phrase "engineering polymers" refers in this thesis to those synthetic polymeric materials used in a solid state within an engineering context, for example a particular Nylon (polyamide) as used for the manufacture of car parts or a particular PVC (poly(vinylchloride)) as used in the construction of drain pipes and guttering. These materials are commonly referred to as plastics or engineering plastics despite the fact that several texts distinguish "plastics" by their particular thermal response and form, i.e. as separate from elastomers or films. This study concerns all solid, synthetic polymers with relevance to an engineering perspective: plastics materials should be assumed to refer to the engineering polymers as thus described.

The domain of engineering polymers stands to gain from a detailed information analysis for several reasons. These materials are of increasing relevance to current design activity in a number of fields, as plastics succeed metals in a variety of applications (generally because of production, cost or weight criteria). Engineering design is making universal use of computerised assistance as is evidenced by the large numbers of CAD and CAE software packages on the market [4], and materials data are of crucial importance to many of these applications.

The use and organisation of such data for design with metals are well established but plastics are relatively new products. Although the first commercially viable such material, celluloid, came into use in the 1880's [5], the market for plastics was not properly developed until after the second world war when the advent of a highly productive petroleum industry provided the raw materials. Even then plastics were not accepted as a class of potentially high performance materials until approximately thirty years ago.

Engineering polymers are now becoming increasingly popular for unusual and demanding applications and are often tailor-made to fulfil certain functions. They behave in a very different manner from metals, resulting in new challenges for the design process. A wide variety of behaviours, and methods of measuring them, has resulted in vast quantities of published data on engineering polymer materials.

1.4 Engineering polymer data

1.41 The nature of the data

The polymer domain differs significantly from that of metals due to the emphasis on individual material grades (the final commercial product): minor differences in chemistry and molecular structure result in significant differences in observed properties, leading to large numbers of grades, each with a trade name and a unique set of behaviours. This is unlike metals, where small chemical changes to grades result in comparably small changes in property values.

Engineering polymers can take any of a wide range of forms, from structural foams to flexible sheathing for cables. Documenting the behaviour of all of these materials requires a variety of approaches and the information describing them may be presented in a number of different forms, including, for example, mathematical models of engineering response, numerical data, textual descriptions (of appearance or resilience within certain environments, for example) and graphs.

Engineering polymer information may be loosely divided into two types: qualitative and quantitative. Qualitative information is that which can be described in words but is difficult to represent numerically, such as the fact that polystyrenes are easily coloured. Often this information describes groups or families of plastics, applying to many grades. The representation of qualitative information is an important issue and some examples of how this information is currently disseminated are offered in the next section. However the incorporation of this information into the proposed system has not come within the bounds of this study.

The majority of available quantitative information relating to commercial engineering polymers takes the form of properties. A property, most simply, comprises an attribute, such as density or melt viscosity, and a value associated with that attribute for each individual polymer grade. These data are prolific and, historically, presented in the simplest format, often neither recognising important relationships between different properties nor similarities between their values for groups of polymer materials.

Property data may be single value (that is, one datum value for each property quoted for a grade), or multi-point, where a number of values of a property are quoted, illustrating its variation with respect to another parameter such as temperature (usually, in the literature, in the form of graphs or mathematical models). The representation of multi-point data in graphical form is not covered in this thesis as it is not considered to introduce additional issues relevant to the research. The representation of relevant engineering models within an information system does, however, merit consideration and this aspect is introduced in section 2.6.

The large amount of available information relating to engineering polymers [4] can, without consistent data organisation, be confusing for the engineering designer to use. An analysis, from the polymer domain perspective, of the possibilities for improving on existing methods of information organisation has lead to an alternative approach. This has been used to develop a computerised polymer information system, which will be introduced in section 2.7 and described in depth in chapter 4, the implications and testing of which provide the main theme of this research. First, however, existing information formats are discussed in greater depth.

1.42 Examples of existing methods of polymer information organisation

Data pertaining to engineering polymers are usually disseminated by means of supplier data sheets; printed, commercial information on the products of a certain manufacturer, designed to show them in their best light, and distributed on request. The frequency of updates and formats of these are determined by the supplier and are often tailored to different types of user. This results in a wide variation in the form and level of detail of the information. Usually the grades found together on a sheet are of a single "family," as defined by the supplier; this is likely to be a subset of a chemical family, such as polypropylenes, and may comprise grades that are similar because they share an application, because they are of the same form, or because of other reasons deemed important by the manufacturer.

A simple data sheet may comprise nothing more than a table of the values of a number of selected properties for a list of grades. A typical example is the chemical company Hoechst's publication, sheet HFKS 599 E 9060/042: an A4 sized folding leaflet with ten sides of information about their "Hostalen PP" range of polypropylenes. This covers seventy nine grades of Hostalen PP, each designated by a series of three letters and four numbers after the name Hostalen. These grades are linked by little more than their membership of the polypropylene group; four methods of processing (extrusion, blow moulding, compression moulding and thermoforming) are featured and their applications cover a wide range including pipes, films, textiles and tanks.

The values of thirty nine properties are offered for each grade. Each property takes up a row of the table; they have been ordered so that general, mechanical, thermal and electrical properties are grouped together.

The grades head the columns. It is noted that some columns are used for more than one grade, implying that the quoted property values are shared by some of the grades, even though they are named differently. A table on the back of the leaflet describing the processing and applications of each grade explains this: either the use, or the process, or both, differ for grades with different names but the same property values.

This data sheet offers a relatively limited information format: there are no multi-point data, no diagrams, and very little text (which, where it occurs, explains the naming conventions and introduces qualitative information relating to the family as a whole, concentrating on beneficial aspects such as good chemical resistance and high toughness).

At the other end of the spectrum are found more detailed data sheets, for example document no.1-40-01 produced by the Dutch fibre company D.S.M. High Performance Fibres B.V., pertaining to their "Dyneema" products.

This contrasts strongly with the Hostalen data sheet. The document is more expensively produced, being a glossy, colour brochure in A4 booklet format. Again there are approximately ten sides of information, but this time only three grades are covered, namely Dyneema SK60, Dyneema SK65 and Dyneema SK66, all high performance polyethylene fibres. This narrow scope, in terms of both the number of grades and the range of forms and applications, allows a large amount of detail for each grade.

A lengthy introduction to the background and production of the fibres - including product photographs and descriptions of the materials' microstructure with technical diagrams - is followed by the properties. These are introduced category by category. A textual description of the grades' performance in respect of each property is offered together with tables of values, graphs (of stress versus strain for example) and two dimensional plots, such as specific strength versus specific modulus. For each property category, coloured boxes summarise the main points. Sections on the processing and various applications of Dyneema are all accompanied by lengthy written descriptions, data tables where appropriate and photographs.

This clearly provides more in-depth information than the Hoechst document but it does assume that the user is uniquely interested in Dyneema: there is no scope for comparison with other equivalent polyethylene materials or even fibres. The simpler, more economical form of data presentation such as the Hoechst leaflet does have advantages: an overview of all polypropylene grades supplied and broad property, process and application comparisons are easily achieved.

The May 1991 publication by Weston Hyde Products Limited, relating to their "Darvic" PVC (poly(vinylchloride)) sheet products is different again. It covers seven grades of Darvic, some of which may be supplied in different colours, and is a large and professionally produced booklet, of some twenty eight pages, offering considerable detailed information in the form of data, graphs, and text. Large sections of the booklet are given to design, fabrication and shaping descriptions and the grades' resistance to a number (several hundred) of chemicals.

This illustrates how the format of a data sheet is strongly influenced by the products themselves and their eventual applications. The Darvic products are destined for use as containers (both for food and chemicals), glazing, protective shields and engravable signs. Although all common properties are covered and divided into categories, most property values are given for the Darvic range as a whole and not for individual grades. This shows a distinct shift of emphasis from the previous two examples.

The wide variation in available information is apparent and makes comparing grades from the same manufacturer easier than comparing grades from different manufacturers. This may be partly attributed to differences in the style and level of detail in their publications, and partly to different degrees of processing to which their grades are subjected, but also important are points relating to comparability of the information itself. For example, even for grades of similar form, manufacturers will have different priorities for the behaviours they wish to illustrate, and will use different property lists. Problems also arise from the use of different units for properties, and different test methods for establishing those properties.

Other variations between manufacturers' information arise with qualitative data, for example the data relating to resistance to chemicals. In Weston Hyde's Darvic sheet, resistance to each chemical, for the family, is denoted by the codes A, B and C, which denote satisfactory, some attack or absorption, and unsatisfactory, respectively. More specific interpretations of these descriptions are given in preceding paragraphs and the concentrations of chemical for which the code is valid are given in some cases. No exposure time has been given for these tests. By comparison, D.S.M.'s Dyneema sheet quotes resistance to a smaller number of chemicals, at a given pH, by means of a star rating: one star means seriously affected, two means slightly affected and three means unaffected. No further explanations of these descriptions are given but the exposure time is six months in all cases.

So, for a designer seeking information about a number of materials, perhaps in order to make a discriminating decision regarding their selection, the task of comparing manufacturers' printed information is a formidable one, exacerbated by the problems of data incomparability, considered in more detail in section 2.2. This task is usually accomplished by means of preliminary filtering, often based on previous experience of similar products or accepted knowledge, followed by consultation with one or two proposed suppliers or a consultant in the field, such as RAPRA Technology [6]. Problems can arise when assumptions are made on the basis of available data without the expertise necessary to, say, judge the relevance of those data, or to infer the correct information from them.

The use of computers to ease the task of materials selection and comparison is now becoming widespread; a number of materials suppliers and consultants issue their data in magnetic form and a variety of databases and selection software packages have been produced.

These use database formats that provide a model close to the table format of supplier data sheets (see section 2.3). Many invoke simple selection routines based on property values to propose individual grades as appropriate for the user's needs. The grades from one or several companies may be represented on a system, with the widest selection (and the highest price).

usually to be found in the packages sold by independent consultants. In some cases more sophisticated methods are employed with the aim of producing knowledge-based systems. In addition, there is evidence of the increasing popularity of the object-oriented paradigm to be found in some alternative approaches to the materials information representation task. All of these approaches are described in current literature and a critique is given in the Literature Review, chapter 2.

Outside the commercial world of plastics manufacturers, for example in academic research establishments, the emphasis is no longer on property values for individual grades. Equally there is no particular need to group together information about grades made by the same company, or made for similar end uses. Nevertheless the polymer information that is available must still be organised. Some polymer texts and publications introduce various methods of classification as a means of organising information about plastics materials. Many use some form of loose classification to order their chapters. Much of this work is detailed in section 5.2. A number of different classifications, based primarily on the more scientific approach to plastics characterisation, and aimed at the needs of different users, have been identified and analysed.

1.5 The objectives of this study

1.51 The overall task

It was proposed that some of the advantages offered by each of the information dissemination methods described in section 1.42 could be combined if a general, user- and supplier-independent, extensible classification of engineering polymer materials was implemented in a computerised information system existing independently of a database of polymer data. The object-oriented paradigm has a number of advantages to offer in this context, discussed in sections 2.6 and 3.4. It was therefore chosen as the basis for the polymer data modelling software, POISE [2], written in the language Smalltalk 80™ [1], which was partly developed when this study began.

The aims have been firstly, to research a principled classification system for engineering polymers, designed to create useful and practical groupings of the grades to ease the task of seeking information about them, and, secondly, to build appropriately on the design of POISE, so that the classification structure may be implemented within this system.

For the purpose of testing POISE the CAMPUS™ database [7] has been used to provide information on grades of engineering polymers. CAMPUS™ has been developed, populated and maintained by five large polymer suppliers. It therefore contains a large number of commercial grades (over a thousand), is regularly updated, and although it does not provide a complete data set, is fairly representative of the commercial polymer data domain. CAMPUS™ is described in greater detail in section 2.51.

1.52 Dealing with a particular challenge to data representation: property proliferation

The issue of data incomparability has already been raised. Attempts to confront this issue are described in the standardisation literature referenced in the following chapter. Important though this work is, it fails to deal with the fact that there are cases where a specific, unusual or additional property is needed to identify the fitness of a grade for a certain use, when the commonly accepted standard properties - although good for general comparisons - are not helpful.

Convenient and efficient access to those properties excluded from standard formats, in a manner that does not result in useless property specifications for grades not described by them, is an important issue. This is discussed later in the context of the design of the information structure. Highlighted by insights gained from an analysis of property types, the issue has exerted some influence on the final architecture.

2. Literature review

2.1 Perspectives

The context within which any representation of engineering plastics information resides is that of engineering design. Materials information is simply one perspective amongst others in the design environment.

The importance of using multiple perspectives to model design in a way that preserves the particular character of each is discussed elsewhere [8], and contrasted with the dangers inherent in creating systems of mixed perspectives driven by specific user requirements, such as that created by the Alcoa Technical Centre [9]. There it was decided to address the issues associated with having a number of diverse information systems and data formats, which had arisen within the establishment over several years. In order to unify their data sources, standardise the formats and make the data accessible from a number of viewpoints, Alcoa created a conceptual data model, based on hierarchical and network relationships using the software tool "CODE," written in Smalltalk 80™. The backbone of the model was a single hierarchy with five "root concepts" from which all others inherited. These were Application, Data Source, Entity, Material & Surface Property and Process Parameter. Clearly this model is at odds with the policy of separate perspectives employed for this research, for five distinctly different perspectives are merged into a single hierarchy.

In contrast, this study concentrates on the single perspective of engineering polymer materials. Other perspectives relevant to the domain (such as manufacturing process information and product description information) would, if required, be modelled separately (using different class hierarchies) and the design information would be distributed across these different perspectives. If general domain information or calculations are required, properties from different perspectives may have to be combined: a means of achieving this within the object-oriented framework by object-to-object message exchange, known as message delegation, has been developed by Zucker et al [8].

2.2 Polymer data standardisation

It is well known that a major stumbling block encountered during the process of comparing engineering polymer materials is the fact that the data used to describe them are not in comparable forms. This may be because of a trivial reason such as the fact that different units have been quoted, for example dynes/cm^2 for Young's modulus as compared with MPa; it may be that different test conditions have been used to determine the value of a property, such as a different temperature range for the measurement of a coefficient of linear expansion; or it may be that an entirely different property is being used to illustrate some general behaviour, for example the Vicat softening temperature as compared with the crystalline melting temperature.

In an attempt to alleviate this problem a number of organisations have been set up to introduce some uniformity into the type of data that are used to describe a polymeric material, i.e. the properties and the test methods devised to determine values for those properties. The CAMPUS™ database uses a standard list of general engineering properties drawn up by the standards committee for plastics in the German DIN standard no. FNK-UA 102.1. These are the properties most commonly specified for engineering polymers and are listed in Appendix 1. Standard test methods have been drawn up by various national bodies such as ASTM (American Society for Testing and Materials), BSI (British Standards Institution), DIN, (the German standards authority), and also by the international body ISO (International Standardisation Organisation). ISO also runs STEP (Standard for Electronic exchange of data on manufactured Products) which is concerned with standardising aspects of CAD/CAM data exchange [10].

However these efforts have not always resulted in comparable data. Lockett [11] suggests that the reasons for this are that standard tests drawn up by different organisations for the same property may be significantly different, and that each standard permits a significant degree of user choice in the selection of test parameters. He outlines ongoing work by the British Plastics Federation in conjunction with French and German organisations and ISO to "standardise the standards."

It will be years, however, before much of this work comes to fruition, and for the purposes of this research it is proposed that those properties used within the CAMPUS™ database are the nearest to an internationally standard list to be found at present. It is partly for this reason that the CAMPUS™ database has been employed as the provider of real world polymer grades and data within this project.

2.3 Data and databases in general

Frost [12] defines data formally as "the symbolic representation of simple aspects of some named universe of discourse." The emphasis here is on the word simple: data are pieces of knowledge that cannot be reduced further into smaller components. Knowledge is regarded by Frost as being a "model of some named universe of discourse." It is therefore more complex than data.

Much progress has been made in the development of a number of data formats suitable for the electronic storage and retrieval of data, aimed at simplifying and speeding up the task of sifting through large quantities of information.

Frost defines a database as a large collection of regularly formatted data accessed by more than one person and/or used for more than one purpose, and a database system as a set of resources designed to store the database, maintain database security and provide the necessary access facilities. A database system must also have an underlying data structure, that is, a method of arranging the data that is appropriate to the needs of the users or uses of the database and the nature of the data itself. Frost states that there are seven commonly used and accepted data structures, also known as data models, of which three, the entity relationship attribute model, the relational data model, and the hierarchical data model merit discussion here.

The entity relationship attribute model consists of three concepts: entities, values, and relationships. Where an entity has associated with it a value, that value is known as an attribute of the entity, and different entities are linked by relationships. This model is based on the notion that relationships between entities are considered distinct from relationships between entities and values. While this is valid for a number of cases, there are times when it is unclear whether a concept should be termed an entity or an attribute: the definition often depends on the relationship it has with another concept.

The hierarchical model bears considerable resemblance to the above in that it also regards the universe as consisting of entities, attributes and relationships. However there is a clearly delineated architecture for structuring these concepts with respect to one another, with consequences of both greater organisational capability and increased restraints. Entities are related to other entities in inverted tree structures, where the nodes of the tree are the entities and the branches that link them are the relationships between entities. Entities at the "top" of the structure are called roots and may be related to any number of lower-level dependent entities, each of which may be related to any number of lower-level dependents, and so on. If an entity X is a dependent of entity Y, then Y is called the parent of X, and X the child of Y. An attribute is regarded as a property of an entity and may be related to many entities (an entity may also be related to many attributes).

An application of the hierarchical data model to a polymer database might result in something like figure 1:

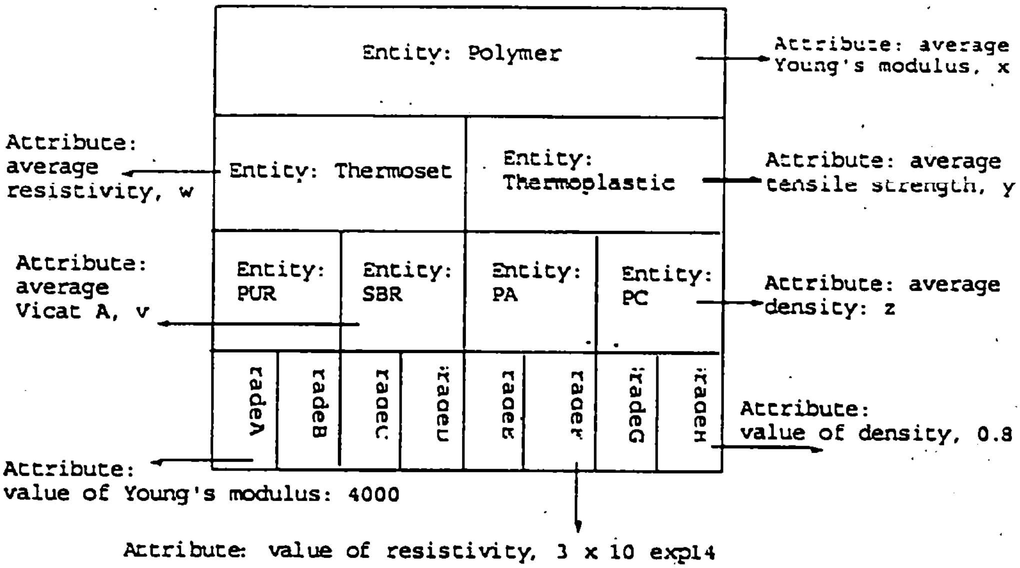

Figure 1: A simple application of the hierarchical model for polymers

Although this would appear to model the polymer world well, there are a number of shortfalls. The main one is that the data structure would be permanently slotted into the prescribed hierarchy and adding to or altering the structure to accommodate new data would be cumbersome, since the attributes and attribute values of each entity would also be fixed. For example, an attribute "average tensile strength" belonging to the entity "thermosets" would remain the same regardless of additional thermosets being added lower in the hierarchy.

The major constraint of the hierarchical view outside the world of polymers, however, is considered to be that entities may not be related to more than one parent entity. Other fallbacks of this model are that the structure implies that relationships between entities have direction, and that things must be classified as either entities or attributes (often an impossible task). The hierarchical model is considered by Frost to be of use only when the situation to be modelled is truly hierarchical and when the required access to and manipulation of the database is also hierarchical, i.e. access to data is most efficient if it involves traversal down through the tree and from the entities to their attributes. Despite this, and the fact that the hierarchical model is not accompanied by a mathematical formalism, it has none the less achieved some popularity for use in appropriate situations.

The most commonly used model today is the relational model, introduced by Codd in 1970 [13]. In this view the universe is regarded as consisting of entities, entity sets and relations. According to Frost [*ibid*] a relation is a set of n-place tuples, each of the form <e1, e2, e3,.......en> where entity e1 belongs to entity set E1, entity e2 to entity set E2, and so on. In other words, each entity in a tuple is of a certain predefined type, and their presence in the tuple indicates a relationship between them. A relation may be represented by a table as illustrated below in the context of polymer material information.

Grade name (Entity set E1)	Density (Entity set E2)	Modulus (Entity set E3)	Resistivity (Entity set E4)
<Superplas	3.2	10,000	5>
<Wonderplas	1.5	15,000	6>
<Duropol	0.8	9,000	7>

Table 1: An application of the relational model to three hypothetical polymer grades.

Here each tuple represents a plastics material grade.

A notable feature of this structure is that each entry in a relation is "flat" : every tuple has an entry for every entity type. This can result in large amounts of redundancy where the same relationship occurs in a number of places. This problem can be overcome by a process of normalisation, which factors out the important dependencies and creates multiple relations (i.e. multiple tables) for a single data set, which are related to each other. This process can be performed by the systematic application of a set of well defined normalisation rules. The resulting structure is relatively symmetrical, compared to the hierarchical model, and acknowledged to be a powerful model capable of accommodating a wide variety of situations.

The relational model has gained considerable popularity due to the similarity between "Codd relations" and mathematical relations, which means that well-defined operations from relational theory can be used to manipulate relational databases. The presence of a mathematical formalism has lead to the construction of query languages that perform valuable selection and joining operations.

Relational databases are therefore employed widely as the basis for the storage and dissemination of polymer materials data, but are considered inappropriate for this application for a number of reasons, discussed in section 3.1.

Both relational and hierarchical models are both essentially rigid structures, where an initial data analysis will permanently decide the arrangement and volume of data. In reality, database systems are often hybrids of the two, containing relational and hierarchical features. Their structure is still fixed, and they possess no algorithmic capabilities.

2.4 Knowledge-based systems

The difference between a knowledge-based system (a KBS) and a database is that a KBS contains knowledge, in the form of rules, in addition to data. This knowledge is used to enhance the information content of the data. KBS research has been described [14] as having the aim of making computers more useful by providing them with some of the attributes of human intelligence. An expert system is one type of KBS, being a computer program that performs a task that represents some limited area of human expertise, and that makes use of stored representations of knowledge as a means of providing solutions and explanations. In the context of materials data KBS systems, described in the following section, knowledge is used to interpret and compare the data, usually with a view to providing some insight into the comparative merits of different materials for certain purposes.

2.5 Polymer data systems

2.51 CAMPUS™

The CAMPUS™ (Computer Aided Material Preselection by Uniform Standards) database [7] has been developed jointly by a number of large companies in the plastics industry, namely BASF, Bayer, Hoechst, G.E.Plastics, and Du Pont. It is designed for use on personal (IBM-compatible) computers and delivered free of charge to prospective customers in magnetic disk format. Data are maintained and updated by the contributing companies who send out the latest versions of their own data independently of one other, although there is some effort to keep versions synchronised across the database. Each company's disk may be viewed independently or with the other companies' data that it complements.

The CAMPUS™ handbook states that the advantages of CAMPUS™ are:

> A uniform interface and data structure for different plastics manufacturers;
> Comparable data, resulting from uniform selection of properties, specimen preparation and test conditions;
> Constant updating of the families, extension of the test methods and adaptation to standards developments.

Thus CAMPUS™ aims at data and interface standardisation and up-to-date information provision. Unfortunately, however, there are areas where CAMPUS™ fails in this endeavour. In particular, the units of measurement it employs are often obsolete and do not follow SI (Systeme Internationale) protocols. For example, minutes and millilitres are frequently (but not consistently) used instead of seconds and litres; the property melt volume rate is measured in ml/10min and viscosity coefficient is in ml/g. This makes comparison with data from other sources cumbersome and relationships between property values difficult to ascertain.

Most of the data on CAMPUS™ are single point data, but there are some multi-point data that may be viewed graphically, and also the option of plotting two-dimensional scatter diagrams of one property against another to see where chosen grades fall on both scales. CAMPUS™, however, relies on a flat-file database structure and when the data are viewed by normal means this is quite apparent: the display takes the form of long, unmanageable lists of grade names and data. These are viewed by selecting a particular manufacturer or chemical family (the family name appears as a value of one of the fields in each entry) and the properties whose values are to be displayed for each grade in the list. Individual grades may be viewed by marking those of interest in the list and selecting a function to display every property and its value.

This is obviously an inefficient process and the database contributors have arranged the incorporation of facilities to allow searching of the database and selection of grades by means of a querying process. Grades with values of specified properties outside a designated range will be eliminated, leaving those of interest. This is an acceptable, if slow method of viewing the data if, and only if, selection on the basis of physical property values is the primary need of the user.

CAMPUS™ is also limited in terms of the properties specified. All are general properties measured on a standard test sample, with a strong bias towards thermoplastic materials. Despite these limitations, CAMPUS™ was used as the source of data for the polymer information system under development because of the size and availability of the dataset. Version 2.3 ©1991 was used throughout, supplied to us in ASCII format by each individual manufacturer. Normally users of CAMPUS™ would not have access to the raw data in this manner as the system is offered in compiled format. The data were extracted from the CAMPUS™ disks and exported to an object-oriented database more appropriate to the needs of the system. Only the single point data were used.

In addition to properties and their values, each grade has a comment in text format: these too were extracted and transferred for display on a suitable interface. These comments are very supplier-dependent and vary widely in the detail and quality of their information. Many grades have no comment at all. Some examples of comments are given below.

Two examples from Bayer follow, the first being little more than an extension of the grade name and the second offering considerably more, categorised information.

1. DURETHAN AKV 35 conditioned
   DURETHAN AKV 35 as moulded
   PA6,6.
   35 % glass fibres.

2. POCAN KU1-7315
CHARACTERISTICS
PBT, V-0 type, thermoplast modified; reinforced,
5% glass fibres
PROCESSING & DELIVERY FORM
Injection moulding, pellets
ADDITIVES
Release agent, flame retarding agent
SPECIAL CHARACTERISTICS
flame retardant, UL 94 V-0 in 1.6 mm, heat stabilised, excellent surface quality
Applications: housing components e.g.

Two examples from BASF show that their commenting ranges from a discursive annotation to a minimal extension of the grade name:

1. LUPOLEN 1810 E PE-LD. Used preferably for extrusion of hollow mouldings, sections and blown films. Can be injection moulded to produce articles having good impact resistance. Good resistance to environmental stress cracking.

2. ULTRAMID A3WGM35, Dry NYLON 66-GF15-M25

This is a clear reflection of the variation in information style and quality that is found in the supplier data sheets, and illustrates a need for some standardisation and improvement in the representation of textual information as well as numerical information; however that has not been an objective of this thesis.

2.52 Other polymer data systems

There are many other commercial databases catering for plastics materials data, for example EPOS™ [15], M/Vision™ [16] and Plascams-220™ [6]. The data within these databases are, as with CAMPUS™, organised using database format, and as such would be presented to the user in the form of long lists of numbers with little ordering or guidance, were it not for the searching facilities that are included in each, whereby the selection and sorting of materials that most closely satisfy the property requirements of a chosen purpose are facilitated by means of an algorithmic search process imposed over the entire data set [2]. The selection is often performed by elimination of those grades with values of certain properties outside numerical ranges followed by a matching of the material characteristics of the remaining grades with the user's product requirements. A weighting function is sometimes included so that properties may be ranked according to their importance, Hopgood [17]. Such databases work on the basis of a fixed-size data structure for each grade (i.e. limit the number of data types available for consultation).

Plascams-220™ (produced by the Rubber and Plastics Research Association, RAPRA) is an example of a large, comprehensive database dedicated to plastics materials that uses chiefly numerical, single value representations of properties. In this system the user volunteers an estimate, on the decile scale, of the relative importance of relevant properties for use within an optimisation procedure, once elimination of inappropriate candidates has been performed. The products of these weighting estimates with the property scores of the shortlisted grades are summed to give an overall rank position for each grade. Hopgood, incidentally, suggests that this method is inadequate for the selection of plastics materials and proposes an alternative inference mechanism ("AIM") for selection [17].

RAPRA recommends that the final selection is confirmed by reference to additional information on their database, in the form of text descriptions and full data sheet type entries for each grade, followed by consultation with suppliers.

M/Vision™, a product of PDA Engineering, a U.S. based company, is a materials information system with a much wider scope, drawing on extensive material databanks for plastics, metals, ceramics and composites. It also offers standards information, the possibility of user-defined databanks and the opportunity for integrating with CAD and CAE software. An additional facility enables information management within a company, so that duplication of data can be avoided and uniformity may be introduced into the test methods and units used. The main function of this system, however, is materials information manipulation. Selection is performed using a standard query language over a database, although there are many sophisticated tools to enhance this process, such as the ability to use spreadsheet software, to plot graphs, to select sections of graphs in order to focus on a reduced number of grades, to predict property values using models and/or linear regression, and to select grades on the basis of keywords in their textual description. M/Vision™ probably offers one of the most ambitious and comprehensive materials information systems on the market but nonetheless does not offer abstraction of general information, nor browsing options, nor functionality specific to a material, class of material, or context.

The representation of expert knowledge in the form of rules imposed over low-level data to facilitate materials selection is also well documented. Ahari et al [18] describe the application of an intelligent knowledge-based system to the task of materials selection which improves upon existing search techniques by incorporating a degree of classification, so that, for example, only plastics in a chosen class such as polypropylene are considered. It also allows flexible prioritising of properties together with the ability to select on qualitative or vague information (by creating property values such as high, medium or low). An additional feature still under development at the time of writing was the inclusion of geometry factors so that, for example, a designer may be guided towards thickening a specific section of his design to allow the use of a low cost material.

Bullinger et al [19] describe a knowledge-based system for materials selection specifically for application to design with fibre-reinforced composite materials. It combines a typical CAD functionality with direct access to a materials database and incorporates rules to take account of complicating features such as production technology and cost characteristics. Its fundamental difference when compared with a standard database is the incorporation of geometrical factors into the selection process together with a more sophisticated set of selection criteria.

A different approach is taken by Surkan et al [20] in their expert system for materials selection, in which geometry is not considered, but the emphasis is placed on facilities that offer a reduced representation of the database, to save time, and to partition this reduced form into categories, obviously in recognition of the worth of some degree of classification.

Ashby [21] concerns himself more with appropriate ways of interpreting the data relating to materials to determine their suitability for certain functions, and identifies "performance indices" as a means of narrowing down the choice to those materials that will perform as required given certain generalised geometrical and loading constraints. Performance indices take the form of arithmetic functions of properties; those materials satisfying the required criteria can be easily identified by graphical means, using two dimensional plots of one property against another, as facilitated within the "Cambridge Materials Selector" software.

Much of the work in materials information representation appreciates the need for improved guidance in the materials selection process and occasionally incorporates a degree of classification of materials. However the direction of development is generally towards increasingly sophisticated selection methods combined with geometry considerations. Browsing and abstraction, key aspects of this thesis, are not supported by the foregoing models.

2.6 Object-Orientation

Object-orientation gained popularity as a computing technique in the 1980's, pioneered by the creators of Smalltalk™, the Learning Research Group at Xerox Palo Alto Research Center [1]. There are now many programming languages based on the idea of fundamental computational entities, known as objects; for example CLOS, C++ and Simula [13]. In all of them the fundamental concepts are data abstraction, behaviour sharing and evolution.

These concepts are implemented within Smalltalk 80™, the language with particular relevance to this research, using a hierarchical code structure that organises the objects by providing a classification system with inheritance. Objects can represent any real world entity and may include a descriptive part, relevant variables, data, and/or functionality in the form of algorithmic expressions.* Because objects are encapsulated, i.e. may only be altered in any sense by means of carefully controlled access routes, it is possible to make changes to one object in the system without causing disruption to the others. Thus evolution of the system is supported. Behaviour sharing is enabled by virtue of the inheritance facility: since the subclasses of a class will inherit its behaviour, this behaviour need only be encoded once. As a corollary to inheritance, data within subclasses may be abstracted, or summarised, in a superclass, enabling generalities to be modelled.

The object-oriented framework has been extended to object-oriented databases. Like other database models, these allow the storage, manipulation and retrieval of data. This is done either by incorporating persistence into a language (so that the data structure is preserved over a number of program runs), the approach taken by POISE, or by adding language capabilities to a database management system. Object-oriented databases have different application areas from conventional databases and use a different data model from those already described; this is currently poorly formalised but uses typing to organise the data, as outlined by Goldberg [1].

For applications requiring the straightforward processing of large amounts of static data, for example pay-roll programs, conventional database models provide adequate support and management, for once the initial data analysis has been performed, the structure of the database tends not to change significantly. For situations where the structure of the data and programs is subject to frequent alteration, however, conventional databases do not cope easily with the required evolution of the system. Object-oriented databases are much better suited to these

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* This ability to include functionality as part of individual objects, i.e. together with their private data space, is a particularly important aspect of the object-oriented structure, with useful implications for this research, discussed further in sections 3.4 and 4.2.

demands. Blair [13] suggests that an example of such an application would be an engineering design environment. The design process is an evolutionary one requiring a data facility amenable to mutation and extension. In a design environment, objects are likely to be complex (i.e. built up from other objects) and it will be necessary to view these objects from every level of detail, or resolution. Clearly an object-oriented approach is suited to a number of aspects of the design environment, including the materials perspective.

It is for these reasons that the existing polymer information system, POISE, introduced in the following section, is written in an object-oriented language, namely Smalltalk 80™. A number of other systems for representing materials data using the object-oriented paradigm have also been developed.

2.7 Existing object-oriented work relating to materials data

McCarthy [22] discusses the need to organise material properties data in a more rigorous way than is achieved by current database management technology, and suggests that the standard relational model may not be suitable for implementing some of his solutions.

He reports a prototype materials properties data system that allows the networking of multiple databases, the implementation of a thesaurus facility and the representation of tables and graphs and different levels of data abstraction. He also proposes the use of class hierarchies, for both materials and properties, arguing that users need abstraction and summarising mechanisms to aid navigation of the information space. He suggests a modular architecture for this complex and ambitious system, and uses an object-oriented representation for the data due to its evolutionary capacity, ability to accommodate functionality and hierarchical structure as previously outlined. Nonetheless the fundamental objective of this system is still data retrieval.

Hansen et al [23] describe their investigation into new data models and database architectures that will allow flexible, extensible and transparent interfaces between application programs and applicable sources of data in the context of scientific domains. They use the object-oriented paradigm for its rich data definition and manipulation facilities and the ability to construct complex data types and store methods together with data. Their data model for materials science (specifically crystallography) is a hierarchical structure whereby a material is split into its component parts. There is also a hierarchy representing the physical states of the material. The data model and database management system are designed specifically to bring together materials data from heterogeneous, non-object-oriented data sources, the primary objective being easy access to multiple external data sources for global information retrieval.

An object-oriented approach to database management is also adopted by Hughes et al [24] for the purpose of creating a knowledge base for materials. They benefit from the ability to define abstract data types, i.e. complex objects over which arbitrarily complex operations may be defined, in a mechanism for the definition and storage of objects that are expressible as mathematical formulae or physical laws. The ability to include functionality within an object is therefore the key aspect here, leading to what they describe as "programmer-defined domains," in which the user can, to some extent, define the rules that make up the expert system.

In the foregoing examples many of the acknowledged benefits of object-orientation are used to improve on existing data models or database architectures. The approach taken by this study shares the views of those cited above, i.e. that objects are useful ways of representing entities, in particular material entities; that the ability to associate specific methods with these objects and their data is a useful feature; and that classification is a helpful means of information organisation. However it also contrasts with them, in that the key aim here is the derivation of a model for engineering polymer data that should be based on polymer domain considerations rather than computing considerations. The result is a hierarchical structure with the sole aim of representing the world of polymer materials, rather than a complex system with the aim of, say, linking relational databases, or extracting the data from them via object-oriented interfaces (often containing complicating factors - such as hierarchies of state - which would be better modelled within a different perspective).

The design of the object-oriented polymer information system, POISE, used and developed further throughout this research, incorporates features to fulfil this aim, such as a polymer materials hierarchy with inheritance, abstraction of general information, and an absence of complicating factors such as geometry, as discussed in detail by Zucker et al [2]. The POISE software architecture, written in the class-based, object-oriented language Smalltalk 80™ [1], is intended to organise plastics materials information to make it more accessible to the engineering designer. POISE incorporates an object-oriented database management system that receives data from an external database. POISE provides a skeleton structure, which organises representations of the entities providing the data (i.e. the polymer grades and classes). It also acts as a screen through which the data may be viewed and manipulated in literal or abstracted form within the constraints of a hierarchical model. Mutation and evolution of the data structure are allowed and functionality may be added at any appropriate point within it.

3. The research direction

3.1 Summary of aims

- To explore the issues arising from the process of developing and testing a computerised polymer information system using the object-oriented paradigm. The system employs a classification of engineering polymers in parallel with a database of polymer data as the basis for its data structure.

This required:

- The development of a principled classification system for engineering polymers, which must create and order hierarchically groups of similar plastics grades; be extensible; and be user independent.

- The development and improvement of the design of the existing object-oriented polymer information system, POISE, to enable it to accommodate, display and manipulate the resulting data structures.

- The population of the resulting system with CAMPUS™ grades and other grades with different data representation requirements, and the testing of the system in action.

3.2 Why the relational model was not used

Previous chapters have suggested that commercial databases dedicated to plastics materials have not confronted all of the difficulties associated with obtaining and handling polymer materials information. Many of the drawbacks arise from the fact that the relational model is not the most appropriate model for polymer data, for the following reasons.

i)The low level information format results in large and unwieldy lists of data with little ordering or guidance. The process of normalisation, commonly used to alleviate this problem, is not helpful in the context of an engineering polymer database, as there is rarely enough data repetition for a useful factoring to be applied.

ii)Property descriptions are over-simplified, taking the form of no more than a name for each data set, and leave the end-user poorly equipped to interpret the significance of each property for the design task.

iii)A fixed, pre-determined data structure is assumed, which does not allow for extension or elaboration.

iv)Relationships between entities (properties or material types) are restricted to the Codd relations between and within records of grades.

v)Attempts at overcoming the difficulties associated with low level information format, to be found mainly in those cases where a service is being sold together with the data, for example in RAPRA's Plascams-220 [6] or PDA Engineering's P3/Materials Selector (which complements its M/Vision Databanks) [16], take the form of algorithmic materials selection based on property values. This has certain drawbacks: structured querying must be performed over the entire data set, and the selected grades are taken out of context. It can be difficult to judge the merits of a single, isolated grade, with no supporting information about the nature of its chemical history, process or additives, for example. Thus these systems require substantial prior user expertise, such as knowledge of criteria for the elimination of grades and the appropriateness of the final list.

This problem is often more pronounced for those databases produced by materials suppliers (of which CAMPUS™ and EPOS™, cited earlier, are examples) whose primary purpose is to publicise information pertaining to their own grades. These organisations will assume that their own expertise will be called upon at some stage and seldom offer sophisticated tools to support the selection procedure. In their favour, however, commercial driving forces mean that such databases often have the advantage of regular updates, with the potential of being available on-line.

To overcome the issues outlined in (i) and (v), this study proposes that by grouping together the data relating to similar grades of plastic and arranging those groups into a family-tree like structure, the user will benefit from browsing through the abstracted information, i.e. the knowledge conveyed in the generalisations about each group, with guidance from the classification structure.

A final, informed decision may made by the user himself and the pitfalls of algorithmic selection methods, such as the "odd fish effect" suggested by Zucker and described in Sargent's book [25], are thus avoided. The "odd fish effect" refers to the observation that an algorithmic selection method, using summed property weightings to "filter and sort" materials grades, fails to band together grades that are related by chemical structure. Instead of appearing in (or disappearing from) the short-list together, a small change in a single property weighting results in a group of chemically similar grades dispersing: individual grades "pop in and out" of the materials shortlist irrespective of any familial connections they have with others in the list.

3.3 Why the hierarchical model was not chosen

The hierarchical data model seems to offer the appropriate architecture for accommodating a system with a family-tree like structure. However, the hierarchical model is based on a fixed-size data structure for each grade. Any system that models design data needs to be extensible and mutatable, so that the addition of new data, in the form of entities or attributes, and the reorganisation of the structure within certain limits, may be supported.

The hierarchical model will not accommodate such flexibility. Properties not initially present in such a database will never be available for consideration, and, should the structure of the chosen hierarchy come under revision at any point, it will not be possible to account for this without complete restructuring.

Thus point (iii) is not satisfied by the hierarchical model, and in fact neither are points (ii) and (iv) since data descriptions and relations within this model are as simple and inflexible as in the relational model.

3.4 Benefits of object-orientation: abstraction and methods

The object-oriented model, in the form of the POISE software architecture written in Smalltalk 80™, was employed for the data modelling task, since it offers the following benefits, all of which are within the language capability of Smalltalk 80™.

- It naturally supports a hierarchical structure, with inheritance of properties.
- It allows browsing of the abstracted information within the hierarchy.
- It offers an extensible database (and is therefore able to extend property lists indefinitely).
- It supports evolution, so the hierarchy may be revised with ease and efficiency.
- The option of adding functionality, in the form of object-specific methods, at any point in the structure means that a complex real-world entity such as a polymer grade, a class of such grades, or a property can be modelled (as an object within its hierarchy) with greater flexibility and detail. (These methods are also naturally inherited and so the behaviour of a class at the top of the hierarchy is automatically present for its subclasses).
- Message passing between objects means that complex relations between them may be modelled, such as the relation between the property objects for stress and strain.
- Annotations, graphs, formulae, and so on can be incorporated at any level of the hierarchy.

POISE allows externally supplied engineering polymer data, currently from the CAMPUS™ database, to be organised and viewed via a class-based hierarchical representation. The benefits of a principled navigation facility are therefore combined with the ability to refer to up-to-date information, since the system can link up to and gather information from the most recent supplier databases. POISE and its development are described in chapter 4, which includes discussion of more sophisticated use of the behavioural aspects of object-oriented systems, in particular their appropriateness for interaction with other perspectives.

3.5 The need for a principled classification

Having opted for a hierarchical data structure, it was necessary to create a suitable classification of engineering polymers for implementation within it that satisfied the criteria outlined in section 3.1. The development of this classification and the accompanying analysis provide the primary thread in this thesis. This is described in chapter 5, paying attention to the issue of different categories of properties and the requirements for a useful factorisation of the grades for which they are specified. It is shown how conflicts arising from these considerations reflect more fundamental issues behind the principles of classification itself. The resulting structure was explored and discussed.

4. Developing the object-oriented system, POISE

4.1 POISE

4.11 The existing system

At the start of research, POISE had already been written in its basic form on Apple Macintosh II computers, from work on an overlapping DTI sponsored project [26]. It was developed further throughout the course of the project.

The basis of the information structure, the polymer materials object hierarchy, had been implemented with a temporary classification in place. Interactive facilities to enable viewing of the hierarchy and manœuvring of the polymer classes within the structure as deemed appropriate (while ensuring that they carry with them all their subclasses, grades and data) were also in place. This functionality allows the end-user of POISE to change the class ordering within the hierarchy, thereby supporting evolution.

Plate 1 shows a snapshot of the Hierarchy Editor window. The final hierarchy (discussed in chapter 5), implemented within POISE, is in the top half of the window. Here it is being altered by the user to relocate the class PAtsp (signifying transparent polyamide grades) from a position outside the Partly Crystalline class to a new position as a subclass of the class PA (polyamides), which lies within the Partly Crystalline class. Such changes are easily performed using "drag and drop" techniques with the computer mouse.

The object-oriented database was in operation and was developed further throughout the course of the research. Means of importing properties, data and comments from CAMPUS™ into this database had been implemented. Information is dynamically analysed during the translation process into initial positions in the class hierarchy, based on the materials family names given by the supplier companies. Further structure changes introduced incrementally to the model using the Hierarchy Editor are seen by fresh releases of the CAMPUS™ data. The system was designed so that it enables persistence of data and the data model from one session (or one user) to another, and from one platform to another [27].

Access to a visual display of the class and grade information within POISE is facilitated by a feature of POISE (already in existence but further developed throughout this research) termed the Property Comparison tool [2]. This may be employed to explore the nature and consistency of the data within the classes and to compare data between classes, by displaying one or more labelled histograms, with axes, in a resizable window. A histogram shows the data distribution for a class in the hierarchy, for any property specified for the class. Data and distribution information is stored in the class object, rather than retrieved at the time of querying. Browsing of the abstracted, or class information is thus facilitated.

Plate 2, for example, shows the nature of the display: it is apparent that the user can, without any form of numerical interpretation, see the property ranges for any class, compare them with other classes at the same or a different level in the hierarchy, and pinpoint immediately anomalies, or the best and worst performers in the range.

A mouse click on one or more histogram bars enables access to a list of the grades in the property range represented by those bars. Selection of one of the grades from the list results in a Grade View window, with the name of the grade and all of its property values, to be displayed.

At the point of data capture, all properties are introduced at the top of the hierarchy, i.e. the property objects are located within the most general class, Polymer, and inherited down through the hierarchy to the subclasses and finally to every grade, where the individual data values are held. Property objects take the form of Partial Template Objects, or PTOs, so called because they define part of the data structure of an object onto which they are "installed," or attached [28]. A PTO for, say, density, installed onto the materials class object Polymer, provides a datum location for the density value of each of the members of that class and its subclasses. PTOs for other properties will complete the data structure for the Polymer class.

Methods (or functions) may be added to property and materials class objects via the interface within the Smalltalk™ programming environment.

Three main components of the POISE architecture may be identified as particularly relevant, namely the persistence environment, concerned with the automatic storage and maintenance of object transactions; the raw data acquisition environment, providing the gateway to third party data; and the high level classification environment, offering a means of experimental information structuring. These components enable POISE to provide a hierarchical model of the domain, with inheritance, that has an extensible database and may be allowed to evolve according to user requirements. It also offers abstraction, the ability to model complex entities (such as materials classes and properties) and the relationships between them, and the ability to replace existing data with more current data (without disturbing the model).

4.12 Further developments

To allow a user to exploit the extensibility feature, it was necessary to modify the interface and incorporate mechanisms to enable new classes, new grades, new properties and new data to be added. This was achieved by means of menu options at the appropriate point in the interface.

The menu for adding new classes and grades, for example, may be found by clicking on the narrow bar above the hierarchy in the Hierarchy Editor window, Plate 1. These options, when selected, trigger the creation and initialisation of new objects (or access to existing ones for modification); self-explanatory windows on the objects concerned allow entry or alteration of the specifications in a very straightforward manner. For example, definition and redefinition of properties are achieved as illustrated in Plate 3, which shows a window on the property object for density. Its units and datatype may be altered at any time, together with information on the display of density data and general comments about the property itself as required. Whether it is a general or a special property (i.e. whether it has general applicability to families in the hierarchy or relevance to polymer categories not specified in the hierarchy) is also noted here: this matter is discussed in depth later on.

A tool to move properties within the hierarchy structure was developed. Clicking on a class in the hierarchy - see the upper part of the Hierarchy Editor window, Plate 1 - causes a list of the properties specified for that class to be displayed on the lower half of the screen. Simple promotion and demotion facilities enable any property, once selected, to be relocated up or down the hierarchy as appropriate. This control is particularly important whenever a superclass has been repositioned. In this case selection of the class PA has resulted in the property water absorption, which is defined by this class, to be displayed.

An important task at this stage was to refine the hierarchy so that suppliers' classes fell in line with the chosen structure and to manœuvre the properties to appropriate positions within it. It was found that most properties apply to all polymer grades, and so should be defined at the top level, but that some are redundant for certain classes of polymer. For example, melting point is of no use in describing thermosets, and so is more usefully defined within the Thermoplastic class, which is where it was placed. This is a good example of the sort of optimisation that is difficult within a flat-file database.

Also incorporated into the system was a facility for searching through the database so that shortlists of grades could be produced on the basis of certain criteria. For example, those grades with a particular property defined, those with values of a property within a certain range, or those with specified keywords in the text of their comments can now be shortlisted.

Searching is not a primary aim of this system but it proved a useful system development aid when it came to checking the data, comments and grades that were in the system. Searching by name allowed known grades to be accessed. Once the shortlisting facility was established it was a natural step to extend it to the Property Comparison function; it is now possible to create shortlists on the basis of selected bars in the histogram and then view those shortlists on a different Property Comparison window for a different property. This allows a process of incremental "zooming in" on a group of grades, which is performed under the complete control of the user. Plate 5 shows this in action.

These were the initial improvements on the POISE system: all were based on the perceived requirements for a generic polymer materials information system.

Further analysis of the representational problem revealed inadequacies in the classification structure implemented within POISE, which failed to group together grades similar by virtue of certain engineering properties and their shape or form. Further modifications were required to deal with this, involving the incorporation of an additional classification structure. This is discussed in section 6.4.

4.2 The use of methods - a costing algorithm

An important feature of object-oriented systems is their ability to accommodate functionality (numerical models or algorithms) at appropriate points in the structure. In the context of Smalltalk 80™ and, specifically, POISE, this aspect can enable complex modelling of the polymer domain entities in the hierarchy. Thus an object may comprise, in addition to data, "methods" that employ those data and describe some behavioural aspect of the entity represented by the object: the polymer grade or class.

As a simple example, a property object for density may incorporate methods enabling the translation of its units from g/ml to kg/m^3. Not only would these methods cause all displays of the density units to change, they would also calculate the new values of the property for those grades with density defined. Clearly this algorithm would have no relevance for other property objects nor for any other sort of object and would be redundant and confusing if specified across the system: realistic modelling of the domain and its entities is therefore made possible by this feature.

A more sophisticated use of object methods has been proposed [27]. This involves adding functionality to estimate the cost of an injection moulded plastic component. A number of formulae relating to this calculation have been sourced. Barrie [29] suggests that the production cost per part (P) can be found from the following:

$$P=\{(1.1).w.p.\ 10^{-6}\} + \{mhr/3600\ .\ \text{cycle time}\} +$$

$$\{[mhr/\text{units per month}]\ .\ 1000\ .\ [0.013\ .\ (w.N)^{1/2} + 0.34]\}, \qquad (1)$$

where

w = mass of one component (grams);

p = raw material cost per tonne;

mhr = machine hourly rate;

N = number of impressions per mould;

cycle time is in seconds, and units per month is in thousands.

The first term is the materials cost experienced by the moulder (the factor of 1.1 is to allow for waste); the second term is the production cost associated with making one part; and the third term is an estimate of general machine costs, combining the intensity of use with overall costs based on machine quality.

Cycle time can be calculated from material properties as follows [30]:

$$\text{Cycle time} = \text{Filling time} + \text{Cooling time} + \text{Demoulding time}, \qquad (2)$$

where:

Filling and Demoulding time are machine dependent, and

$$\text{Cooling time} = (\text{Material constant}).t^2 \qquad (3)$$

Here

t = wall thickness (mm), and

$$\text{Material constant} = 1/[16a]\ .\{(\text{Melt temp.} - \text{mould temp.})/(\text{Freeze off temp.} - \text{mould temp.})\}^2, \qquad (4)$$

where

a = thermal diffusivity ($10^{-7}m^2s^{-1}$);

Freeze off temperature may be taken as the crystallisation temperature for partly crystalline polymers and the glass transition temperature for amorphous polymers.

A number of the values of these parameters can be found by consulting tables, for example of wall thickness and machine time with respect to machine size, in appropriate texts [31], or may be obtained from in-house information if the user is a manufacturing company.

This algorithm transcends the boundaries of the materials perspective, but the calculation draws on a number of materials properties: for example, thermal diffusivity, freeze-off temperature, and density (in the context of component mass). Thus methods for accessing data within polymer material objects will be useful for providing the correct information about the relevant material, with the appropriate units, for insertion into the algorithm.

It is helpful to consider how such an algorithm - an example of data manipulation across more than one perspective - may be implemented. The other perspectives required to model the non-material data are:

A manufacturing perspective, which will have class definitions for:

Production Schedule (holding such information as units/month and number of impressions per mould);

Processing Machine (the machine in question will be an instance of the Injection Moulding Machine subclass and will have information on the machine hourly rate and machine time), and

A product perspective, which will have a class definition for:

Product Description (giving a class of components and their exact geometries, the wall thickness, etc.).

A prototype such implementation has been created by Ogden and Demaid [26], using basic models for manufacturing and product perspectives with hypothetical machine and artefact examples. The algorithm itself was split up so that its parts could be calculated in the relevant perspectives and classes.

The final calculation was performed in the Production Schedule class of the manufacturing perspective, which responded to the message "cost" using a process called delegation [8] to share out various tasks between other classes and perspectives and bring together the returned data to calculate the cost per artefact.

For example, the mass of the artefact was calculated within the Product Description class of the product perspective, using the value of its volume and taking its density value from the material grade within the class PA in the materials perspective. Cycle time was calculated in the Processing Machine class of the manufacturing perspective, which had to delegate to the Product Description class of the product perspective for the wall thickness value and to the materials perspective for the material constant (calculated by methods installed on the PA class).

5. Developing a principled classification for engineering polymer materials

5.1 Classification

According to Simpson [32], classification is "the ordering of organisms into groups (or sets) on the basis of their relationships, that is, of their associations by contiguity, similarity, or both." Taxonomy is "the theoretical study of classification, including its bases, principles, procedures and rules." Taxonomy has also come into accepted use to designate the end product of the taxonomic process. Carl Linnaeus (1708 - 78) is widely credited with having created the first classification of living organisms, although Adanson, his contemporary, is thought to have formalised the structure of the biological taxonomy. Since then there have been few rigorous applications of formal taxonomy outside the field of biology. There is [33] "remarkable agreement among various authors in the field that the present system of taxonomy attempts to fulfil too many functions and as a consequence does none of them well. It attempts (1) to classify, (2) to name, (3) to indicate degree of resemblance...,(4) to show relationship by descent - all at the same time." Nevertheless biological taxonomists have developed an organised body of knowledge that is both useful and consistent to a high degree. It is the intention of this study to apply some of their theory to the domain of plastics materials.

Aristotelian logic [34] emphasised the need to discover and define the "essence" of a taxonomic group, which should give rise to properties that are inevitable consequences. This brings to attention the distinction between "natural" and "arbitrary" classifications. Gilmour [35] emphasises that the nature of a taxonomy depends on its purpose: if the purpose is restricted, then the resulting classification is a special classification ("arbitrary"), and will convey less information than a general or "natural" one. It has been the aim of this research to find the most natural classification for plastics materials and to define classes that best convey the "essence" of the grades of engineering polymer they subsume. Such a classification should then approach the ideal of being a user-independent representation of engineering polymers.

Using the elements in place of polymers, as an analogy, the periodic table is a system that gives rise to "natural" classes, by virtue of the fundamental principles on which it is based (the arrangement and numbers of subatomic particles). The groups (e.g. the halogens) contain elements that exhibit consistent behaviour regardless of the context in which they are viewed.

A useful taxonomy for plastics materials, then, should group together similar grades of engineering polymer and abstract important information, which summarises the behaviour shared by the grades, into classes in a principled fashion. In a computer information system it will be populated with property names and their values as provided by polymer grades. Classes must be carefully chosen so that they form, in this case, a hierarchy that covers the domain completely and will not be invalidated by the addition of unforeseen new materials or properties, thus ensuring extensibility. It is through the ability of the taxonomy to accept and group together plastics, as described by their properties, in a well-conditioned and extensible form, that the underlying precepts are shown to be useful.

Fundamental decisions regarding the principles that control the definition and naming of classes and their position within the classification structure to create a taxonomy are needed.

The above requirements mean that classes should be:

- Distinctly bounded
- Exclusive (no overlap between classes)
- Fully complementary (no "gaps" - all sub-classes should be subsumed by the super-classes and should not violate their ancestry).

i.e. obeying the semantics of strict inheritance as described by Blair [13]. In the attempts to devise viable taxonomies it has been recognised that there is a need to cater for a minimal number of exceptions while avoiding such complicating features as multiple inheritance (where a class may have more than one parent) [36], [37], [1].

5.2 An analysis of existing polymer classifications

In order to obtain an understanding of the fundamental principles generally considered to give rise to the character of a polymer, which therefore determine which polymeric materials may be considered as similar, an analysis of existing classifications was performed. This revealed an apparent tension between classification for science and classification for use, which accords with a conflict found during the investigation of the principles behind the creation of a plastics materials taxonomy (detailed later) and inspection of the nature of plastics materials properties. This conflict arises from the fact that two requirements, namely the need to base classes on fundamental polymer domain principles to ensure extensibility and high level abstraction, and the need to reflect similarities relevant in an engineering context, appear to be mutually exclusive.

Books with a strong reference theme are represented well by Brydson [5] who assumes a fundamental division within plastics materials between:

- Thermoset and Thermoplastic
- Amorphous, Partly Crystalline and Rubber-like

The first classification reflects differences in degree of bonding: the long-chain molecules of thermoset plastics are extensively cross-linked during processing, resulting in a material that cannot be made to melt or flow. There are no primary bonds between molecules in thermoplastics and the materials can be made to soften and take on new shapes by the application of heat and pressure.

The second classification is based on microstructure for the distinction between amorphous and partly crystalline, while degree and type of bonding and molecular forces are more important for the rubber-like category. Thus inconsistencies are introduced into classification criteria at an early stage. All of the factors considered, however, are influential, i.e. affect a wide range of properties that describe the physical behaviour of plastics under certain conditions, and have implications for the appropriate use and processing of plastics.

Brydson divides these classes one stage further into families based largely on the primary monomers in the polymer chain, e.g., PVC, polystyrenes, etc.

The Rubber and Plastics Research Association [38] includes an elastomer class on the same level as thermoplastic and thermoset in order to separate out and provide a grouping for materials with rubbery characteristics at a high level.

Books written from a teaching perspective, e.g., Billmeyer [39], emphasise differences in molecular structure by classifying heterochain thermoplastics (i.e. those polymers whose backbone contains atoms other than carbon) as separate from those which have a continuous carbon backbone ("homochain" thermoplastics), in addition to the aforementioned partly crystalline, amorphous, thermoset and thermoplastic distinctions.

Plate and Papisov [40], take Billmeyer's approach a stage further. They divide Heterochain and Homochain thermoplastics into subclasses depending on which main chain atoms and functional groups are present. However only polymers of a relatively simple structure are considered and the classification of those with combinations of different main chain atoms and functional groups is not attempted.

Boenig [41] describes a classification based on molecular mass using terminology coined by Staudinger in the 1920's:

Name	Hemicolloids (Low Polymers)	Mesocolloids (Meso-polymers)	Eucolloids (High Polymers)
Molecular mass.	1,500 - 5,000	5,000 - 10,000	> 10,000
No. of segments	20 - 100	100 - 1,000	> 1,000
Chain length (Å)	50 - 500	500 - 2,500	> 2,500
Comments	If linear, dissolve without noticeable swelling. Low viscosity solutions.	Soluble if linear and exhibit swelling depending on chain length.	Dissolve with intense swelling if linear. Dilute solutions are very viscous.

Table 2: Staudinger's polymer classification

This classification is based on a very important feature of polymers and results in clear divisions between polymers in terms of those properties affected by molecular mass, particularly solubility related properties. However engineering polymers fall almost entirely within the eucolloids class and their solubility characteristics are rarely their most important feature.

In some cases polymers are distinguished by the technique used to produce them. These techniques fall into three main categories: addition polymerization, condensation polymerization and rearrangement polymerization, with addition polymerization being divided further into free radical, cationic and anionic polymerization [5]. The reaction environment may also produce a further factoring in some cases, depending on whether polymerization is performed in bulk, in suspension or in emulsion form. Billmeyer [*ibid*] prefers to distinguish polymers by the mechanism of their polymerization reaction and divides them into step-reaction and chain-reaction polymers. Although some of these factors result in a factoring according to chemical features of the polymer, this approach fails to give insight into possible groupings of plastics with similar engineering properties.

An unusual classification based primarily on a combination of microstructural properties (crystallinity and degree of cross-linking) and temperature (T is use temperature, T_g is glass transition temperature and T_m is crystalline melting point) is given by Van Krevelen using Leuch's nomenclature [42]:

Polymer Class	General Properties	Range of Use Temperatures	Degree of Crystallinity	Degree of Cross Linking
Molliplasts	ELASTO-VISCOUS LIQUIDS	T > Tg	0	0
Mollielasts (ELASTOMERS)	SOFT & FLEXIBLE RUBBERY SOLIDS	T > Tg	0	Low
Fibroplasts	TOUGH LEATHERY-HORNLIKE SOLIDS	Tm > T (> Tg)	20-50	0
Fibroelasts	TOUGH AND FLEXIBLE LEATHERY SOLIDS	Tg < (T < Tm)	0	INTERMEDIATE
Duroplasts	HARD & STIFF SOLIDS	T < Tg	0	0
	HARD AND TOUGH STIFF SOLIDS	T < Tm	INTERMEDIATE TO HIGH	0
Duroelasts	HARD SOLIDS	T < Tg	0	INTERMEDIATE TO HIGH

Table 3: van Krevelen's classification

This is based on fundamental polymer features but takes into consideration only those aspects and properties that cause plastics to be divided into classes with similar mechanical behaviours and so, despite its formal approach, still results in a classification with a specific end-use bias. (For example, those with a primary interest in the electrical properties of plastics would not benefit from such a classification). It highlights the fact that a biased classification cannot remain constant under all conditions: use temperature, T, is a crucial variable on which the entire classification depends. It is conceivable that a grade that is a molliplast at one, high temperature above its glass transition point, may also be classified as a duroplast if it is used at a lower temperature, below its glass transition point.

National and international standards give good examples of classification methods considered useful to industry, e.g., ASTM D4000 [43], which does not abstract information from groups of materials but classifies with emphasis on nomenclature, identifying key features on an individual grade level and acknowledging a strong performance imperative. For example, ASTM D4000, PA120G33A53380 refers to a grade with features indicated by the following keys:

PA120: Nylon 6,6 heat stabilised
G33: Glass reinforced with 30% glass, nominal
A: Table A (D 4066) for property requirements
5: Tensile strength, 175 MPa min
3: Flexural modulus, 7500 MPa min
8: Deflection temperature, 235°C min
0: Unspecified

Another such example is found in the ISO standard for the classification of vulcanized rubber [44]. To each material is assigned a designation from each of three categories simultaneously, referred to respectively as "Type," based on resistance to heat ageing, "Class," based on resistance to swelling in oil, and "Group," based on low temperature resistance. Thus a material can have a designation BCD implying it is of Type B (referring to the range of temperatures to which it is resistant, in this case up to 100°C), Class C (referring to a volume swelling not exceeding 120% in oil) and Group D (indicating that it is non-brittle down to -10°C). A further two stages of categorisation may be attained by considering another two groups of basic physical properties. There is no hierarchical structure to this classification and again the description is solely in terms of measured physical properties.

It is important not to mistake trends in behaviour for distinctions between separate classes; Billmeyer, for example, says that increasing intermolecular forces result in a tendency to go from amorphous to partly crystalline to fibrous. This is not a statement of clear boundaries between these three states: intermolecular forces are not the only factor and material types defined by microstructure are being confused here with material forms defined by process (a fibre being a partly crystalline thermoplastic that has been extruded under the conditions necessary to impart the required alignment of molecules and shape of the final product).

In a different approach Boenig [41] reiterates this classification but bases it on the values of the initial elastic modulus:

TYPE	RUBBERS	PLASTICS	FIBRES
ELASTIC MODULUS (dynes/cm^2)	$10^6 - 10^7$	$10^8 - 10^9$	$10^{10} - 10^{11}$

Table 4: Boenig's classification

Confusion arises here because a classification based on the value of a single property results in classes of material that are commonly discriminated because of their likeliness to take a certain physical form, where the usefulness of that form depends on the property in question. It is therefore a circular description and would be more accurately expressed simply by referring to the property itself.

It is seen that existing classifications are often shallow and seldom principled; many that arise from conventional terminology comprise classes that overlap, often because of the need to address both molecular structure and use and because these two factors do not always run in parallel.

The main points illustrated by this analysis are as follows:

- The recurrence of thermoset and thermoplastic classes supports a decision to incorporate them at a high level in the hierarchy. However, further factoring into chemical families defined by their functional groups introduces problems as such families will often subsume both thermoplastic and thermoset grades (for example, the polyurethanes).
- The inclusion of an elastomeric/non-elastomeric distinction is common but the position of the elastomer class varies from classification to classification. It is placed on the same level as the thermoplastic and thermoset classes where use is important but subsumed within thermoplastics, on the level of amorphous and partly crystalline, by Brydson. However,

elastomers can be either thermoset or thermoplastic and furthermore some chemical families may contain elastomer grades without being entirely comprised of elastomers.

Including an elastomer class introduces inconsistency into its level wherever it is placed in a classification defined by molecular or microstructural features, since, although many elastomers share certain molecular features, elastomericity is caused by a complex combination of factors including temperature, and an elastomer class has to be defined according to observed physical behaviour rather than molecular character.

From a scientific viewpoint the class is clearly difficult to define and place, yet for practical purposes it is convenient to consider elastomers in a class of their own, as they have well defined properties and uses.

- The division between partly crystalline thermoplastics and amorphous thermoplastics can be considered principled from a chemical point of view since a partly crystalline polymer is strictly defined (it undergoes a phase change to a regular microstructural form on cooling). Thus the classes are distinctly bounded. However there are still chemical families whose grades may be divided between amorphous and partly crystalline, especially where crystallinity is process dependent, e.g., the strain-induced crystallinity of PET, and there can be a problem deciding at what point the degree of crystallinity becomes important regarding its effects on the physical properties. (PVC, for example, has approximately 5% crystallinity but is generally considered an amorphous polymer). However, if degree of crystallinity were to be included as a property of a polymer, classes that would have been subsumed by the partly crystalline thermoplastics would no longer benefit from the important abstracted information associated with, for example, the absence or presence of a melting point, distinct only for partly crystalline thermoplastics.
- It seems easier to form a classification if a bias towards a particular end-use is acceptable. To cover all conceivable perspectives would, however, result in multiple hierarchies, which

would be contrary to the aim of producing a single structure independent of any user perspective.

- The repeated use of the common chemical family classification supports the view that chemical family names provide a useful reference for meaningful general information to be inferred about the properties of a plastic.

5.3 Engineering polymer materials properties

Inspection of the nature of the numerical information pertaining to engineering polymers provided an insight into the structural requirements of a model that is to represent these data in an easily accessible manner. It also highlighted some important issues to be considered when formulating the principles behind a classification structure.

It was observed that an individual grade of plastic can be described by a potentially infinite list of properties, as new tests and properties are constantly being devised to illustrate material behaviours. A property, most simply, takes the form of an attribute, such as density or melt viscosity, and a value associated with that attribute.

Classes within a hierarchy of plastics materials will specify the properties required to describe the instances (grades) they subsume. The properties will be inherited by those instances via any intermediate subclasses. It must be possible to define properties at any point (class) in the hierarchy without violating the class description. Allowing selective specification of properties as appropriate means that properties are not wastefully specified where they are redundant (which would lead to empty data locations for all grade members of such a class) and therefore enables efficient data structuring. A good example is the property melting point, which would have no place within a class of thermosets nor all of its subclasses.

For materials destined for production into bulk plastic forms a grade is usually supplied in the form of granules for injection moulding. The values of most of its properties will be obtained from tests on a further processed sample, usually one formed from injection moulding into a shape that complies with standard test specifications. Many of these properties are standard, i.e. quoted by most suppliers for their own products and measured using widely accepted test methods and conditions, on a specimen with universally accepted processing conditions and geometry. For grades destined for use in other forms, such as films or fibres, specific tests are performed on differently processed samples. These properties and their values can be considered to be more dependent on process and geometry. The performance properties of a complex, final product will be yet further affected by shape and process considerations.

The divisions between grades in terms of their property characteristics are fundamental to the problem of ordering and classifying plastics materials. Five different types of polymer properties have been recognised:

- Intrinsic properties, such as density, modulus and transparency, which reflect fundamental atomic and molecular arrangements. Such properties are largely independent of whether they are tested on a granule supplied for injection moulding, simple test pieces or fully finished artefacts (subject to some exceptions, such as the modulus of highly aligned polymers).
- Engineering properties, such as tensile strength measured using a specific specimen geometry, which, although they are strictly artefact properties, i.e. subject to geometrical influence and loading type, are taken to be generic properties for the purpose of materials comparison. In general such properties are those of the bulk (3D) material.
- Specific engineering properties, such as the properties used to describe a film or thin sheet, which requires tests especially designed to be applied in 2D, or the properties that describe fibres, and are therefore usually applicable only in 1D. Such properties approximate more closely the geometries and/or loadings of an engineered product.

- Artefact properties, produced by testing final products in a manner similar to the conditions experienced in use (although usually accelerated), for example impact tests designed by a car manufacturer interested in the performance of a plastic car bumper, or tests designed by a kettle manufacturer concerned with a plastic's performance under cyclic boiling.
- Specific process related properties such as the reduction of strength at the weld-line of an injection moulded part.

In general, it is observed that only the first of these five categories encompasses properties that are quoted for a grade regardless of its intended end use, and that may be included by way of any inheritance hierarchy designed to represent generic knowledge. The second category is so broadly quoted (even for those grades that are recommended for extrusion, since these grades can often also be injection moulded) that it may also be considered to be a generic category. The last three encompass properties that are only quoted when the grade is destined for specific applications. In a hierarchy containing only chemically defined classes, therefore, these need to be specified via a route other than inheritance, for example introduced at grade level, as they may not necessarily be relevant to all grades of any class.

This division of properties between generic (for general comparison) and use-oriented (to support selection for a particular use) leads to one manifestation of a fundamental problem encountered during the development of a classification of plastics materials. This is discussed in section 5.8 in greater depth, but, in summary, is the inability of any simple taxonomy to accommodate both the fundamental scientific tenets and a more practical, engineering imperative. The illustration of this provided by the property type analysis highlights the implications for the representation of numerical data. A single hierarchy based on the scientific approach will be implicitly extensible and will accommodate the generic properties but it fails to satisfactorily represent use-oriented properties.

This is an important issue because the number of special tests is very large and materials supplier companies expend much effort conducting tests to industrial customers' specifications. Any plastics information system needs to recognise the presence of these very specific additional property lists and allow access to them.

First the development of an engineering polymer taxonomy of single hierarchical structure that complies with the criteria of extensibility and independence from user bias is detailed.

5.4 Criteria for classifying engineering polymers

To clarify the issues involved in the creation of a generic plastics taxonomy, the definition of "similar" needs to be carefully considered. In extremis, grades of plastic could be considered similar in terms of:

- Physical properties, or:
- Chemical structure.

If physical properties alone are considered, only the observable physical behaviour of a grade is taken into account when deciding the other grades to which it is most similar, ie., to which class it belongs. This approach requires a formal statistical methodology. The resulting classification, based entirely on properties and property values, may or may not reflect trends in chemical composition.

The most simple such analysis would be a univariate one, i.e. based on the values of just one property (or one set of correlated properties). This may produce, for example, a division of grades between those with high, medium and low impact strength.

The diversity in the behavioural aspects of plastics means that any "class" so produced will not demonstrate consistent behaviour overall. In practical terms, plastics that are similar with respect to one set of related properties are quite different when a different set is considered.

Further factoring according to other properties would extend the classification but the resulting structure would be biased according to the order of prioritisation of the chosen properties. The boundary between one class and another (i.e. the difference between "high" and "low") would be, in some cases, arbitrary. Figure 2 illustrates four possible alternative factorings based on physical property sets which result in different hierarchies according to whether structural, thermal or electrical properties are considered to be important.

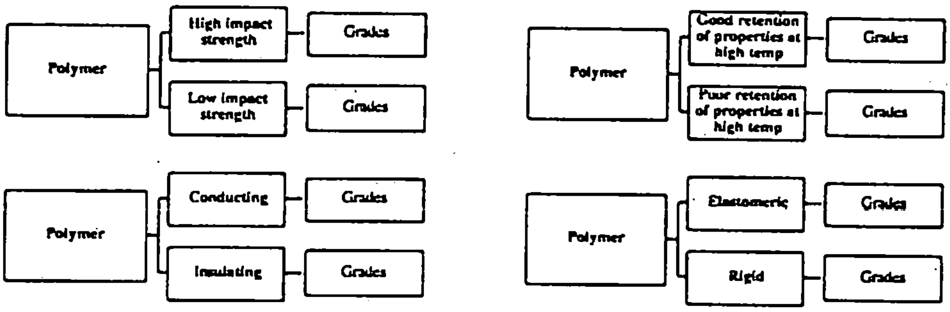

Figure 2: Taxonomies based on physical properties

The ISO standard for the classification of vulcanised rubber [44] is an example of this approach. The system provides a means of nomenclature, by assigning type codes, rather than a classification. The bias towards assumed user interests is apparent: the standard has allocated resistance to three phenomena (heat ageing, swelling in oil and temperature) as the most relevant properties of this class of material; this may not be the case for all users of this classification.

To take all properties into consideration simultaneously would require a multivariate statistical analysis of the available data. The resulting classification would draw together those grades of similar form, process, etc., by virtue of their shared property profiles.

Tatsuoka [45] describes methods of ascertaining profile similarity between individuals for the purpose of psychological research, where the profile is based on a number of attributes. He identifies two problems: the "classification problem" in which the purpose is to ascertain which of several group profiles an individual's profile most closely resembles, so that the individual may be "classified" as a member of that group; and the "taxonomical problem," where the purpose is to *form* groups of individuals who have similar profiles, in which case there are no pre-defined groups and the task is to generate the groups empirically. At this stage we are concerned with the taxonomical problem for plastics materials.

In his description of the "Generalised Distance" method developed by Mahalanobis (1936), Tatsuoka brings to attention two important issues that are relevant to any statistical approach.

Firstly, in deciding the similarity between any two entities based on their numerical attributes, the comparative importance of a given numerical difference between the entities' scores for each variable must be taken into consideration. (For example, when comparing two people, a difference of three inches in height could be considered more important than a difference of three points on the IQ scale). This may be dealt with by means of standard deviation for populations that obey statistical distribution laws, but such a method would not apply to a sample of engineering polymers because of the non-random distribution of their property values (influenced deliberately by the addition of fillers, reinforcements, etc).

Secondly, all statistical methods must take into account any correlation between variables. For many plastics properties this will be significant (for example the correlation between glass transition temperature and heat deflection temperature or between tensile strength and impact strength) but not quantifiable in general, and would therefore render a statistical analysis inaccurate at best. Manly [46] criticises Cluster Analysis in general, of which the distance method is but one approach, as being of use only when the groups are very distinct. An overlap between groups tends to result in structures that are not reproducible from repeated analyses. The assessment of results from any method tends to incorporate a rather large subjective component.

In addition to the foregoing disadvantages, statistical methods fail to take account of properties that may only be described qualitatively.

But the most important point about a statistical, property-based approach is that any taxonomy it creates would not support an extensible data structure: the introduction of new properties would present a new taxonomic problem requiring fresh analysis. This would place the initial taxonomy at risk of distortion or even destruction. Although not immediately obvious, the introduction of new grades could also present a new taxonomic problem (it may appear that this only introduces a classification problem; but new grades could require additional classes high in the hierarchy). Thus the addition of new properties *or* new grades may call for a new taxonomic structure, meaning that the original was not extensible.

A taxonomic analysis based on similarities in terms of physical properties alone was therefore considered an inappropriate approach.

By contrast, a chemical structure approach should result in an extensible structure because it reflects the fundamental elements that make up a polymer molecule. Taking no account of property values or observed physical behaviours, the resulting classification will be based solely on criteria of similar molecular structure and features. The idea is that this will produce a "natural" classification and that grades with similar physical behaviours will be grouped together automatically; though in practice this is likely to be valid only for properties closely dependent on molecular structure, and not for those with dependencies on external factors such as geometry, or fillers. These proposals were explored in detail, as follows.

5.5 Some chemical hierarchies

Detailed attempts at creating a hierarchy based on molecular aspects alone are illustrated below. It is important at this stage to differentiate between two types of hierarchical structures: a) compositional hierarchies of nested entities, which take account of scale, so that a subsuming entity is larger than those part entities it subsumes, and b) control hierarchies, where the entities higher up the hierarchy exercise broader influence than those below it. Control hierarchies may or may not be nested.

Salthe [47] proposes that the world is ordered in both of these ways simultaneously. The following illustrations may appear on first viewing to depict nested hierarchies of polymer components (bond types, main chain atoms, functional groups, etc). However they are all control hierarchies, wherein fundamental features of molecular structure are the primary criteria for factoring, assuming they will exercise influence over the properties of the materials subsumed. Descending through the hierarchies, divisions are based on smaller and smaller differences in molecular structure, but the entities subsumed are not those molecule parts specified, but rather molecules *containing* those parts.

Figure 3 shows a hierarchy based solely on chemical considerations, that is, the atoms and groups of atoms (functional groups) present within the engineering polymer molecule.

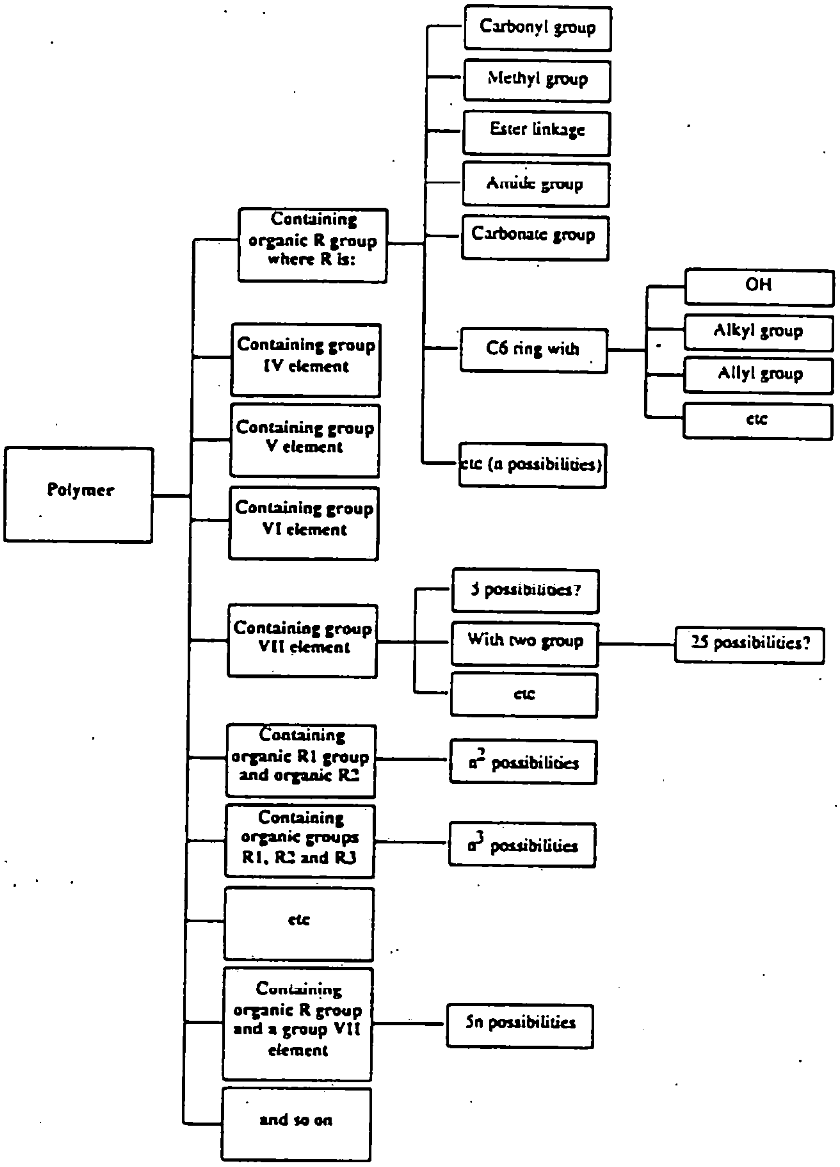

Figure 3: A purely chemical hierarchy

This leads to a very complex structure with an almost endless list of possibilities of atom/group combinations. No consideration is given to whether the combinations exist, or are likely to exist, in real materials: such considerations would undermine the potential for new and currently unpredictable molecules and would therefore preclude extensibility. The approach is too general to offer real organisation and does not group together materials in an insightful way with regard to their observable physical properties. It also ignores many important spatial considerations which are brought into the picture in the next attempt.

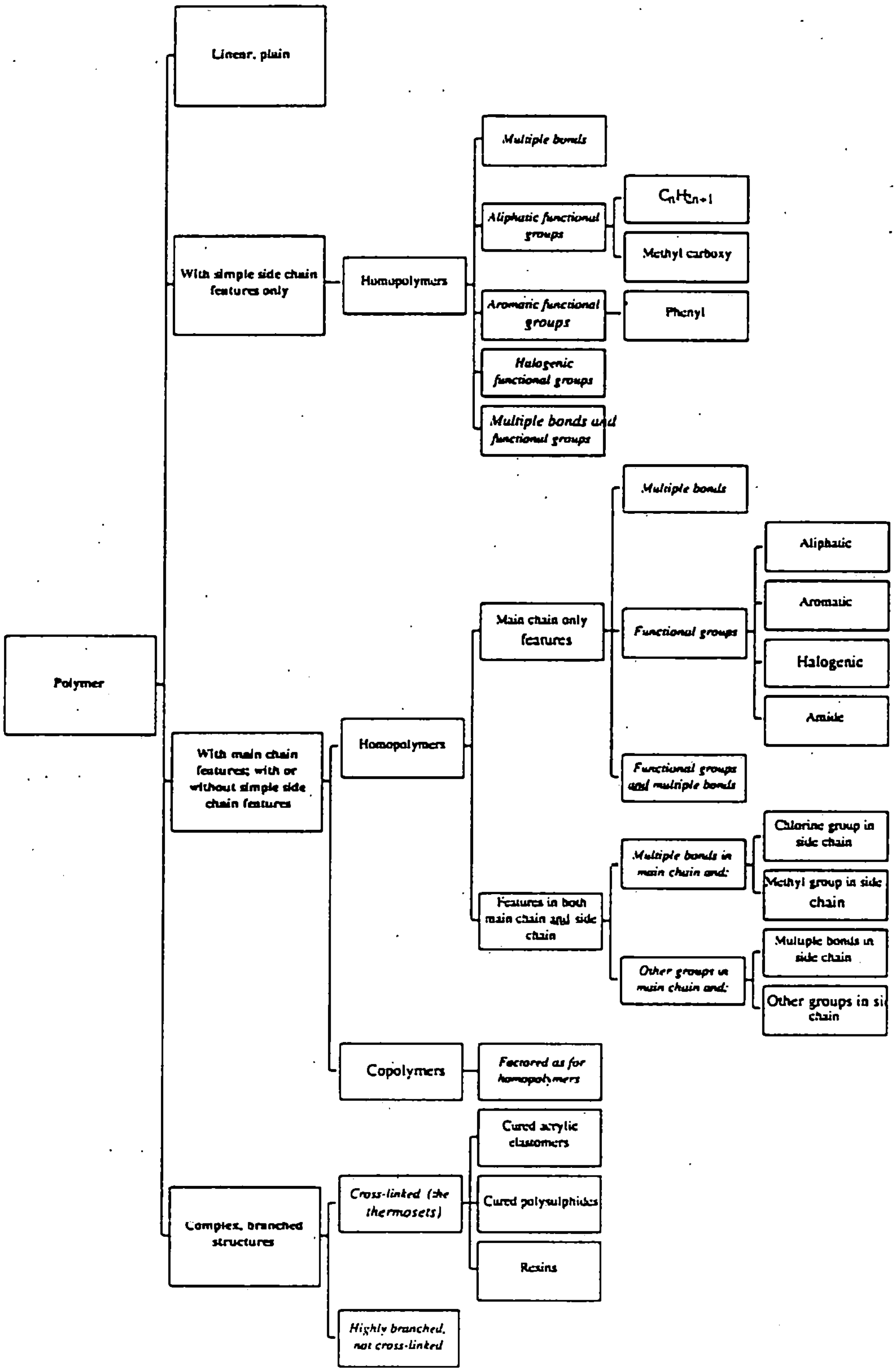

Figure 4: A hierarchy based on molecular features

Figure 4 shows a hierarchy based on chemical features considered to be important within the domain of polymer chemistry, including multiple bonds as well as atoms and functional groups. It is designed to consider sufficient factors to cover the domain completely without introducing unnecessary complexity, and to order the important chemical features within a hierarchy that takes account of the approximate shape of the molecule, the position of the features, the monomer order and the degree of bonding within the polymer molecule. This is a good illustration of the number of factors that need to be considered, and the difficulty of including them in a tree-like structure, even when the issue of the elements/groups present has been simplified considerably.

Inspection of the resulting groups confirms some useful generalisations.

The class of heterochain polymers whose back-bone contains oxygen, nitrogen or sulphur falls neatly out of this classification and, as expected, contains materials with properties that are usually more temperature stable and that display, for the most part, high strength, toughness, stiffness and abrasion resistance. Thermosets and thermoplastics are just discernible as separate groups; the thermosets as the first branch of the "Complex, branched structures" class and the thermoplastics as the rest, although the division is perhaps not given the emphasis it deserves in this classification.

The presence of double bonds in the molecular structure often implies the potential for elastomeric behaviour, but does not delimit any elastomer class (illustrated, for example, by ethylene-propylene elastomers, which are formed from the copolymerization of propylene with ethylene and would not be picked up by the double bond criterion). Fluorine containing polymers often show good resistance to hostile environments (such as acid, organic solvent, etc).

However individual effects can easily be off-set or even negated by other factors and unfortunately it cannot be said that property values generally accord with the resulting classes. Property types are certainly not accounted for by such an arrangement.

In addition, finer details, which have observed effects on the properties of polymers, such as the stereochemistry of those with asymmetric carbon atoms, which has important implications for the crystal structure and related properties, or the configuration around a double bond, (a good example being isoprene in the *cis*-1,4 configuration which has well known rubbery characteristics as compared with other configurations of the same molecule) are difficult to integrate into such a structure without creating excessive complexity. Figure 5 depicts a hierarchy based solely on considerations of molecular structure. The additional level of confusion that would arise if these were included within a hierarchy based on the polymer chemistry, such as that in Figure 4, may be easily inferred.

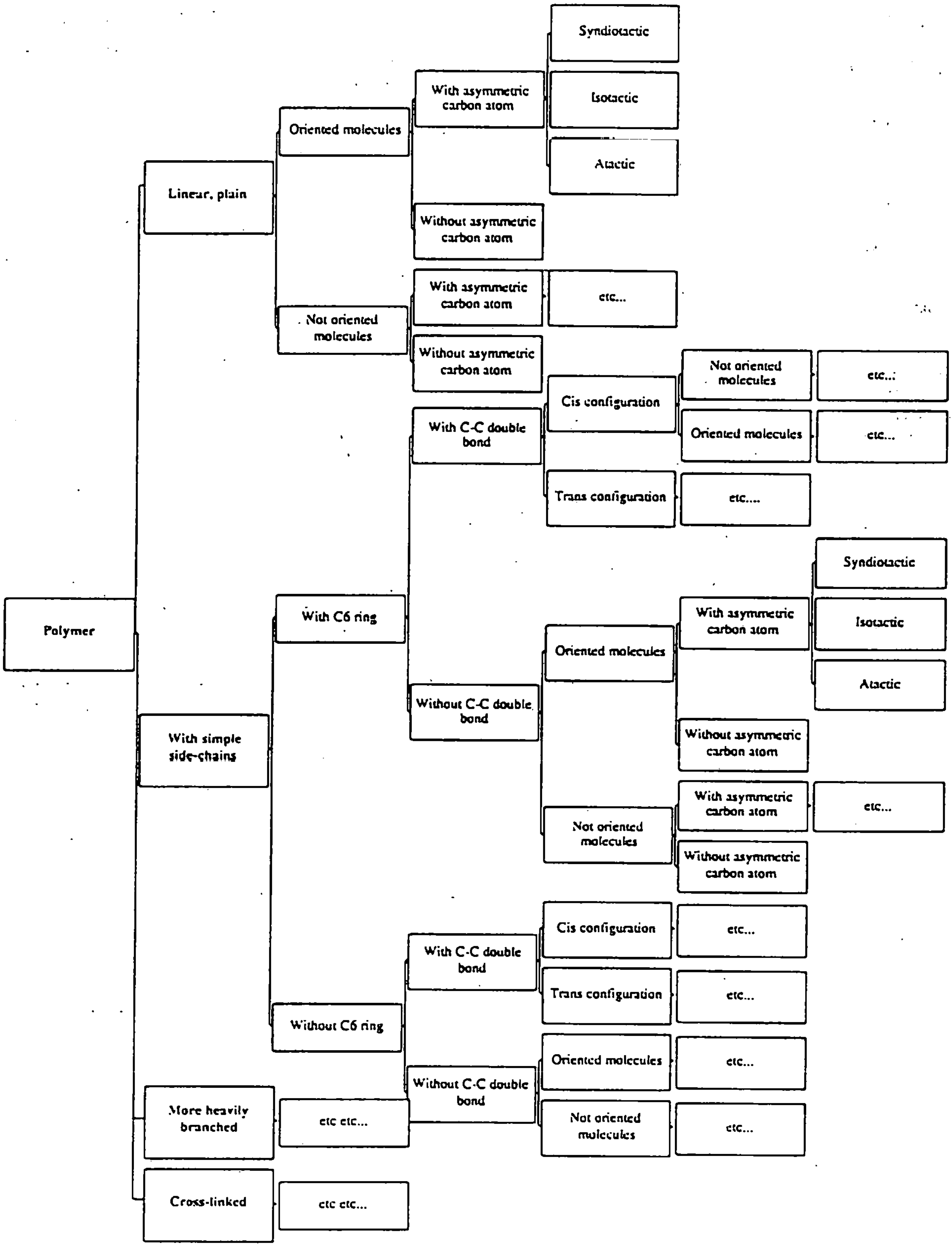

Figure 5: A hierarchy based on purely structural considerations

The true extent and complexity of the full hierarchy based on just these molecular aspects is perhaps better illustrated by the following illustration of the complete structure, outlined in a different format.

- Polymer
  - Linear, plain
    - Oriented molecules
      - With asymmetric carbon atom
        - Syndiotactic
        - Isotactic
        - Atactic
      - Without asymmetric carbon atom
    - Not oriented molecules
      - With asymmetric carbon atom
        - Syndiotactic
        - Isotactic
        - Atactic
      - Without asymmetric carbon atom
  - With simple side-chains
    - With C6 ring
      - With C-C double bond
        - Cis configuration
          - Not oriented molecules
            - With asymmetric C atom
              - Syndiotactic
              - Isotactic
              - Atactic
            - Without asymmetric C atom
          - Oriented molecules
            - With asymmetric C atom
              - Syndiotactic
              - Isotactic
              - Atactic
            - Without asymmetric C atom
        - Trans configuration
          - Oriented molecules
            - With asymmetric C atom
              - Syndiotactic
              - Isotactic
              - Atactic
            - Without asymmetric C atom
          - Not oriented molecules
            - With asymmetric C atom
              - Syndiotactic
              - Isotactic
              - Atactic
            - Without asymmetric C atom
      - Without C-C double bond
        - Oriented molecules
          - With asymmetric carbon atom
            - Syndiotactic
            - Isotactic
            - Atactic
          - Without asymmetric carbon atom
        - Not oriented molecules
          - With asymmetric carbon atom
            - Syndiotactic
            - Isotactic
            - Atactic
          - Without asymmetric carbon atom
    - Without C6 ring
      - With C-C double bond
        - Cis configuration
          - Not oriented molecules
            - With asymmetric carbon atom
              - Syndiotactic
              - Isotactic
              - Atactic
            - Without asymmetric C atom
          - Oriented molecules
            - With asymmetric carbon atom
              - Syndiotactic
              - Isotactic
              - Atactic
            - Without asymmetric C atom
        - Trans configuration
          - Oriented molecules
            - With asymmetric carbon atom
              - Syndiotactic
              - Isotactic
              - Atactic
            - Without asymmetric C atom
          - Not oriented molecules
            - With asymmetric carbon atom
              - Syndiotactic
              - Isotactic
              - Atactic
            - Without asymmetric C atom
      - Without C-C double bond
        - Oriented molecules
          - With asymmetric carbon atom
            - Syndiotactic
            - Isotactic
            - Atactic
          - Without asymmetric carbon atom
        - Not oriented molecules
          - With asymmetric carbon atom
            - Syndiotactic
            - Isotactic
            - Atactic
          - Without asymmetric carbon atom
  - More heavily branched
    - etc etc
    - etc etc
  - Cross-linked
    - etc etc

It is clear that accounting comprehensively for structural factors would be an impractical task: there are many of them and no clear reasons for their prioritisation within a hierarchy. In addition such considerations cannot easily be applied to a set of engineering polymer grades as often the structure is not known to this level of detail.

Yet these finer details of molecular structure can sometimes be the most significant contributors to the properties and uses of a material. Even if they are ignored, the number of combinations of chemical functional groups and bond types is very large, implying the need for an equally large number of classes, since every new combination may result in a new set of characteristics due to the combined, unpredictable effects of several interacting groups. This approach to classification is therefore both unwieldy and produces unsatisfactory results.

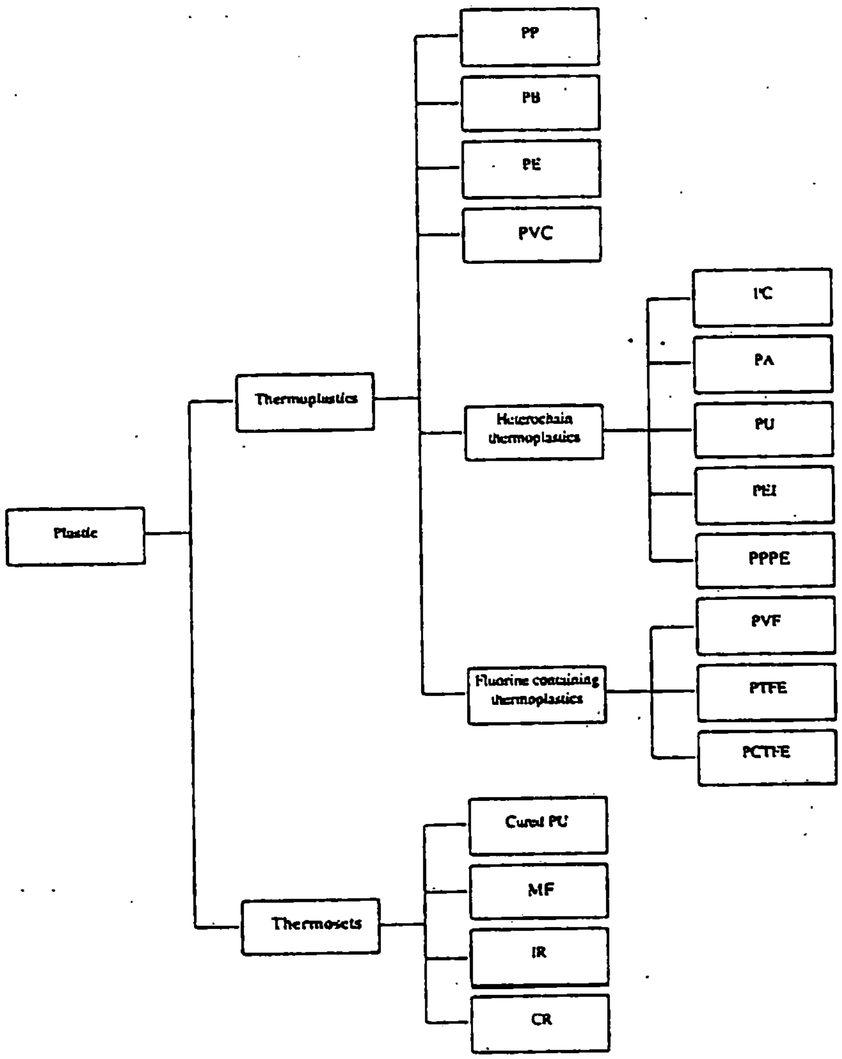

Figure 6: A simplified molecular hierarchy

Figure 6 depicts an attempt at a less detailed classification based on molecular features. The features with important property implications that were brought to attention in Figure 4 have been stated explicitly to simplify the structure. Although this hierarchy appears of more practical use, it is seriously flawed. For example, there is no obvious place for heterochain thermoplastics that also contain fluorine, nor does it give any indication of the presence of crystallinity. There will be other features with important ramifications (for example the presence of highly electronegative groups, which introduce polarity into the molecule) that cannot be included as their classes would overlap with existing ones. All other hierarchies based on this approach were discarded for similar reasons.

5.6 The optimum structure

It is proposed that a taxonomy based on the initial factoring of all plastics into the superclasses Thermoplastic and Thermoset followed by the factoring of Thermoplastic into Amorphous and Partly Crystalline provides the starting point for a classification system that will group together plastics with broadly similar properties, since these are important distinctions which reflect fundamental and far reaching differences between the classes they subsume.

The subclasses of these major classes must be chemical classes, and are chosen so as to describe their members in a broad and straightforward way, i.e. according to the major chemical groups on and in the polymer chain. Such classes, often made distinctive by their behaviour with respect to certain properties only, are already familiar. For example, polyamides (Nylons) share a sensitivity to moisture which acts as a plasticiser. Whilst it is possible for a property of one grade of Nylon to be radically different from that of another because of some reason such as a subtle detail of molecular structure, or process or geometry (highly aligned polymer chains designed to promote stiffness of a thread for example), it is argued that their grades will exhibit broadly similar characteristics for the purpose of materials comparison.

Decisions made early on in the design process use the nomenclature of these accepted plastics classes together with other broad generalisations. Materials selection for a new front panel assembly of a British Rail train is reported by Narraway [48] who describes how design requirements included adequate strength and rigidity combined with ease and economy of manufacture, transparency and the ability to accept paint. This high-level, verbal specification excluded all glass-reinforced plastics; acrylics were considered unsuitable for the impact requirements, and PVCs were eliminated because of their low temperature structural properties.

These chemical family classes have many advantages. They enable the convenience of using an accepted nomenclature and capture the general information considered useful by designers. They convey the essence of a material with a distinctive, recognisable character: something which, for example, the phrases "All plastics with an impact strength over x and Young's modulus greater than y," or "All plastics containing a double bond in an ethyl group side chain" do not achieve.

Grouping the chemical family classes and abstracting their information into designated superclasses requires the ascription of a physical or microstructural type to an entire family. This is not always possible, but a compromise may be reached. Where chemical classes are split between superclasses the problem may be dealt with by appropriate nomenclature: for example two polyurethane classes can be included: Thermoplastic_Polyurethanes and Thermoset_Polyurethanes, the first as a sub-class of Thermoplastic and the second as a sub-class of Thermoset. The resulting structure is extensible because of the implicit knowledge contained in its chemical and physical factoring.

Deeper factoring is possible where broad chemical families clearly subsume other chemical families; polyolefins cover polyethylenes and polypropylenes, for example. A more detailed factoring than this is prevented by the complexity and the number of exceptions it would introduce.

Although an elastomer class would appear to be of practical benefit, justification for its inclusion and positioning is not adequate.

Elastomeric behaviour occurs as a direct result of certain molecular features, such as the presence of double bonds leading to a glass transition temperature below room temperature, or the presence of cross-linking to prevent flow: this suggests its applicability within a primarily chemical/microstructural classification.

But the definition of a material as elastomeric is decided purely by its physical behaviour (e.g. the value of the elastic modulus). This is because there is no single chemical or microstructural feature, or clearly definable combination of such features, that enables a natural factoring of elastomers to be created. To include an elastomer class would therefore be to introduce an approach similar to the physical properties method described earlier, and would introduce a bias in favour of a certain physical behaviour at some point in the hierarchy. The result of these considerations is that no special class has been set aside for elastomers.

Figure 7 shows an outline of the hierarchy that is judged to be the most useful representation of engineering polymers. It also illustrates the specification and inheritance of properties. The full hierarchy in a different format follows.

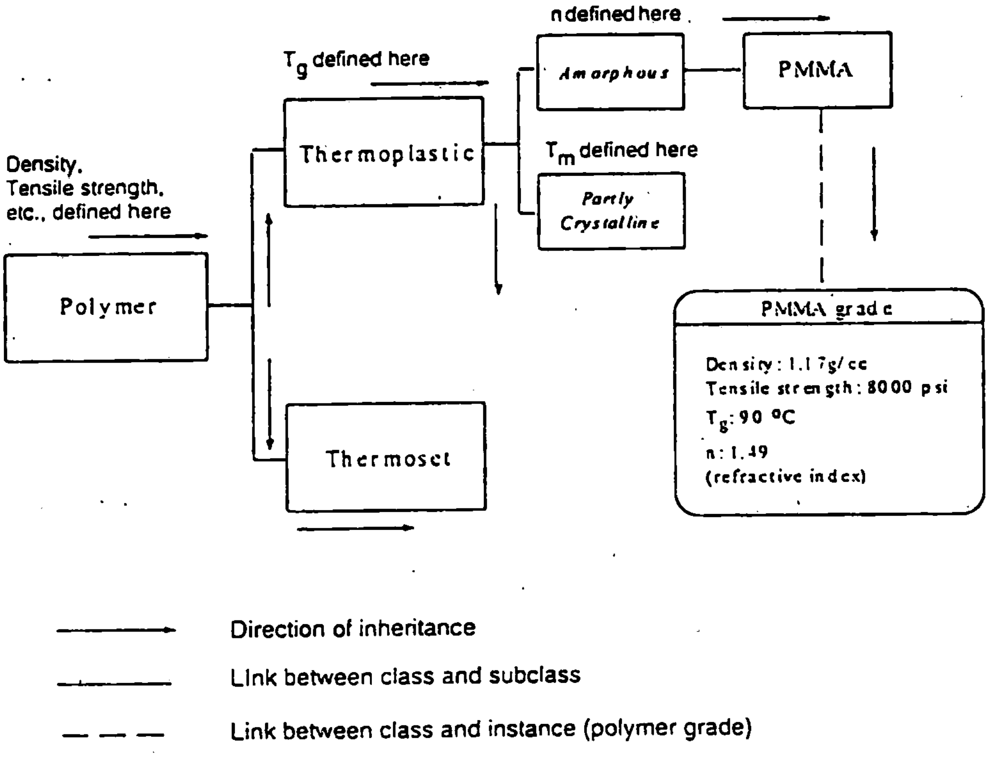

Figure 7: The optimum hierarchy, based on microstructure and chemical class.

A working hierarchy of polymer classes

- Polymer
  - Thermoplastic
    - Amorphous
      - PVC
        - PPVC
        - UPVC
        - CPVC
      - PVCA
      - PVAC
      - PVB
      - Ethylenecopolymers
        - EVA
        - Ionomers
      - PVAcetal
      - PMMA
      - Nitrileresins
        - PAN
        - SAN
      - Styrene-basedpolymers
        - Homopolymers
          - PS
            - HIPS
            - XPS
        - Copolymers
          - SAN
          - ABS
          - MBS
          - ASA
          - SMA
      - PVP
      - Poly(vinylesters)
      - MediumMWtPEO
      - Polyarylate
      - PAS
      - PES
      - PEI
      - PAPI
      - Polyarylether
      - PC
      - Polyphenylsulphone
      - Phenoxyresins
      - Poly(parabanicacids)
      - Polyhydantoinresins
      - ModifiedPPO
      - PSU
      - Thermoplastic_PU
      - Cellulosics
        - CP
        - CAP
        - CAB
        - CA
        - EC
        - CN
      - Polymethacrylimide
    - Crystalline
      - PPS(linear)
      - Polyolefins
        - PE
          - HDPE
          - LDPE
          - LLDPE
          - MDPE
          - UHMWPE
          - XLPE
          - CPE
        - PP
          - CPP
        - Polybut-1-ene
        - PB
        - PIB
        - PBT
          - akaPTMT
      - CrystallinePVC
    - Polyfluorocarbons
      - Homopolymers
        - PTFE
        - PCTFE
        - PVF
        - PVDF
        - PFA
      - Copolymers
        - FEP
        - PECTFE akaECTFE
        - PETFE akaETFE
    - PVA
    - EVA
    - Polyvinylidenechloride
    - PA
      - PA6
      - PA6/6
      - PA6/10
      - PA6/12
      - PA10
      - PA11
      - PA12
      - Transparentnylons
      - Aromaticnylons
    - POM(Polyacetal)
    - PEEK
    - LinearPPS
    - AlkylsubstitutedPPO
    - PET
    - HighMWtPEO
    - PBTB
  - ThermoplasticElastomers
    - PMP
    - Copolyesteretherelastomers
    - TPU
    - PETP
    - PPPE
      - EPR
      - ETFE
    - SBS
    - PolyepichlorohydrinEOcopolymers
    - Elastomericpolyamides
  - Thermoset
    - ThermosetElastomers
      - Dienerubbers
        - BR
        - SBR
        - IR
        - IIR
        - CR
        - Naturalrubber
      - Acrylaterubbers
        - MBS
        - NBR
        - NCR
      - AcrylicRubbers
        - Alkyl2-cyanoacrylates
        - Dimethacrylates
    - Acrylic adhesives&resins
    - Polyimides
    - Vulcanisedpoly(epichlorohydrin)
    - Vulcanisedpolysulphides
    - Cross-linkedPPS
    - DAP
    - DAIP
    - ADC
    - Epoxides
      - DGEBA
    - Thermoset_PU
    - Polyisocyanurates
    - Furanes
    - PFresins
    - RF
    - Aminoplastics
      - UF
      - MF
      - Melamine-phenolformaldehyde
    - PolyesterResins
      - Orthophthalic types
      - Isophthalic types
      - Terephalic types
      - Bisphenol types
      - Vinylester types
    - SiliconeResins

5.7 Testing the structure

5.71 Implementing the hierarchy into POISE

The implementation of the final hierarchy within POISE is illustrated by a snapshot of the hierarchy screen in Plate 1. The tools available for the restructuring of this hierarchy, the movement of properties and viewing the abstracted data have already been discussed in section 4.1. These were used extensively for organising the classes to correspond to the final hierarchy and for placing certain properties (such as refractive index) selectively.

5.72 Properties, and the available data set

The data used within the POISE system originate from the CAMPUS™ database. Although relatively large, specifying approximately fifty properties and containing over one thousand commercial grades, CAMPUS™ is typically an incomplete and imperfect data set. Its particular weaknesses have been revealed through exploration of the data with the Property Comparison tool, and these weaknesses prevented a complete testing of the hierarchy.

Specifically, it was found that a large number of properties are universally unpopular: invariably, grades do not have values specified for these properties. This has limited useful exploration to a few commonly measured properties that give good distributions for most classes. These properties are:

Creep modulus at 1000h
Density
Heat Deflection Temperature A
Izod Impact Strength at 23 °C
Relative Permittivity at 1 MHz
Specific Volume Resistivity
Strain at Break (50 mm/min)
Strain at Break (5 mm/min)

Strain at yield

Stress at yield

Tensile Strength

Young's Modulus

Short though this list may seem, it gives a good broad idea of the behaviour of a polymer material, covering mechanical, thermal and electrical properties.

Other weaknesses in the CAMPUS™ database arise because of the particular manufacturing biases of its contributors. Most are primarily in the business of thermoplastics, with the result that thermosets are under-represented. Within the thermoplastic genre, only a few classes are well populated (polyamides being the largest class). Investigations were restricted to those classes with a substantial amount of data. In addition to the abstract classes Polymer, Thermoplastic, Thermoset, Partly Crystalline Thermoplastic and Amorphous Thermoplastic, three subclasses each of both the Partly Crystalline Thermoplastic and the Amorphous Thermoplastic classes have been considered in depth. A lengthy inspection of all other classes revealed insufficient data to test the structure. However the wealth of polyamide data enabled a thorough inspection of this particular class and its subclasses. In addition a small exploration of the copolymers present in the database has been performed.

5.73 The abstract classes

For each of the above properties, two Comparators were employed to illustrate the nature of the abstract classes. One showed the distributions for the all-subsuming class Polymer against its subclasses Thermoset and Thermoplastic, and the other showed Thermoplastic in juxtaposition with its subclasses Partly Crystalline and Amorphous.

This investigation revealed so little data for the class Thermoset that it was not discernible on the large scale necessary for the display of the Thermoplastic data. The two cases where data were discernible were for the common properties density and tensile strength; these distributions are illustrated in Plate 3. They show that thermosets have densities approximately in the middle of the range for all polymers, but their tensile strengths tend to fall below the average for polymers in general.

For each of the selected properties, a comparison of the classes Thermoplastic with its subclasses Amorphous and Partly Crystalline (indicated on the Comparator screens as simply "Crystalline" for convenience) proved more worthwhile.

For the properties creep modulus at 1000 hours, density, and heat deflection temperature A, it was found that the range of values covered by the Partly Crystalline and Amorphous classes was approximately the same, but slightly wider for the Partly Crystalline class in all cases: see Plate 4.

A similar situation applies for the property Izod impact strength at 23°C, but one particularly high value for the Partly Crystallines was evident. This was inspected by selecting the bar and calling up the grade view window, which showed the two grades in question to be of the family PESU; see Plate 5. These have obviously been classified in CAMPUS™ as polyethylenes, probably wrongly as the acronym is more likely to stand for unplasticised polyethersulphone, although it has been difficult to verify this. Even if they are Amorphous grades, they are still clearly of unusually high performance; there was no comment provided that might explain this observation. However the exercise did show both the importance of accurate classification mechanisms in an automated system such as this, and also the worth of informative commenting.

The property relative permittivity showed nothing of note for the selected classes (again the range for the Partly Crystalline class was slightly wider), and the same applied to the properties strain at break (50 mm/min), strain at break (5mm/min), stress at yield, Vicat A and Young's modulus. However for strain at yield the Partly Crystalline class showed some significantly higher values: these turned out to be polypropylenes but again there was no supporting commentary to suggest why their performance should be so noteworthy; see Plate 6.

Tensile strength showed some high values for the Amorphous class which turned out to be of the PAPPE family (again probably wrongly classified as this is a copolymer of polyamide and a polyolefin elastomer which could have exhibited a degree of crystallinity).

Finally specific volume resistivity showed a large split between the thermoplastics, reflected across both the Amorphous and Partly Crystalline classes, see Plate 6. Inspection of all parts of these distributions showed, however, that the same polymer families were present in both the high and the low bars, implying that the division was not family based, and in addition there was no description for the grades that explained their electrical behaviour (although the high resistivity partly crystalline ones did have electrical applications, see Plate 7 for an example). It is considered that the shape of this particular distribution could be as a result of the very large values of the property itself and the way in which it is expressed: different units or a logarithmic scale would perhaps be more appropriate.

The overall conclusions drawn from this survey of the abstract classes, for those properties with significant data associated with them, are that partly crystalline polymers are likely to exhibit slightly higher values of modulus and tensile strength properties than amorphous polymers. However the ranges are broadly similar and the lower values are also taken by partly crystalline polymers. This could be due to the directional dependence of their strength properties (because of molecular orientation) and the effect of the method of measurement on the result (despite standardisation attempts). Partly crystalline polymers also seem to perform better under impact tests and tests of tensile stability to heat, but are not distinguished by their electrical behaviour and are perhaps not as significantly different from amorphous polymers in terms of their measured behaviour as might have been expected.

5.74 A selection of amorphous thermoplastic classes

The amorphous thermoplastics are not well represented on the CAMPUS™ database and so classes have been selected by virtue of the presence of their grades and data, for the exercise of exploring the potential of the hierarchy. In this case the classes PS, PVC, PMMA and MABS have been investigated for the selected property list, although only the three most populated classes of these four were inspected for any one property.

For the properties creep modulus at 1000 hours, density, heat deflection temperature A, relative permittivity, strain at break and stress at yield, the different behaviours of the selected classes were illustrated clearly, with polystyrene, PS, generally offering lower values than the other classes, in accord with its commonly low performance rating and cost. PVC performed well for heat deflection temperature A and relative permittivity but was inferior to PMMA for strain at break, and showed a generally wider spread than all others for stress at yield, the one property for which PS performed well. These trends are illustrated in Plates 8 and 9.

The properties density and Young's modulus yielded more interesting results. For density, (also shown on Plate 8) a wide spread was shown for PVC. Inspection of a high value revealed that it was from a grade with lead stabilisation. A high density value for PS showed that it came from a grade noted for its dimensional stability and rigidity, suggesting that the high density was designed in to facilitate this. See Plates 10 and 11 for the selected grades from each of these classes.

The property comparison for Young's modulus revealed similar distributions for PMMA, PS and PVC (see Plate 12) except for one very high value for a grade of PS. On inspection this turned out to be the same grade that gave a high density value, confirming that the rigidity requirements had been attained. This may suggest some loose correlation between density and modulus in certain cases.

Other properties either had insufficient data for judging their distributions or revealed no noteworthy aspects. However it is noted that an absence of data for the properties strain at yield and strain at break can be because some grades actually don't yield or break under those particular test conditions: a high performance phenomenon with important implications for system design: it is essential that a data display system does not neglect values simply because they are not numeric, and an alternative to the Comparison Tool is desirable in these cases.

The main conclusions drawn from this particular investigation, however, are that different amorphous polymer family classes behave differently for many properties. For a simple (i.e. unmodified) material, a family will display an easily identifiable range of likely property values that is noticeably different (even if only shifted somewhat) from that for other families. However there are cases where the ranges overlap considerably, making it difficult, on the basis of just a few properties, to characterise that family as distinct from another. In addition, modification, by means of fillers, reinforcements, chemical fine-tuning, etc., (discussed in more detail in the following section), is common, and distorts property values significantly, as illustrated by preceding examples.

5.75 A selection of partly crystalline thermoplastic classes

For the Partly Crystalline class investigation, the polymer families PA, PBT and POM were chosen on the basis of data availability.

Creep modulus at 1000 hours gave a very similar range for all three classes with the exception of an outlier in the PBT class with a very high value. Inspection of the source of this datum revealed a grade with glass fibre modification, designed especially to have a reduced tendency to warpage, see Plate 13.

Izod impact strength and relative permittivity produced overlapping distributions for these classes; variations in the range resulted simply from the difference in the quantities of data present, as with many other of the properties. Strain at break and stress at yield both showed a few high values for the PA class but inspection of the grades in question gave no insight as to the reasons, since there were no comments available. It was noted that grades that lack commentary are invariably BASF grades, showing the supplier dependence of useful information.

Young's modulus gave a more interesting result: although the distributions were similar for all three classes, a few very high values were apparent for PA and PBT. Inspection of the grades revealed nothing for the PA (as they were not commented) but showed the PBT grades to have 45% glass fibre reinforcement; see Plate 14.

Heat deflection temperature A also showed a distinctive distribution, shown on Plate 15. For the classes PA and PBT the distributions are bimodal with null points at approximately the same value (about 150°C). This pattern is possibly also reflected for POM but there are insufficient data to be sure of this.

Further investigation revealed that all of the grades in the top halves of the distributions for PA and PBT have some degree of glass fibre reinforcement: 12 - 45% for PA and 15 - 40% for PBT. The POM grades were not commented. This provides clear evidence of the potent effects of reinforcement.

The property density, also on Plate 15, showed a wide range of values for all three classes (bearing in mind that POM has less data) and illustrates little more than the variety that is possible within these classes (an important observation nonetheless, as density will affect other properties) and the overlap between them.

Overall the conclusions are the same as for the Amorphous families, except that the differences between property ranges for these particular Partly Crystalline classes are not as distinct.

5.76 A closer look at the PA class

The class PA and its subclasses merited further inspection due to the number of polyamide grades and data available in CAMPUS™: A comparison of PA with its subclasses PA6 and PA6,6 was performed for a number of properties.

No significant difference was found between these subclasses: PA6 and PA6,6 cover very similar property ranges and the commonly accepted differences (such as the fact that PA6,6 generally has a higher modulus than PA6) are not apparent from these data. This could be because the crystallinity and the molecular mass distribution - which have far-reaching effects on other properties - of both polymer types may be easily and widely varied during process. Property ranges for both subclasses will therefore be wide, resulting in overlap between them. Selective production of popular grades may skew the distribution to hide the true subtleties of difference betweeen these polymer families, see Plate 16.

5.77 An investigation of a few copolymers

Copolymers result from the simultaneous polymerization of two or more monomers and comprise a sequence of these monomer units along the polymer backbone. The units may be alternating, random, or arising in blocks. Copolymers have been given little attention so far in this study, primarily because they are considered to exhibit overall behaviours distinct from those of their related polymer families, despite inheriting certain characteristics from each contributing monomer. The issue of whether they should be subclasses of one of those "parent" polymers is therefore an awkward one: they cannot be subclasses of both simultaneously and justification for inheritance from either "parent" would be difficult to find. For the purpose of the classification they have therefore been treated as individual polymer families in the same way as the above-mentioned families.

However it was thought that a limited exploration of the properties of copolymers as compared with those of the polymers produced from their constituent monomers may be of some interest. See Plates 17 and 18, which show histograms for the classes ASA, PC, and ASAPC.

These comparisons accord well with the idea that each monomer contributes some of its own character to the resulting copolymer, since the property values of the copolymers are approximately mid-way between those of their related polymers. However this concept does not extend to the property notched impact strength, where the copolymers in each case show a potential for much higher values than their equivalent monomer polymers.

5.78 A search for evidence of an accepted "rule of thumb"

The Property Comparison Tool may be used to confirm some generalised behaviours of polymers. It had been hoped that some algorithms or "rules of thumb" could be found that related only to certain classes of engineering polymer, enabling exploitation of the object-based functionality of Smalltalk™. However, although some trends of physical behaviour are unique to certain polymer families, they are not easily amenable to mathematical modelling (they usually employ scientific parameters describing, for example, the change in the enthalpy of dissolution with respect to the number of carbon atoms on the polymer backbone: quantities not typically quoted by polymer suppliers). The engineering rules of thumb that were sourced generally apply to metals and, again, use properties not found on a polymer database.

However, Pugh's Rule [49], usually applied to hexagonal close-packed metals, offered a chance to test the system since it showed remarkable similarity to another rule of thumb employed by Barrie [29] in his plastics consultancy work. Pugh's Rule predicts the deformation behaviour of crystals and states that a knowledge of their ductility as well as their fracture strength is required for this. Pugh proposed that the extent of the plastic range of a pure metal could be deduced from the ratio of the elastic bulk modulus, K, to the shear modulus, G. This gives the following:

High K/G implies ductility

Low K/G implies brittleness.

Barrie suggests, without physical explanation, that for engineering polymers a high value of Young's modulus (over 3500 MPa) implies ductility and a low value of Young's modulus (below 2500 MPa) implies brittleness. Since Young's modulus is an elastic modulus this is identical to Pugh's Rule where the shear modulus is constant.

Barrie's hypothesis was tested by inspection of the Comparators for Young's modulus and notched impact strength for the classes PC, PS and PMMA. In fact only PC had enough data in both of these properties to offer a useful insight.

When high values of Young's modulus and notched impact strength were selected for PC, it was discovered that there were five grades (one a PCHT grade and the others PC) that occurred in both of the shortlists of these selections, out of a total of about ten grades in the high range of each. See Plates 19 and 20. When the lower values of each property were inspected, all twenty three grades from the low end of the notched impact strength distribution were to be found in the low end of the Young's modulus distribution. See Plates 21 and 22.

There is no documented physical connection between elastic properties and fracture behaviour, but these results do suggest that Pugh's Law can have some value when applied as a rule of thumb to this particular class of engineering polymers, and that the Property Comparison Tool can be used to provide confirmation or otherwise of general or specific rules of thumb for the available polymer data.

5.79 Summary of the exploration of POISE

The above exercise has illustrated the benefits of forming abstract representations of engineering polymers. The Property Comparison tool provides a useful means of displaying the data relating to an abstract polymer class in a visually accessible manner, presenting a picture of the physical nature of that class and how it compares with other classes.

Property value distributions can be seen to vary from class to class and show a generally tight spread for any class except where fillers and reinforcements affect the property values. The use of such additives is, however, a widespread phenomenon, and may be considered a distracting influence on the ability of the system to reflect the fundamental character of a material type. Their effects on property values are significant and it is important that the designer is aware of the factors influencing these values, whether the effect is beneficial or otherwise.

Some common examples of additives and their property effects follow.

(a) Impact modifiers, usually other polymers or copolymers, which increase values of impact strength properties, as illustrated below for polystyrene.

PROPERTIES	STANDARD PS	SEMI IMPACT RESISTANT PS	IMPACT RESISTANT PS	HIGH IMPACT RESISTANT PS
DENSITY (g/cm^3)	1.05	1.04	1.04	1.04
IMPACT STRENGTH @ 20°C (kJ/m^2)	10 - 16	40 - 60	60 - 80	NO BREAK
IMPACT STRENGTH @ -40°C (kJ/m^2)	-	35 - 50	50 - 70	70 - NO BREAK
NOTCHED IMPACT STRENGTH @ 20°C (kJ/m^2)	APPROX 2	5 - 6	5 - 8	8 - 14
NOTCHED IMPACT STRENGTH @ -40°C (kJ/m^2)	-	3 - 5	4 - 6	6 - 12

Table 5: Effect of impact modifiers on polystyrene [50]

(b) Plasticisers, which lower the elastic modulus and second order transition temperature of polymers without altering the chemical nature of the macromolecules;

(c) Extender fillers, which increase the density, elastic modulus, heat deflection temperature and hardness of a material, while lowering shrinkage and reducing cost;

(d) Reinforcing fillers, such as glass and carbon fibres, which generally increase the tensile strength and stress at break, the elastic modulus, the flexural modulus and the stiffness, and cause an improvement in creep behaviour and bend-creep modulus, though the effects are usually anisotropic;

(e) Many other types of additive such as anti-static agents, colourants, flame retardants, whitening agents, cross-linking agents, antioxidants, processing aids and stabilisers, all of which may have significant effects on the values of some properties.

The amount and type of additive are usually known or can be ascertained. It would be feasible to incorporate functionality into the system to take account of its effects by separating out those grades with comparable reinforcement to enable a fairer comparison, for example. Alternatively an algorithm could be devised to predict the effect of an additive on property values to enable "fair" comparison by calculating the theoretical value of the property for the unmodified material. Such methods are not currently in place but could be added with relative simplicity due to the object-oriented nature of the system.

There are, of course, cases where the factors influencing the spread of data are too subtle to quantify or model, a good example being stereochemistry, whose effects would be difficult to predict numerically. Such effects are illustrated below for density and crystalline melting point using polypropylene and poly 1-butene.

	Polypropy-	Lene	Poly1-	Butene
Property	Atactic	Isotactic	Atactic	Isotactic
Density	0.85	0.92	0.87	0.91
MP (°C)	- (softens at ~80)	165	- (softens at ~62)	128

Table 6: Density and melting points of atactic and isotactic polyolefins [41].

In cases such as this, it seems reasonable to consider these effects as characteristic of the polymer material class itself. For example, if stereochemistry results in a wide spread of density data for polypropylenes, polypropylenes are simply characterised by this fact.

The problems associated with accommodating different property types, i.e. generic (for general comparison) and use-oriented (to support selection for a particular use), into a polymer data system are considered in more depth, since these are particularly relevant to the design of a useful data structure, and represent a concrete example of the same conflict as that illustrated by the phenomenon of data distortion due to additives: that is, the inability of any simple taxonomy to adequately represent and abstract information that is relevant in both scientific and engineering contexts.

5.8 The property dialectic

An inheritance hierarchy based on principles of chemistry and microstructure is extensible and effective at abstracting the general, essential information about types of engineering polymer. It is nonetheless poor at gathering together and abstracting information from those grades that are similar from an engineering perspective but dissimilar from a scientific perspective.

Where additives affect the data, this means that, for example, a reinforced grade of Nylon may be more similar in a certain engineering context to a reinforced grade of polyester than to another grade of Nylon. So the chemical family grouping does not reflect all engineering similarities in this case. But such examples do not call for changes in the data structure, as the same properties are quoted throughout and comparison is still possible given methods of filtering out the additive effects.

Other examples of this phenomenon do have implications for the data structure of the system, however. For grades with special geometries, processing methods or artefact design factors, additional properties are required to those specified by their chemical family class in order to describe them.

The existing structure does not accommodate these additional properties and does not group together those grades specifically described by such properties, exemplified well by sheet and fibre grades where the surface to volume ratio is high and the effects of processing are extreme. In contrast it will accommodate scientific and generic engineering (3D) properties into the data structure well, because they are most resistant to variation due to geometry, processing and application specific effects.

Some examples of such specific engineering properties, in this case used to describe the behaviour of film and fibre grades, are to be found in Appendix 2.

In order to deal with this conflict without sacrificing the primary criteria of extensibility and independence from user bias, a way of enhancing the generic structure of Figure 7 is suggested. This enables it to accommodate and organise a population of grades that have been subjected to specific processes and tests and that are described by specific, use-oriented properties such as the above, without compromising the inherited, generic information arising by virtue of chemical characterisations.

6. Enhancing the structure: a property combining strategy

6.1 A formal outline of the problem

It has been established that a hierarchy based on chemical principles will be extensible but will not reflect similarities between grades from the point of view of specific, additional engineering properties. Thus, due to geometrical factors in particular, there will be properties appropriate for some grades of a chosen class but not for others, and yet the property representation of all of the grades in the class, as decided within the class definition in the hierarchy, will be the same if a hierarchical representation alone is used.

It is argued that this need to represent generality and at the same time to distinguish between some specifics of engineering significance is a generic informational analysis problem, leading directly to mixed hierarchies [9], criticised previously as being contrary to the principles of information representation.

There is therefore a need to provide a technique for organising grades that have associated with them the potential of more than one property type (the inherited generic properties and additional specific properties). For example, Dyneema's SK60 polyethylene fibre is described by the fibre property tenacity, which is never used for bulk materials: it represents strength per unit size where size is measured in denier and denier is the mass in grams of 9km of fibre.*

Here fibre-form plastics are used to illustrate the problem in general:

- There may be many fibre-form intances of one particular materials class and of scientifically dissimilar materials classes.

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* Although still widely used in the textiles industry, tenacity has become obsolete in other fields of engineering and has been replaced by specific stress, measured in N/tex where tex is the mass in g of 1km of fibre.

- Any one materials class that has fibre-form members may also have members that are not of a special form.

6.2 A possible solution: multiple inheritance

One approach to this problem is illustrated in Figure 8 which presents a multiple inheritance classification strategy to deal with the need for a dual factorisation. The Fibre definition adds the properties associated with being "fibrous" through the mechanism of inheriting both from the materials class and from the abstract class Fibre, so enabling the construction of instances of multiple property type definitions.

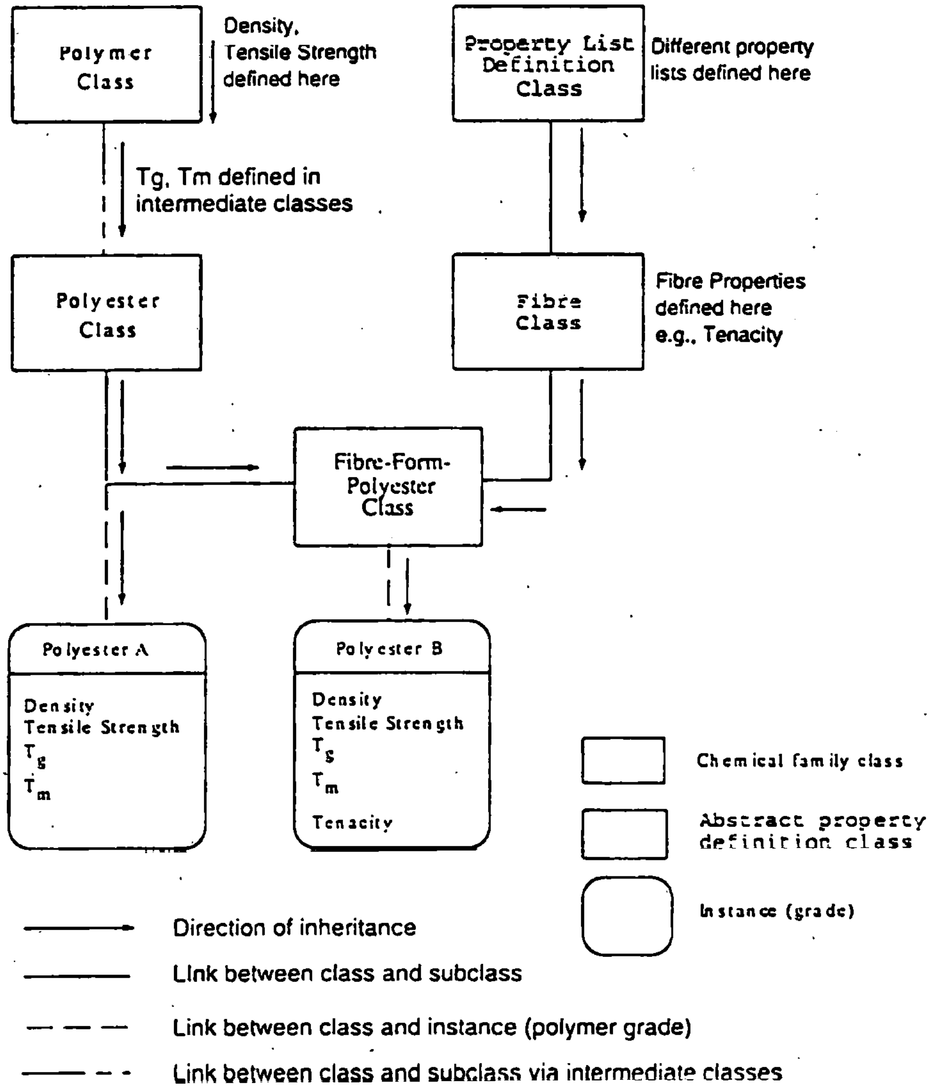

Figure 8: Multiple Inheritance

The effect on the classification structure of allowing the dual definition of classes of grades is to replace the single-inheritance class hierarchy, corresponding to the foregoing domain analysis, with a class network.

The key problem with the class network of Figure 8 is the proliferation of subclasses such as Fibre-form-Polyester, etc. Each such class will be a subclass of both the particular - form class and of any one of numerous materials classes. So for a full hierarchy there will be a vast number of these classes: Fibre-form-Nylon, Fibre-form-Polyethylene, Fibre-form-Polystyrene, Film-form-Polyester, Film-form-Polyethylene, Film-form-Nylon,and so on. What results is barely an organised grouping: the chemical families will be split into numerous form sub-classes; the form families will be split into numerous chemical sub-classes. All sub-classes will have a mixture of the properties they have inherited.

The applications that have been implemented in the POISE system make use of materials classes as entry points to collected data about materials families, through the previously described tools to help analyse their comparative characteristics. Abstracting use/form classes away from materials classes is at odds with the philosophy on which the generic structure is based and does not easily support the use of these comparison tools.

The difficulties introduced by multiple inheritance, therefore, are that:

- multiple inheritance demands that use/form classes are abstracted away, as subclasses, from the more general purpose class definition.
- the use/form grades that it constructs do not include a structural separation between their general-purpose properties and their use/form properties.

6.3 The proposed solution: orthogonal classification

These considerations have led to an implementation that preserves a single-inheritance class hierarchy that groups together grades and classes similar by virtue of chemistry and microstructure.

The materials classes, in POISE, are allowed to be partial, incomplete, extensible definitions of the data structures relating to their instances (the grades). The special-form grades include extensible property definitions that are independent of and supplementary to the inherited property definitions of all the grades that are occurrences of that materials class.

The terminal classes of the materials factoring will now be (partitionable) classes comprising both tailored and untailored grades of that materials family, where the tailored grades have associated with them their supplementary property definitions. Users of a plastics materials information system would expect grades to be defined firstly as occurrences of the materials family that offers their primary description [2].

The method of organisation for grades of the materials class Polyester, is shown in Figure 9. Polyester grades are partitioned between:

1. Instances of Polyester that connote general-purpose grades, as PolyesterA. This instance (i.e. its "property space") is fully defined by its class. Properties accessible through it such as density, tensile strength, T_g, T_m, are either expressed in the definition of Polyester or in a superclass of Polyester in the class hierarchy.

2. Instances, as PolyesterB, that exhibit not only the behaviours common to all Polyester grades, but also have associated with them additional use/form information. PolyesterB is constructed from a merger of two instances: an incompletely defined instance of Polyester containing the information conveyed by the Polyester class, and an instance of a fibre properties definition class which holds the additional information in the form of extra properties, in this case tenacity. These merged instances may be considered a single grade, whose property space is partitioned between the property set inherited through the materials hierarchy and one or more supplementary property sets.

PolyesterB serves as one illustration of how a grade may be generated both from a class definition and from a definition of behaviours that are extraneous to the general classification principle. Similarly, sheet form or foam form polymers could be constructed. In each case they will be linked conceptually to their materials class by membership, and linked officially to their use/form definition object by virtue of its supplementary behaviour contribution.

Specific grades of Polyester such as those used for the production of fibres are identified by the fact that they have additional, separate property lists to those of untailored grades. Thus the Polyester class is itself partitioned between its general purpose members and those specified additionally by the definition object used to supply the use-specific properties. What therefore results from this strategy is an additional classification of plastics grades, one entirely independent of the generic hierarchy and based on different criteria: a classification that provides an orthogonal factoring of plastics materials at the grade level of the existing taxonomy.

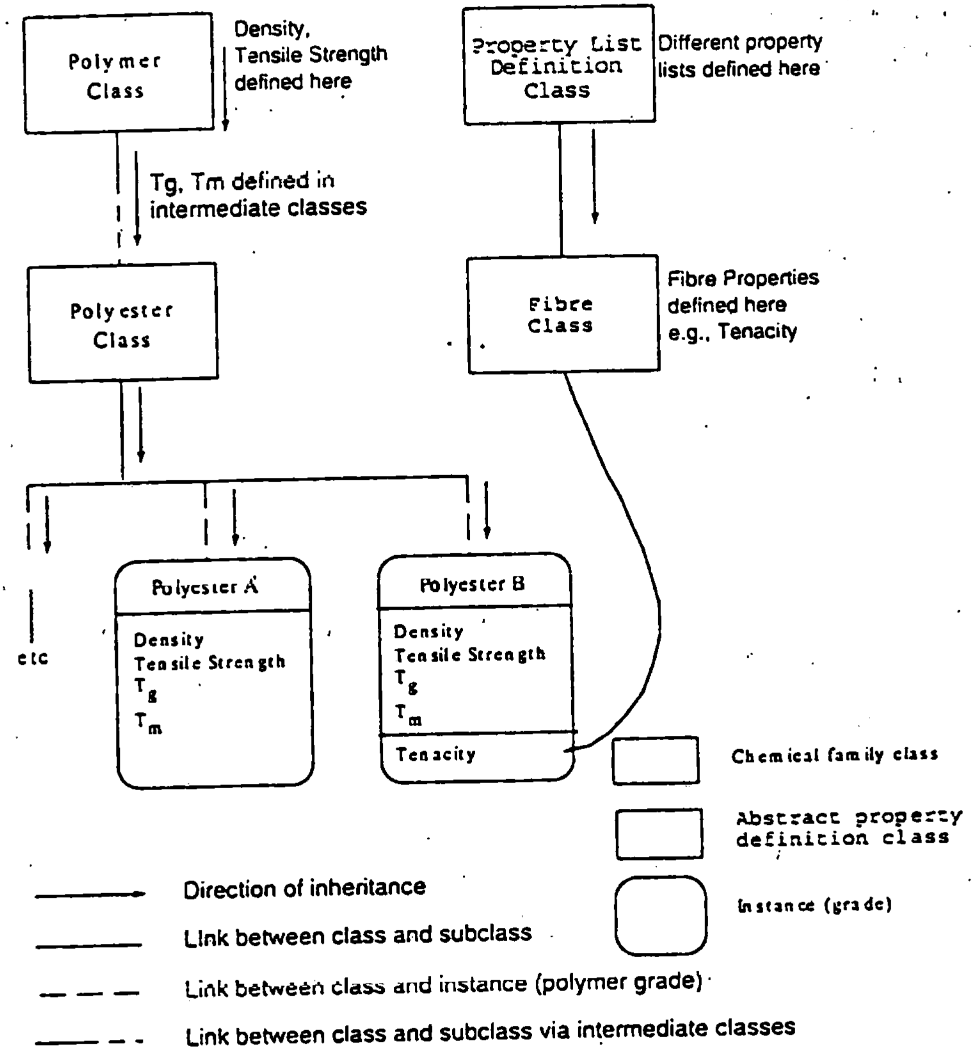

Figure 9: Adding properties selectively, thereby introducing an extra factoring of grades

This new mechanism facilitates further functionality for property comparison using the Property Comparison tool. For example, if a grade has reference to the source of its additional property lists, grades from different classes that share the same additional property may be compared. Thus the Comparator will function across selected grades of selected classes for selected properties.

6.4 Further development of POISE to incorporate the orthogonal classification mechanism

POISE was modified to incorporate this extra feature within the data structure [51]. A hierarchy of definition objects to create use-property-lists was developed, whose instances would provide the partial property space definitions to be appended to the general property spaces, inherited from the materials hierarchy, of the polymer instances. The link from an instance to a definition object is inherently dynamic: if a definition object is modified (e.g. to include previously unspecified properties) this is automatically transmitted to its dependent objects. Since the property space of each updated object remains sorted, their classes will remain partitioned, just as before the update.

The mechanisms within POISE that facilitate the merging of the two types of instance are discussed by Zucker [52] and make use of a Smalltalk™ "Access Enhancer object," which intercepts and manages the behaviour of the complete entity that acts as a single grade.

The interface was extended to allow use-specific properties to be defined and added to their appropriate lists. Plates 23 and 24 show the fibre menu within the property selection functionality and the property window on the fibre property tenacity, with comment, respectively.

If a grade requires an additional property list to be specified for it, a simple menu option within the Grade View window allows any number of these lists to be added to the data specification of that grade alone: the data relating to those special properties must be input after this operation has been performed, and, when viewed, will be seen as distinct from the data pertaining to the generic properties, whose specification has come via the polymer materials hierarchy.

POISE automatically records grades that have additional property lists associated with them, and was modified to enable selective viewing of those types of grades, using the

Property Comparison tool, within any chemical family class that contains one or more of them. For example, the values of the general property density or the fibre property tenacity may be compared for the classes Nylon, Polyester and PET, but considering the fibre grades only. This therefore facilitates the orthogonal classification aspect of the mechanism, illustrated in the next section.

6.5 Testing the new mechanism

6.51 Some sample special grades

To implement the data structure of the "special," partitioned grades described above, examples of such grades and their data were input into the system.

Initially, real supplier data were sought, and a number of suppliers of films and fibre grades were contacted to this end. This produced a variety of data sheets relating to real grades, such as the "Dyneema" Ultra High Molecular Weight Polyethylene fibres from DSM, Cellulose Acetate fibres from Novaceta, the 'Trespaphan' PP film range from Hoechst and the "Biafol" PP films from TVK.

However, in accordance with the general findings on data sheets, there was considerable inconsistency regarding the specialist properties specified for these grades, in respect of the test methods employed, the units, and the names of the properties themselves.

In addition there was little coherence in the generic properties: the only such property consistently specified was the intrinsic property density. It could be argued that the general engineering properties, suited primarily to bulk material grades, should have no place within film or fibre grade data, but many grades destined primarily for these applications can also be injection moulded and the general engineering properties are included as a matter of course. This applies to many grades on the CAMPUS™ database as has been confirmed by communication with a representative of BASF [53]: the absence of specific engineering properties for grades destined for specific uses can be explained by the limitations resulting from the standard data structure in this case.

There are also grades dedicated to use as films or fibres, such as the Hoechst grades Hostalen PPR 1060 F1 and PPN 1060 F3 (films) and Hostalen PPU 1780 F2 and PPU 1080 F(P) (fibres) which, on the supplier's original data sheet, have no specialist properties specified but have the full complement of general engineering properties. Communication with a representative from Hoechst [54] confirmed that in the majority of cases, such data were of no relevance to these grades. Clearly there is a need for more consistent and useful data specification: difficulties also arise when the same material has multiple grade names because it takes multiple forms.

But standardisation of data and nomenclature has not been the objective of this research and it is apparent, despite the confusion amongst published engineering polymer data, that there are cases where a single polymer grade can be processed in a number of ways to produce commercial materials of different forms, and that for such a grade different types of property are simultaneously appropriate, for the purposes of studying the performance of the material, as a standard sample, in its different forms. To illustrate this phenomenon simply, some hypothetical grades have been devised, based on intrinsic and specific engineering property data from real grades and supplemented with generic engineering property data taken from chemical family averages where it was lacking. The data in italics are specific engineering data, particular to grades of the stated form, and not inherited via the polymer materials hierarchy. See Tables 7 and 8.

PROPERTY	FILM 1	FILM 2	FILM 3
DENSITY (g/ml)	1.12	1.12	1.12
HDT/A (°C)	70	70	-
NOTCHED IMPACT STRENGTH (IZOD) @ 23°C (kJ/m^2)	60	60	60
TENSILE STRENGTH (MPa)	85	85	85
THERMAL EXP. COEFF. LONG. 23-80°C (exp-4/K)	0.82	0.82	0.82
WATER ABS. (%)	1.6	1.6	1.6
ELONGATION @ BREAK MACHINE DIRN. (%)	*425*	*350*	*350*
ELONGATION @ BREAK TRANSVERSE DIRN. (%)	*425*	*350*	*350*
MAX SERVICE TEMP (°C)	*93*	*93*	-
0$_2$ PERMEABILITY *(cm^{3}cm/cm^{2}s(cm hg) exp -11)*	*NA*	-	-
TEARING STRENGTH (N/m)	*30*	*70*	*90*
TENSILE STRENGTH MACHINE DIRN.(N/mm^2)	*80*	*71*	*100*
TENSILE STRENGTH TRANS DIRN. (N/mm^2)	*80*	*71*	*100*

Table 7: Three PA6 film grades

PROPERTY	FIBRE 1	FIBRE 2	FIBRE 3
DENSITY (g/ml)	0.908	0.903	0.907
HDT/A (°C)	72	55	55
IMPACT STRENGTH (IZOD) @ 23°C (kJ/m^2)	65	65	85
YOUNG'S MODULUS (MPa)	1500	1400	1450
STRAIN @ BREAK (50 mm/min) (%)	> 50	> 50	> 50
THERMAL CONDUCTIVITY OF MELT (W/mK)	0.118	-	0.118
VICAT A/50 (10N) (°C)	154	151	154
WATER ABSORPTION (%)	0.1	-	0.1
ELONGATION @ BREAK (%)	*17*	*15*	*20*
MOISTURE REGAIN (%)	*0*	*0*	*0*
TENACITY (g/denier)	*8*	*10*	*7*

Table 8: Three PP fibre grades

The Grade View windows on POISE for two of these grades are shown in Plate 25.

6.52 Use of the Property Comparison Tool to explore the data

In addition to the above hypothetical grades, some real grades of films and fibres and their corresponding data were input into the system for testing purposes. These included the commercial grades previously mentioned, which suffer inconsistency in terms of the properties specified for them. This has limited the data available for useful comparison, particularly those pertaining to the general engineering properties. However, some examples of the types of comparison that may be performed with a more complete data set are offered.

Use of the orthogonal classification facility is facilitated on the Property Comparison screen by the button to the left of the polymer class button. This can be seen in Plate 26. When clicked, this button limits comparison to one subset of the polymer database, delineated by geometrical form in these cases, and transcending the existing chemical family classification, which is effectively separated into multiple classifications. Plate 26 illustrates the comparison of fibre grades only, for the fibre property tenacity, across three chemical based classes.

Also illustrated in Plate 26 is the comparison of film grades only for the film property tensile strength in the machine direction. Due to the limited data available, little can be ascertained about the nature of the classes viewed in these cases.

This facility can be used to find those grades of a desired form within a class, by selecting a special property from the appropriate additional property list and investigating the class for that property. Only those grades with data pertaining to the property will be picked up by the Property Comparison tool. This is illustrated by selecting the film property tensile strength in the machine direction for all grades of the Thermoplastic, PA and PP classes. See Plate 27.

Here the film grades of the respective chemical family classes have been sifted out by virtue of the property chosen. PA films with high values of tensile strength in the machine direction have been investigated as an illustration of the selection and inspection facilities as applied to this type of grade and property.

Comparison can also be made between all grades of any polymer family and just the film or fibre grades of that family, for general properties, where the data are available. Plate 28 illustrates this for the property density, which is widely specified, for all partly crystalline grades as compared with fibre partly crystalline grades, and for all grades of Polymer as compared with film grades of Polymer.

The general property density reveals markedly more data for film than for fibre grades: this is because a number of film grades have been located in the CAMPUS™ database and classified as such within POISE. They were found by searching for the keyword "film" in the comments field and checking that this was only used to describe an application of the grade. Although a number of fibre grades are also to be found on CAMPUS™, they could not be easily separated out by this method as the word "fibre" also appeared in the description of grades with fibre reinforcements.

The relatively large number of film grades were gathered together, and classified as such by adding the film property list to each, although there were no data to accompany these properties as no such properties are specified by CAMPUS™.

A methodical inspection of the nature of the film grades on the database, in respect of their generic properties, could therefore be performed in a similar fashion to the previous investigation of the general POISE hierarchy.

From comparisons of the Amorphous class for films with the Partly Crystalline class for films and the Amorphous class for films with some amorphous chemical family classes for films (namely ABS and EVA), it was found that there were few amorphous films, and those that existed were all of the chemical family ABS and exhibited generally lower performance than the partly crystalline films, with the exception of the properties Young's modulus and HDT/A, where the ABS films had a wider overall spread.

Comparison of the Polymer class for films with the Polymer class for all grades suggested that grades destined for use as films showed relatively low values of mechanical properties, illustrated by the properties Young's modulus and heat deflection temperature A, in Plate 29.

Comparison was also made of the Partly Crystalline class for films with some partly crystalline family classes for films (namely PA, PP and PE).

This showed partly crystalline chemical family classes for films to be distinct from one another in respect of the properties density, relative permittivity, strain at yield and HDT/A but to show very similar ranges for the properties stress at yield, Vicat A and

Young's modulus. Data for other properties were not available. See Plate 30 for examples.

It can be seen that with a more populated data set, some important generalisations about the behaviours of engineering polymers in correlation with their ultimate applications and geometrical forms could, where relevant, be made by these means.

6.6 Other uses of the mechanism

6.61 User company properties

Other additional properties not easily accommodated by conventional database systems are those specified by users for a particular purpose. User companies will specify properties for which they need to ascertain values for material grades purchased: often these are listed within their purchasing specifications, together with acceptable ranges if purchase is to proceed, and employ application specific tests which are not to be found amongst the widely quoted generic properties.

This presents another example of the information representation problem resulting from data supplied in addition to the generic data quoted for nearly all supplied grades. User properties need to be positioned and accessed in a way that preserves their distinction from generic properties.

By applying the property combining strategy and mechanism to this problem, an appropriate data structure is obtained which serves the purpose of property space partitioning while at the same time classifying as separate those grades that share a common user company. This has been tested on a small scale using Lucas as the example user company.

Purchasing specifications for a selection of materials were obtained, and from them a number of Lucas properties and their acceptable ranges for various materials. Using these ranges, together with some general property data from what were hypothesised to be likely candidates for Lucas grades, three example such grades, all polypropylenes, were created and input into the system, together with a Lucas property list. These are shown in Table 9.

Each of these hypothetical grades is associated with a Lucas specification number, which refers to a specific type of material and the property requirements it must meet. The Lucas property values for the grades were taken by locating the middle of the relevant specification range.

Although this method has only been employed as a convenient means of providing examples, it highlights a useful application of the system: to compare real data of available materials with data for a hypothetical "ideal" grade or with an acceptable range of such data. This would not be difficult to do using the Property Comparison tool. (An alternative approach might be to incorporate an algorithm into each user property object, which provides information on the acceptable range for that property, and effectively eliminates grades outside that range).

Some Lucas properties have the same name as similar properties in the generic properties list, but are distinguished by different test methods or conditions, and these test methods are given a Lucas code number. The code numbers proved not to be enough in themselves to distinguish each property as they are often applied to more than one property: it is the combination of property name and Lucas code number that sets aside the property as unique.

PROPERTY	LUCAS 1 (3-53-102)	LUCAS 2 (3-53-101)	LUCAS 3 (3-53-100)
DENSITY (g/ml)	1.050	0.902	0.914
HDT/A (°C)	131	66	65
GLASS CONTENT, LUCAS H3.1 (%)	*20*	-	-
IZOD IMPACT, -20°C, LUCAS B6.3(J/12.7mm)	*0.9*	-	*0.26*
IZOD IMPACT, +20°C, LUCAS B6.3(J/12.7mm)	*1.1*	*0.1*	*1.7*
MELT FLOW INDEX, LUCAS A1.2 (g/10 min)	*4.0*	*4.7*	*8.0*
TENSILE STRENGTH @ BREAK, LUCAS B1.7 (MPa)	*66*	-	-
TENSILE STRENGTH @ YIELD, LUCAS B1.7 (MPa)	-	*44*	*37*
VICAT SOFTENING POINT, LUCAS E1.2 (°C)	*167*	*149*	*153*

Table 9: Three Lucas grades

Again those properties specific to Lucas are indicated by an italic script. An example of the way in which a Lucas property differs from that of a generic property of the same name is Izod impact strength. As can be seen, it is measured by Lucas at -20°C and 20°C respectively, whereas the CAMPUS™ Izod impact strength is measured at -30°C and 23°C. The units are also significantly different: J/12.7mm for Lucas as compared with kJ/m^2 for the standard form of the property.

A commented property window for the Lucas property glass content is shown in Plate 31.

For illustrative purposes only (due to the nature of the data) the use of the Comparison tool for the inspection of user-classified grades is shown in Plate 32.

Clearly, with the appropriate data to hand, many useful comparisons could be made by user companies for their own purposes, which could not have been achieved with an existing polymer supplier database on its own.

6.62 Ideas for future uses

This system has the potential to be used for other situations where there is a conflict between criteria for class creation and information representation, resulting in additional factorings that are completely independent of an existing, chemical family based hierarchy. It may therefore be appropriate for creating additional factorisations based on the existence and type of reinforcement or chemical filler, for example. Clear decisions must be made as to which factors should influence the main hierarchy and which should be incorporated by way of the orthogonal classification mechanism. It is believed that the primary distinction should be between criteria based on material (polymer) characteristics and criteria based on other, more physical or application-oriented characteristics if the structure is to remain principled.

7. Future work

In addition to the foregoing suggestions, it is proposed that the system would benefit from the following:

(i) Further exploration of the potential for utilising the functionality of object-oriented systems. For example, the implementation of appropriate "rules of thumb" within certain polymer classes, in the form of object-specific methods, could be used to predict unknown properties, to establish relationships between properties, and so on.

Most such rules draw on chemical, rather than engineering data and so would not be practical in a system relying solely on CAMPUS™ data. If, however, a database of scientific properties was also associated with POISE, there would be some scope for modelling relationships between properties and perhaps predicting likely property ranges for polymers. Molecular mass and degree of crystallinity, for example, influence a number of mechanical properties, such as hardness and softening temperature; the solubility parameter of a polymer can also be estimated from fundamental properties (density, molecular mass and the sum of the molar attraction constants of the repeating unit in the chain) according to Hildebrand's rule [39].

The relevance of many such rules may be limited to classes or sub-classes of the engineering polymer domain. This is easy to deal with in object-oriented systems since the methods are simply restricted to the appropriate class or sub-class. However care would need to be taken regarding extrapolation to new grades, since many rules have little or no physical basis and could produce misleading results.

Methods could also be written to test for and model relationships between additives and the affected properties; they could be placed in classes partitioned according to additive content.

(ii) Further use of the browsing facility. This is a valuable feature of the system, currently used to summarise and display only quantitative information (property data). However there is much qualitative information pertaining to classes of engineering polymers that is currently available in textbooks, supplier data sheets, and as comments on individual grades in computerised systems (and therefore not easily accessible on such systems). Such information common to the members of a class within the POISE hierarchy could be abstracted and displayed in the form of text or graphs, as annotations for that class. It could be accessed by means of a hypertext tool that would respond when the class in the hierarchy display of the Hierarchy Editor window was selected. This would enable the full potential of the browsing facility to be exploited.

8. Conclusions

The benefits of an object-oriented system for modelling the prolific amounts of data relating to engineering polymers have been outlined and compared with aspects of conventional database models within the same context. Object-orientation is considered to provide greater flexibility in terms of the data model, which is allowed to evolve and does not require a fixed structure in (information) space or time. Object-orientation also allows the introduction of functionality at desired points within the model.

It was also shown that there is a need for existing engineering polymer information systems to acknowledge the benefits of materials classification if the user is to navigate the information space with ease and a degree of guidance. The object-oriented language Smalltalk 80™ is based on a naturally hierarchical organisation of code and data, and has been used to develop an information system for engineering polymers, POISE, which exploits this aspect and employs a single inheritance hierarchy as the main structure for their data. POISE was designed to model the design environment; this project concentrated exclusively on its application to the materials domain of that environment, in the belief that other areas, such as geometry and manufacturing, belong in different perspectives and therefore deserve their own models.

An analysis of the plastics domain lead to the development of a taxonomy of engineering polymers with which POISE has been populated. This taxonomy is based on a hierarchical structure with inheritance, which abstracts generic plastics information into classes. It was argued that for the preconditions of extensibility and independence from user perspectives to be met, classification must be done on the basis of criteria fundamental to the materials domain, i.e. criteria of chemistry and molecular structure, eliminating an approach based purely on physical property values.

It was found that conventional classification systems for plastics are loosely defined and provide a means of nomenclature rather than a principled scientific description of groups of plastics. However the complexity of the factors affecting the properties of plastics precluded the construction of a class hierarchy based purely on detailed scientific reasoning.

A shallow but broad classification based on accepted polymer families, subsumed within superclasses founded on microstructural type, was proposed as an acceptable means of abstracting generic information.

This classification was implemented within POISE and the Property Comparison tool was used to compare the data visually within and between the classes. It was found that generally, chemical family classes exhibited property value distributions that were fairly tightly spread within a class and noticeably different between classes, except where fillers and reinforcements had significant effects. The use of such additives is a widespread phenomenon, and may be considered a distracting influence on the ability of the system to reflect the fundamental character of a material type. However this was not considered to present an insurmountable barrier to modelling the domain, since in theory the effects of additives could themselves be modelled, by utilising the functional capabilities of the system.

The Property Comparison tool was also used to explore the tensile and brittle behaviours of certain materials, and showed that Pugh's rule applies in general to the Polycarbonate class of engineering polymers, and furthermore that the Property Comparison tool was useful in ascertaining the applicability of such rules.

Use of other tools developed for POISE demonstrated that the hierarchy is extensible since new classes and grades can be incorporated without difficulty: the abstract classes cover the domain completely by virtue of the fundamental structural principles on which they are based; and new chemical family classes can therefore be placed easily within the structure.

However the classification was shown not to provide a useful factoring for grades from a specific, use- or form-related engineering point of view.

A manifestation of this point with particular relevance to data representation issues occurs in terms of the different properties defined for a grade of polymer. Grades that are similar in terms of their intended use or the degree of processing they have undergone may be described by properties tailored to their particular use or form, in addition to the general, scientific properties that are specified as a matter of course. Accommodating these properties, without creating redundant specifications for those grades that do not require them, has been one of the aims of the research, and has resulted in a need to separate those grades with a special engineering significance from other, more general material grades.

Thus the chosen classification system is offered in conjunction with an orthogonal classification, whereby the final material classes of the hierarchy are partitioned further according to factors extraneous to the scientific principles used to create the material hierarchy. This orthogonal classification is facilitated by a software mechanism which operates in conjunction with the existing POISE software and introduces the engineering-specific properties as a supplement to the generic properties that are inherited via the main hierarchy. A partition between the different property types for each grade is maintained throughout.

This provides a useful engineering factoring at the grade level together with the ability to utilise this factoring within the Property Comparison tool. A number of demonstrations using example special-engineering grades were performed. These illustrated the ability of the system to compare such grades from selected classes with respect to selected properties, and provided evidence of the orthogonal classification that had been created.

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Appendix 1: Campus™ properties

Mechanical Properties (@ 23°C, 50% R.H.)

Density of the moulding compound (g/ml)
Stress at yield: 50 mm/min (MPa)
Strain at yield: 50 mm/min (%)
Strain at break: 50 mm/min (%)
Stress at 50% elongation: 50 mm/min (MPa)
Tensile Strength: 5mm/min (MPa)
Strain at break: 5mm/min (%)
Young's Modulus: sec. 1mm/min (MPa)
Creep Modulus: 1 hr (MPa)
Impact Strength: Izod, 23°C (kJ/m^2)
Impact Strength: Izod, -30°C (kJ/m^2)
Notched Impact Strength: Izod, 23°C (kJ/m^2)
Notched Impact Strength: Izod, -30°C (kJ/m^2)
Notched Tensile Impact Strength: 23°C (kJ/m^2)

Thermal Properties

Heat Deflection Temperature: HDT/A, 1.8 MPa (°C)
Heat Deflection Temperature: HDT/B, 0.45 MPa (°C)
Heat Deflection Temperature: HDT/C, 5.00 MPa (°C)
Vicat VST/A/50, 10N (°C)
Vicat VST/B/50, 50N (°C)
Thermal Expansion Coefficient, longitudinal, 23-80°C (exp-4/K)
Thermal Expansion Coefficient, transverse, 23-80°C (exp-4/K)

Electrical Properties (@ 23°C, 50% R.H.)

Relative Permittivity, 50Hz (-)
Relative Permittivity, 1MHz (-)
Dissipation Factor, 50Hz (exp -4)
Dissipation Factor, 1MHz (exp -4)
Dielectric Strength (kV/mm)
Comp. Tracking Index, CTI (-)
CTI 100 drops value (-)
Comp. Tracking Index, CTIM (-)
CTIM 100 drops value (-)
Specific Volume Resistivity (ohm.cm)
Specific Surface Resistivity (ohm)
Electrolytic Corrosion (-)

Processing Properties

Melt Volume Rate, MVR, 1st value (ml/10min)
  at test temperature (°C)
  at test load (kg)
Melt Volume Rate, MVR, 2nd value (ml/10min)
  at test temperature (°C)
  at test load (kg)

Other Properties

Viscosity Coefficient (ml/g)
Characteristic Density, 23°C (g/ml)
Isotaxy Index (-)

Behaviour towards external influences

Flammability UL 94, 1st value (steps)
at thickness (mm)
Flammability UL 94, 2nd value (steps)
at thickness (mm)
Flammability UL 94/5V (steps)
at thickness (mm)
Water Absorption, 23°C, saturated, 11 (%)
Moisture Absorption, 23°C, 50% R.H., 11 (%)

Optical Properties (@ 23°C, 50% R.H.)

Refractive Index (-)
Degree of Light Transmission (%)

Specimen Production

Specimen and Properties according to DIN (-)
Injection Moulding: Melt Temperature (°C)
Injection Moulding: Mould Temperature (°C)
Injection Moulding: Flow Front Velocity (mm/s)
Compression Moulding: Press Temperature (°C)
Compression Moulding: Cooling Rate (K/min)

Data for Rheological Calculations

Density of melt (g/ml)
Thermal Conductivity of melt (W/m.K)
Specific Heat Capacity of melt (J/kg.K)
Effective Thermal Diffusivity, a-effective (m^2/s)
No-flow Temperature (°C)
Freeze Temperature (°C)
Power Approximation Constant A (-)
Power Approximation Constant B (-)
Power Approximation Constant C (-)
Carreau-WLF Approximation Constant K1 (-)
Carreau-WLF Approximation Constant K2 (-)
Carreau-WLF Approximation Constant K3 (-)
Carreau-WLF Approximation Constant K4 (-)
Carreau-WLF Approximation Constant K5 (-)

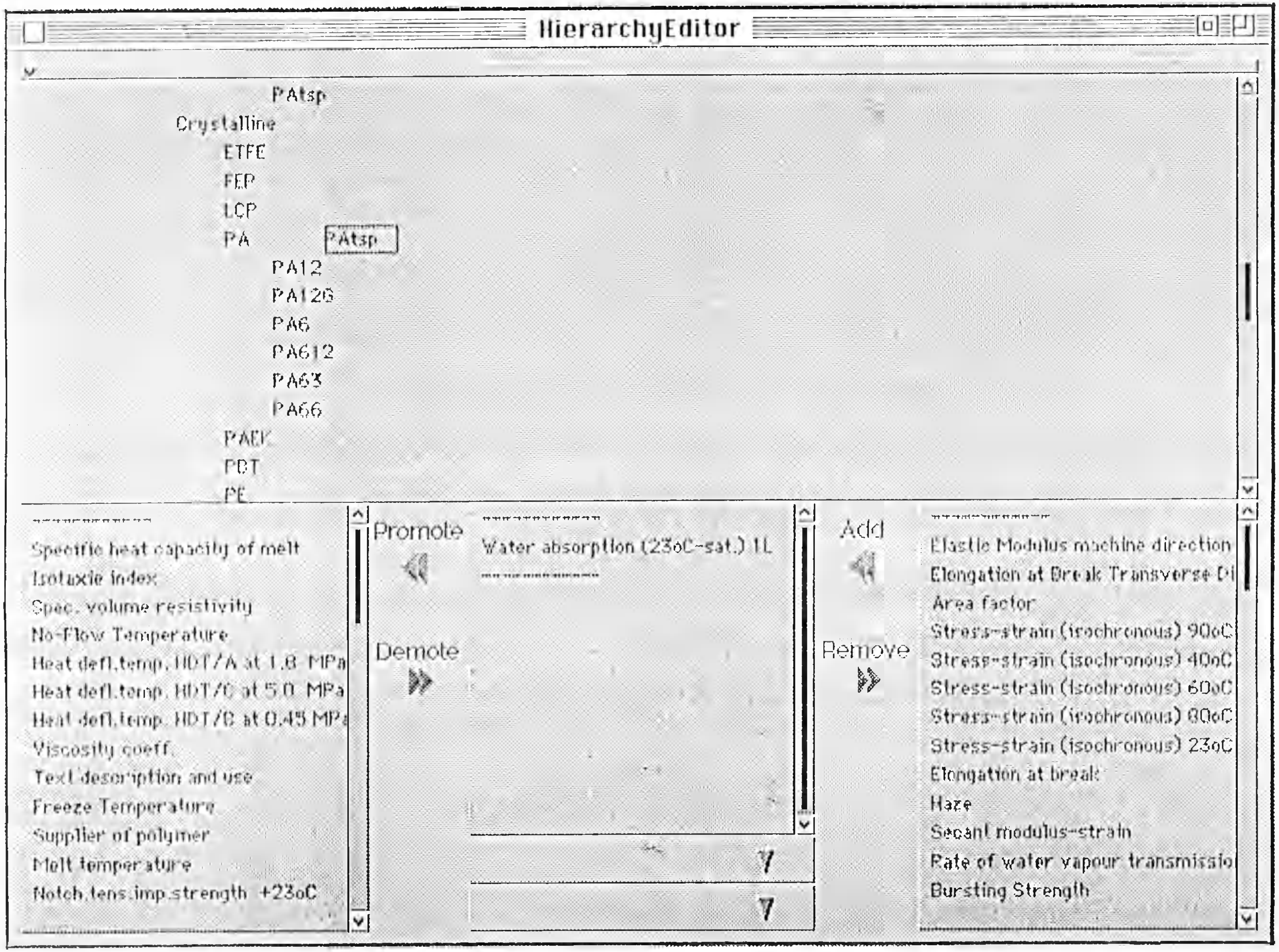
Appendix 2: Film and fibre properties

Film Properties

- Mechanical
    - Tensile Strength, Machine Direction (MPa)
    - Tensile Strength, Transverse Direction (MPa)
    - Elongation at break, Machine Direction (%)
    - Elongation at break, Transverse Direction (%)
    - Bursting strength (Mullen Points)
    - Tearing Strength (N/m)
    - Folding Endurance (-)
    - Seal strength (N/15mm)
- Thermal
    - Minimum service temperature (°C)
    - Maximum service temperature (°C)
    - Heat sealing temperature range (°C)
    - Thermal shrinkage (%)
- Optical
    - Haze (%)
- Behaviour under external influences
    - Gas permeability; CO_2, N_2, O_2 (cm^3.cm/cm^2.sec.(cm Hg) x 10^{-11})
    - Water vapour permeability (cm^3.cm/cm^2.sec.(cm Hg) x 10^{-11})
    - Rate of water vapour transmission, 24 hrs (g.mm/mm$^{2)}$
- Tribological
    - Coefficient of Friction, Machine Direction (-)
    - Coefficient of Friction, Transverse Direction (-)
- Other
    - Thickness range (mm)
    - Area factor, area covered by 1 kg film 1 mm thick (m^2 x 10^6)
    - Maximum width (m)
- Special Characteristics
    - Whether anti-static
    - Whether laminated
    - Whether coated

Fibre Properties

- Mechanical
    - Axial tensile strength (MPa)
    - Transverse tensile strength (MPa)
    - Elongation at break (%)
    - Tenacity (g/denier)
    - Elastic recovery (%, from elongation)
    - Stiffness (MPa)
    - Crimp Level (-)
    - Toughness (g.cm)
    - Cross Section (mm^2)
- Thermal
    - Melt temperature (°C)
- Behaviour under external influences
    - Moisture regain (%)



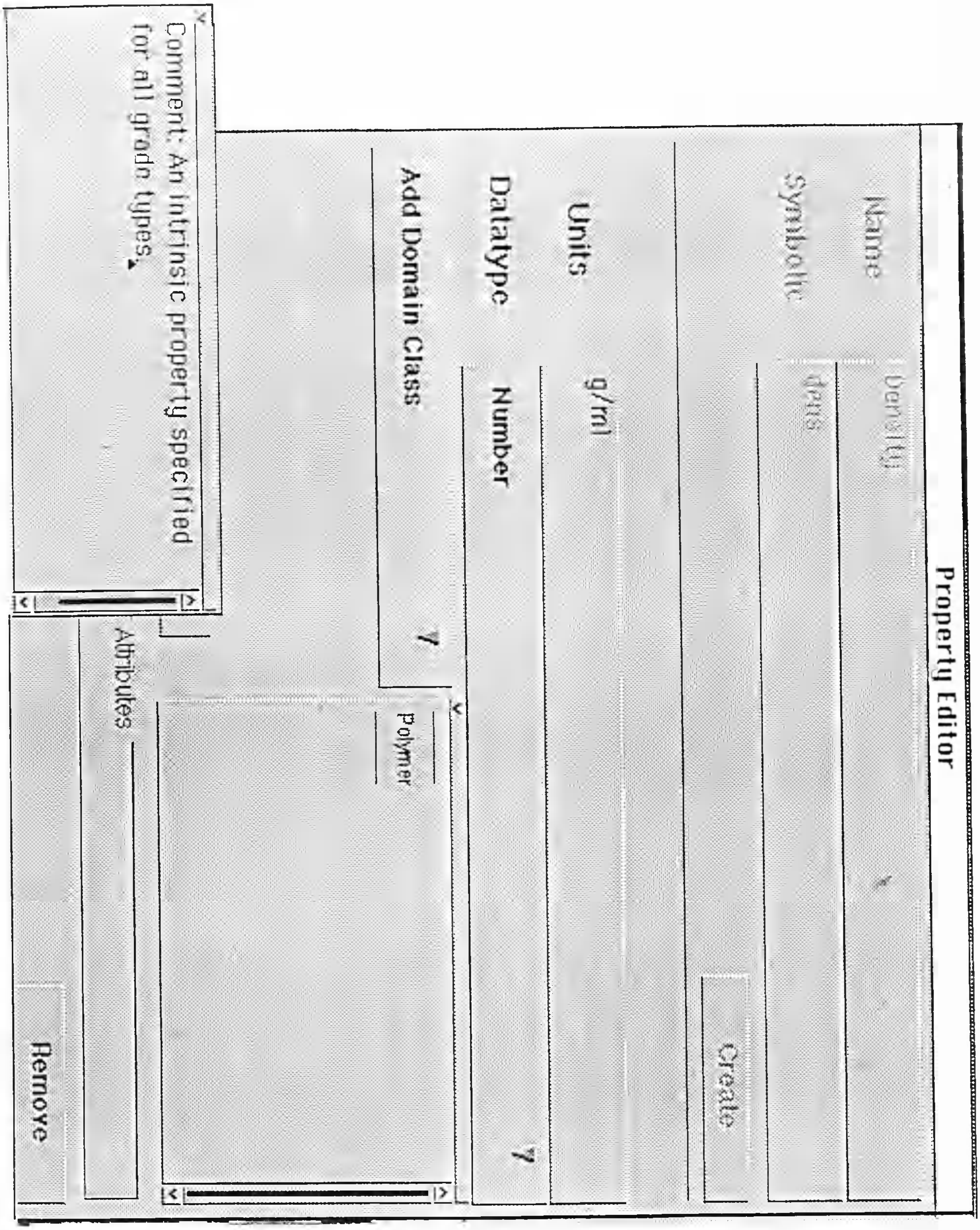
PAtsp
Crystalline
ETFE
FEP
LCP
PA
PAtsp
PA12
PA12G
PA6
PA612
PA63
PA66
PAEK
PBT
PE

Specific heat capacity of melt
Isotaxie index
Spec. volume resistivity
No-Flow Temperature
Heat defl.temp. HDT/A at 1.8 MPa
Heat defl.temp. HDT/C at 5.0 MPa
Heat defl.temp. HDT/B at 0.45 MPa
Viscosity coeff.
Text description and use
Freeze Temperature
Supplier of polymer
Melt temperature
Notch.tens.imp.strength +23oC

Water absorption (23oC-sat.) IL

Elastic Modulus machine direction
Elongation at Break Transverse Di
Area factor
Stress-strain (isochronous) 90oC
Stress-strain (isochronous) 40oC
Stress-strain (isochronous) 60oC
Stress-strain (isochronous) 80oC
Stress-strain (isochronous) 23oC
Elongation at break
Haze
Secant modulus-strain
Rate of water vapour transmissio
Bursting Strength

Plate 1 Hierarchy Editor window



Property Editor

Name: Density

Symbolic: dens

Units: g/ml

Datatype: Number

Add Domain Class: Polymer

Attributes

Comment: An intrinsic property specified for all grade types.

Plate 2 Property Editor window

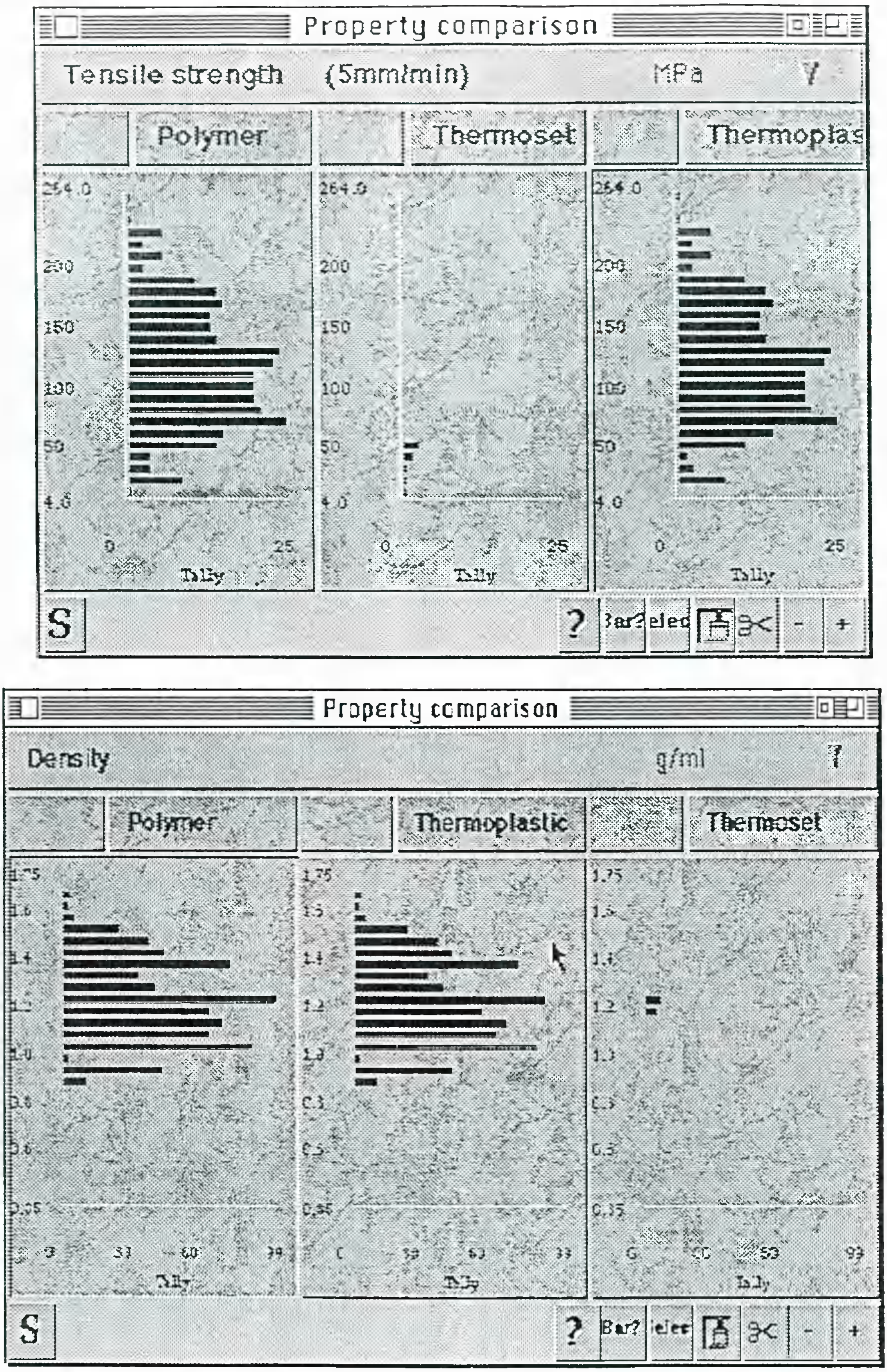
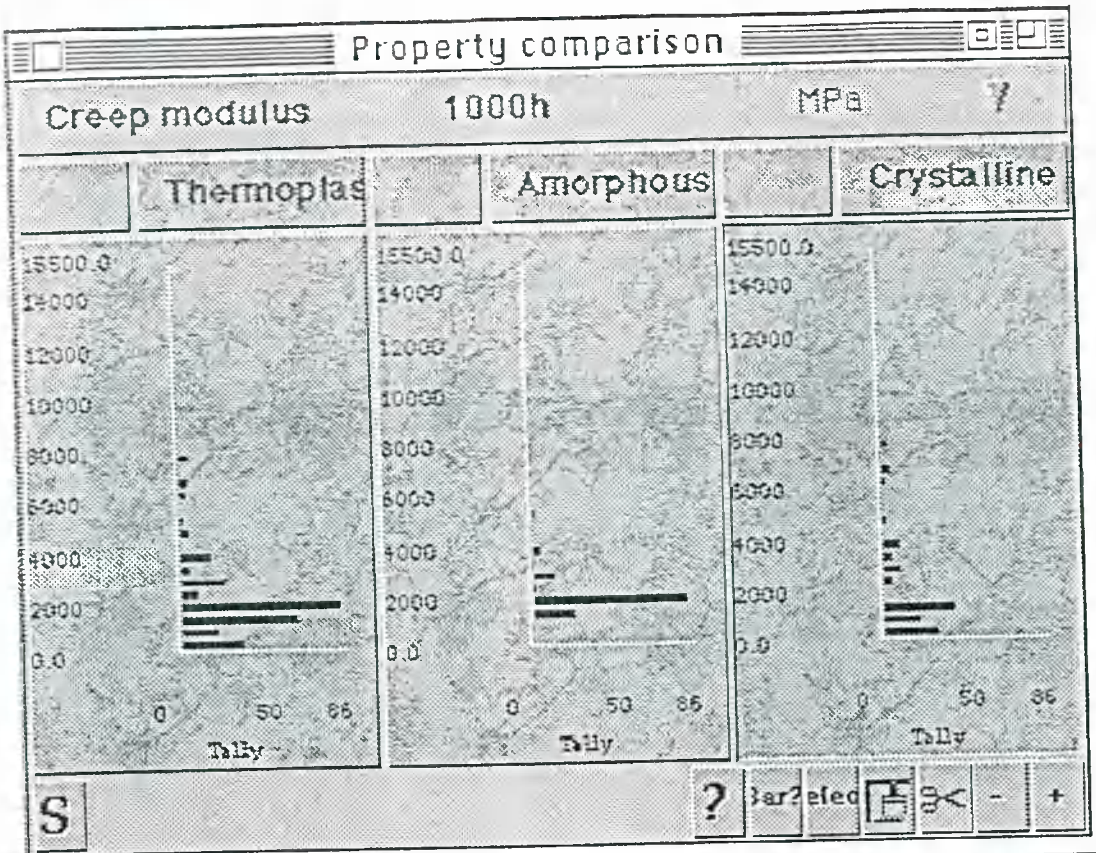


Plate 3 Comparison of density and tensile strength data for the abstract classes Polymer, Thermoset and Thermoplastic



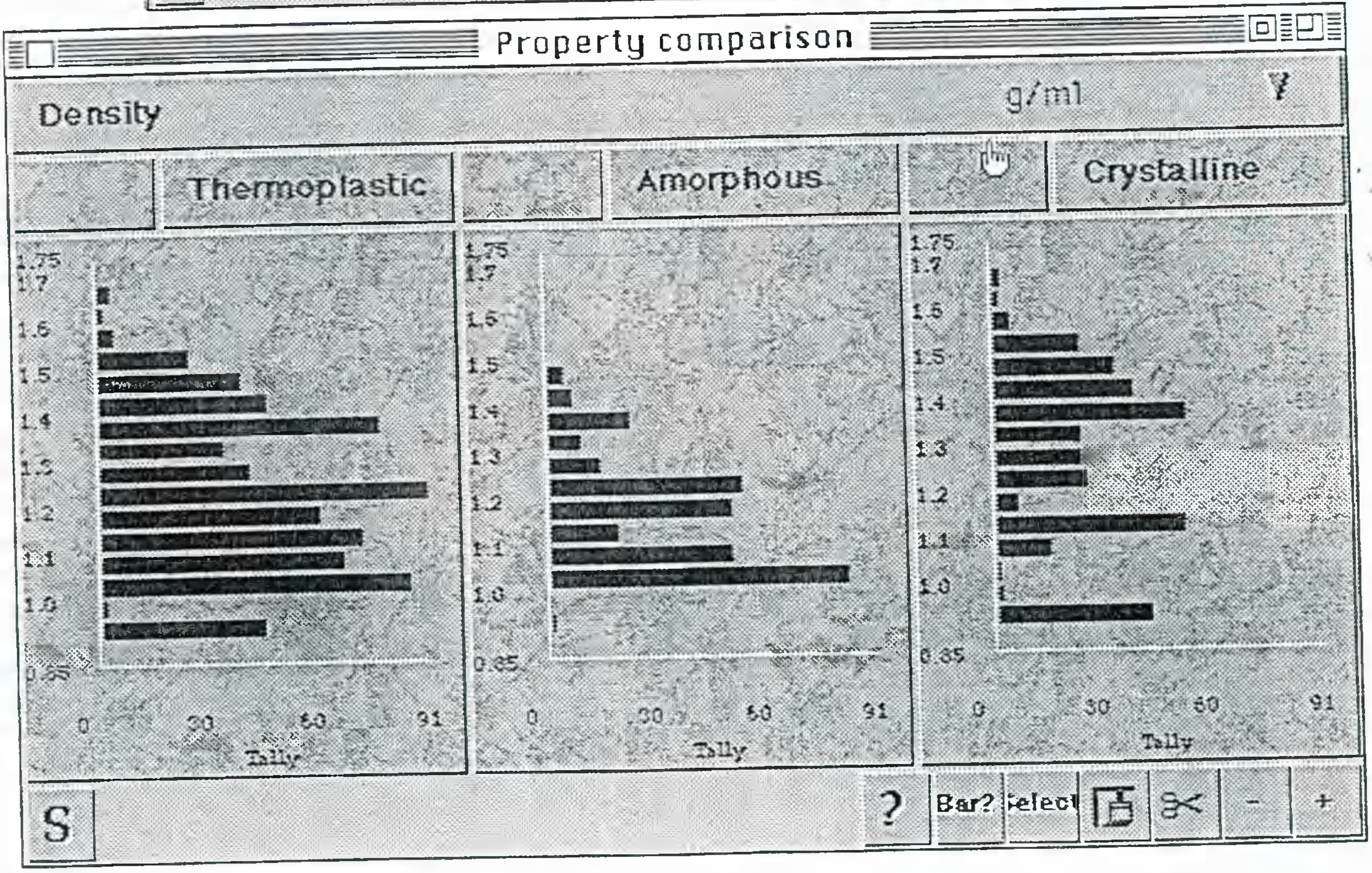
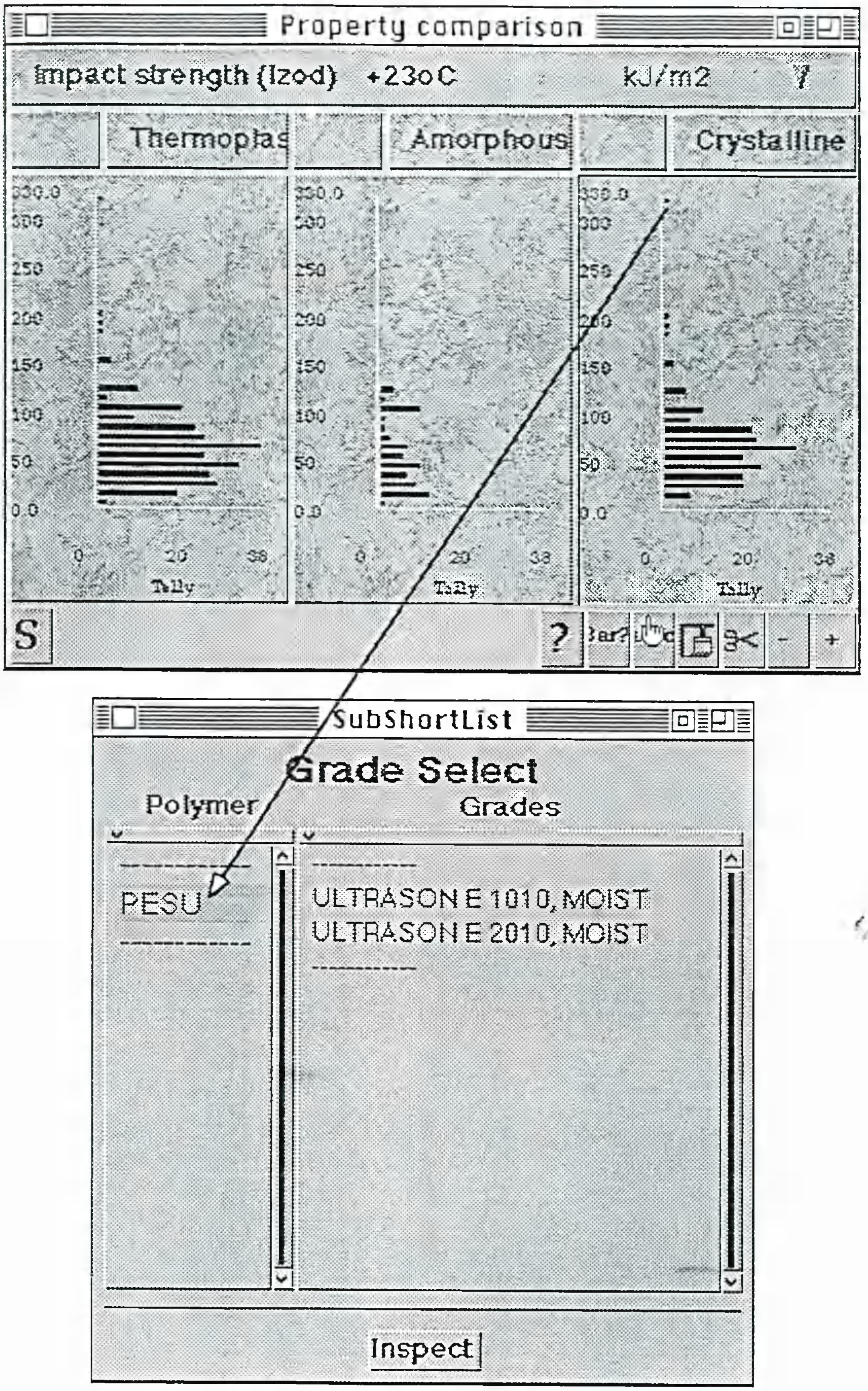


Plate 4 Comparison of density and creep modulus data for the abstract classes Thermoplastic, Amorphous and Partly Crystalline



PESU

ULTRASON E 1010, MOIST
ULTRASON E 2010, MOIST

Plate 5 Comparison of impact strength data for Thermoplastic, Amorphous and Partly Crystalline classes showing bar selection and grades

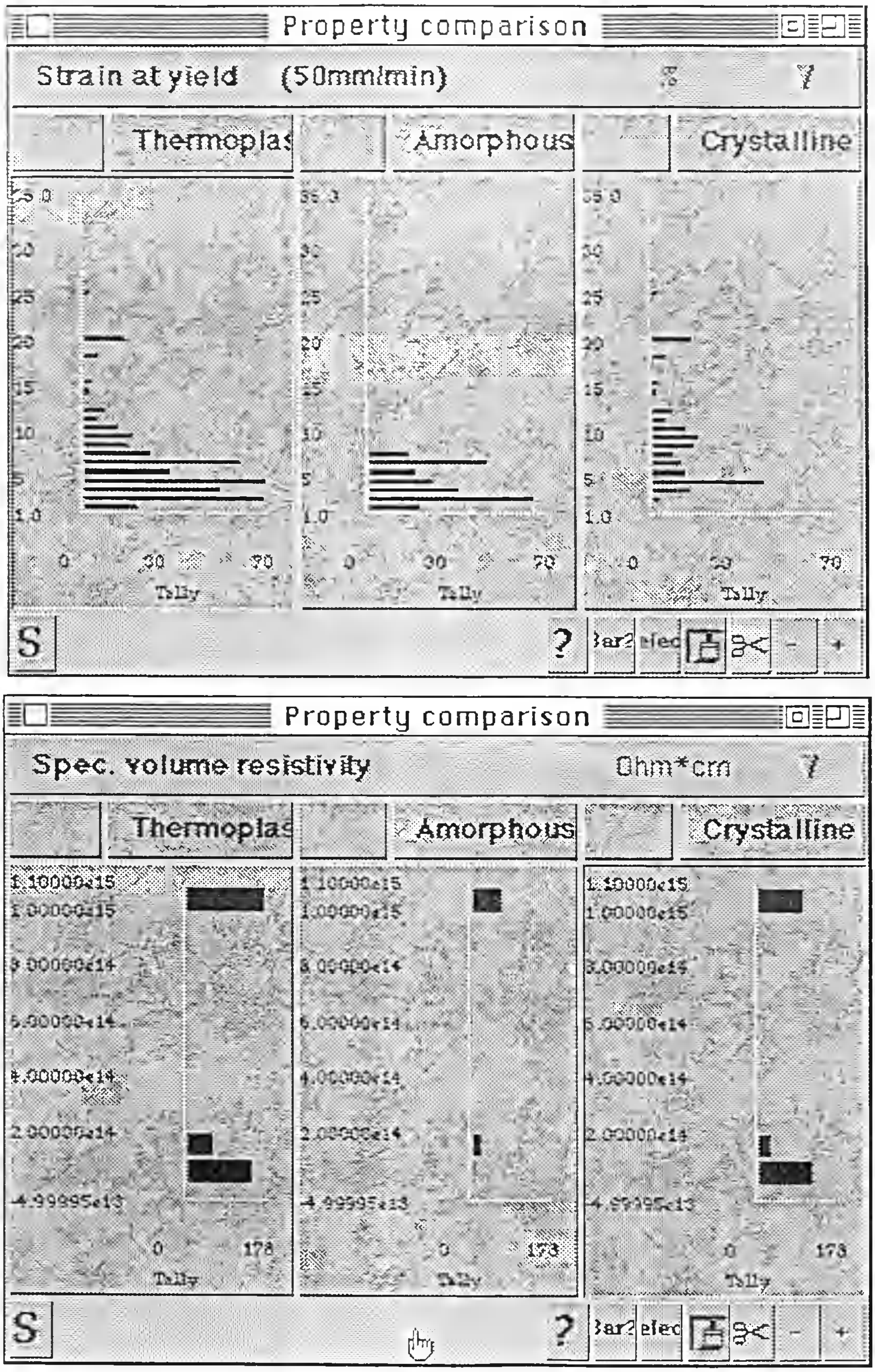
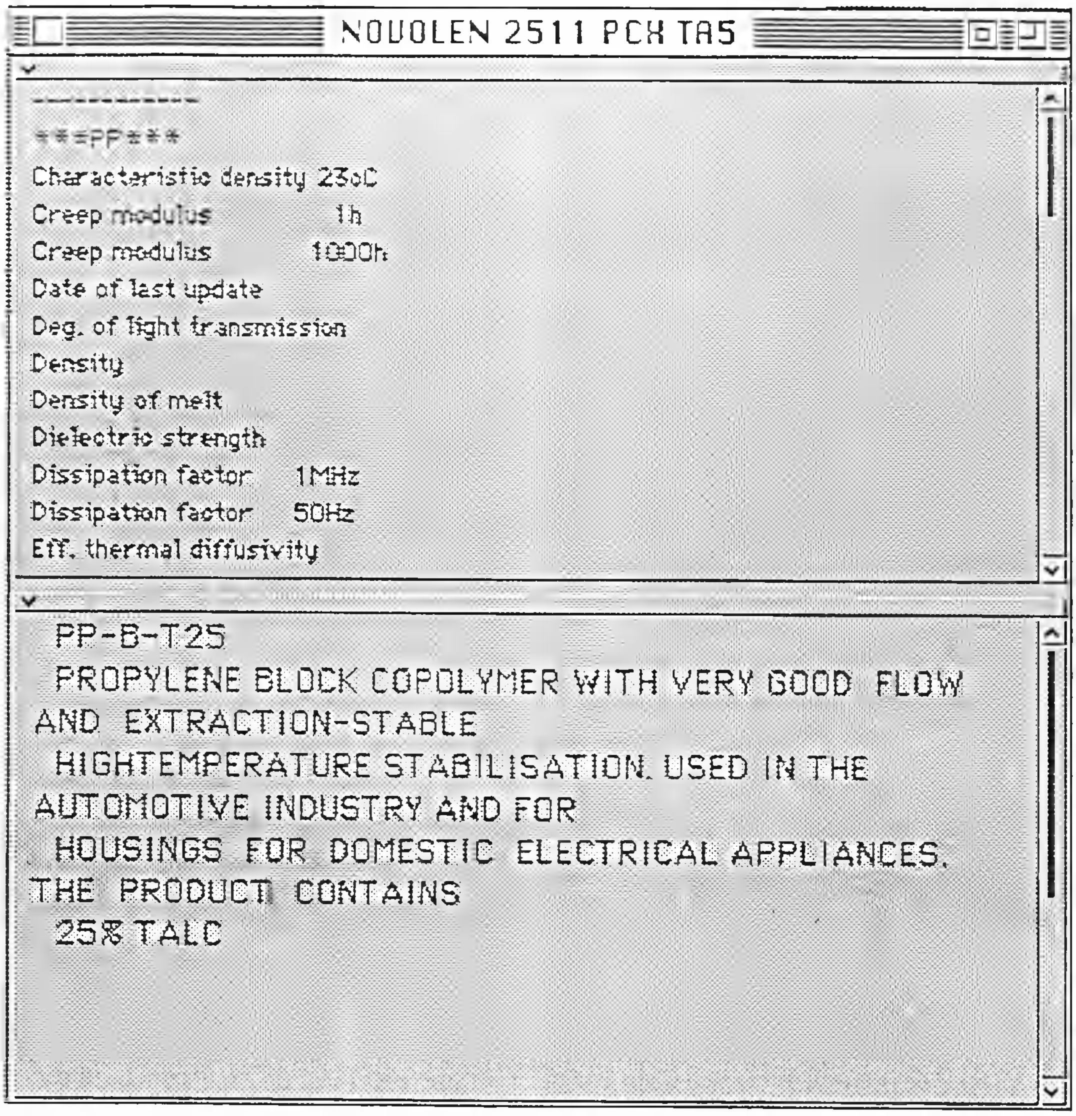


Plate 6 Comparison of strain at yield and specific volume resistivity for Thermoplastic, Amorphous and Partly Crystalline classes



```
------------
***PP***
Characteristic density 23oC
Creep modulus          1h
Creep modulus       1000h
Date of last update
Deg. of light transmission
Density
Density of melt
Dielectric strength
Dissipation factor    1MHz
Dissipation factor    50Hz
Eff. thermal diffusivity
```

```
 PP-B-T25
 PROPYLENE BLOCK COPOLYMER WITH VERY GOOD  FLOW
AND  EXTRACTION-STABLE
 HIGHTEMPERATURE STABILISATION. USED IN THE
AUTOMOTIVE INDUSTRY AND FOR
 HOUSINGS  FOR  DOMESTIC  ELECTRICAL APPLIANCES.
THE  PRODUCT  CONTAINS
 25% TALC
```

Plate 7 A polypropylene grade with high resistivity showing applications

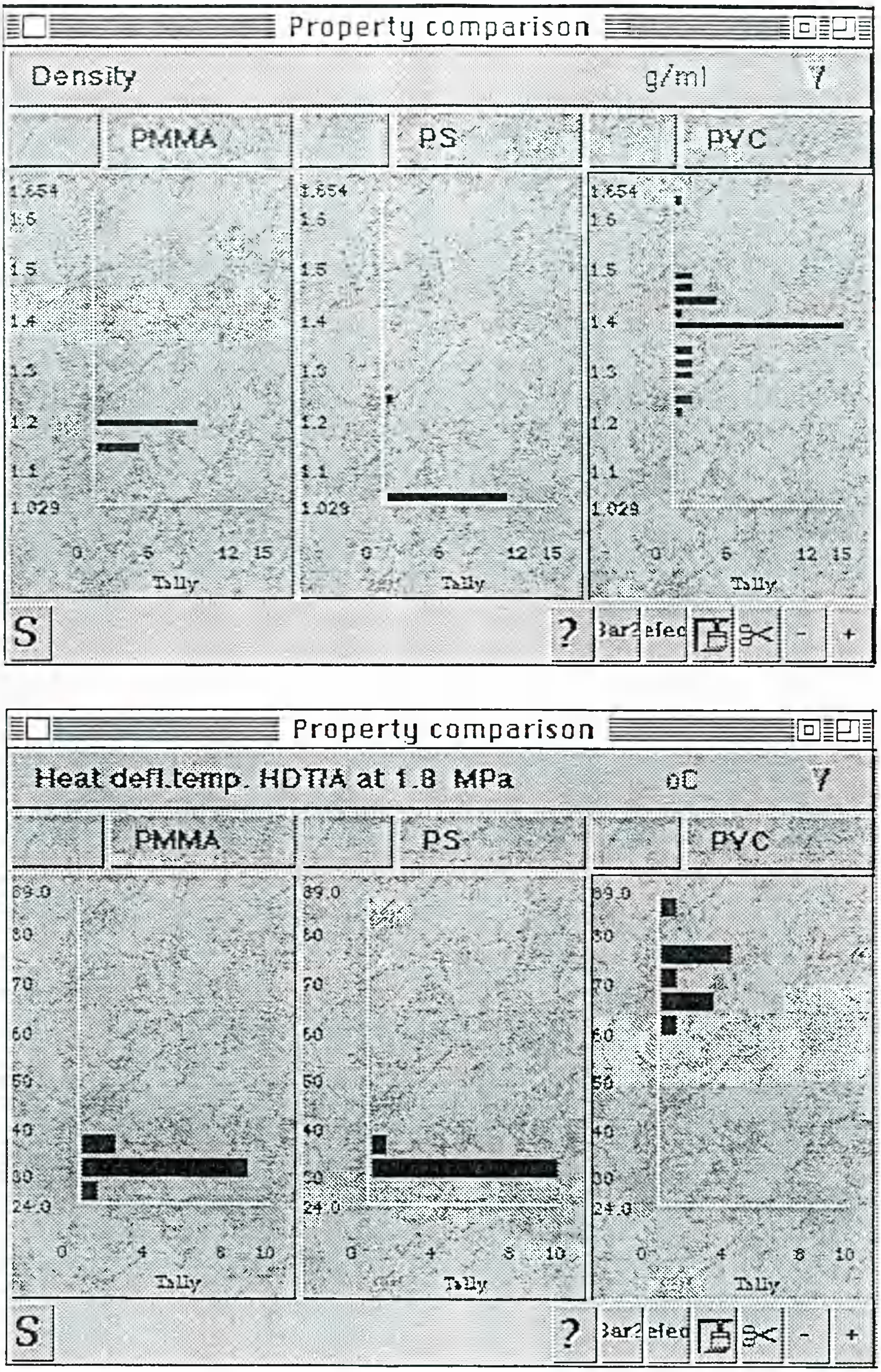


Plate 8 Density and heat deflection temperature data for some amorphous chemical family classes

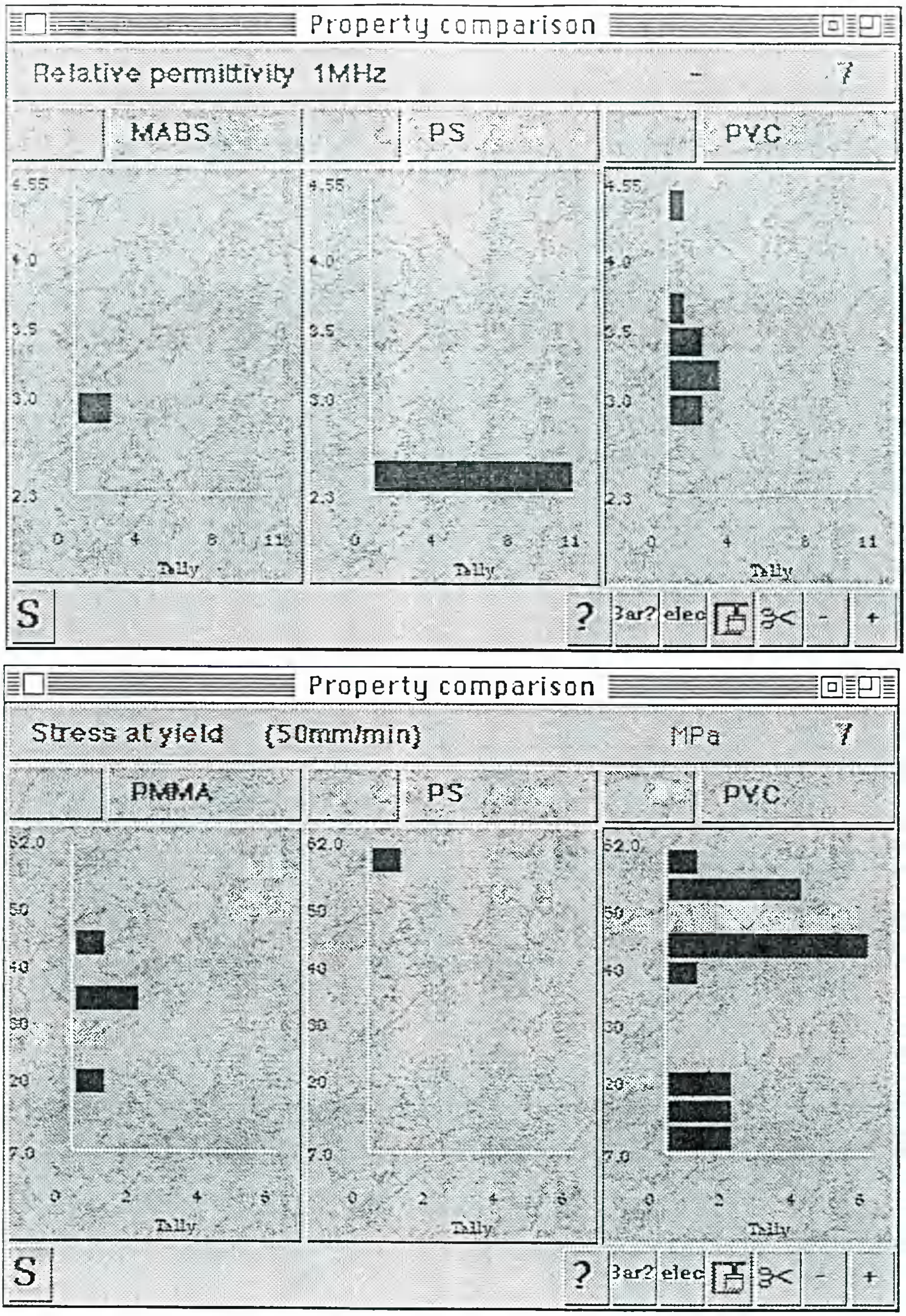
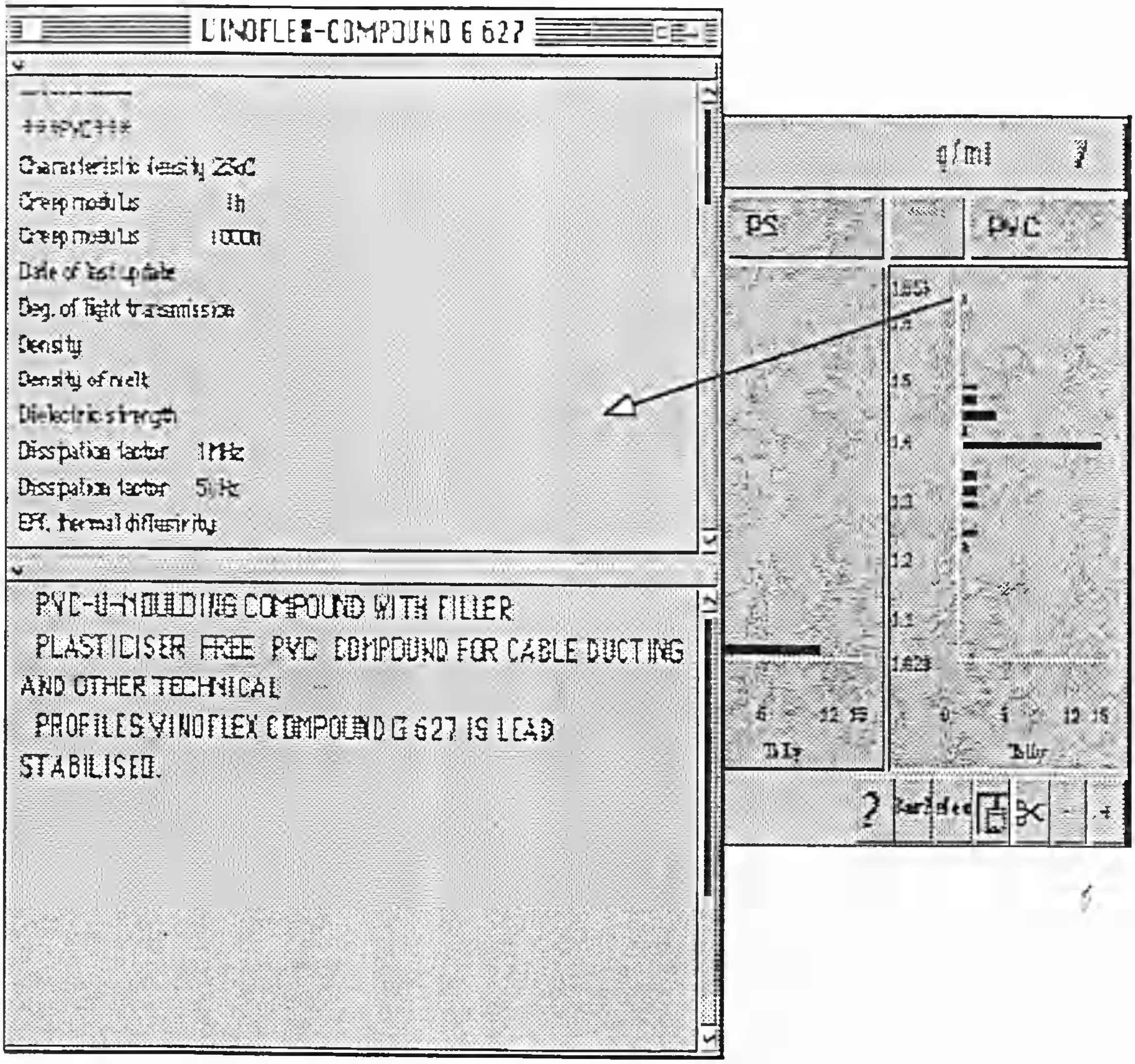


Plate 9 Relative permittivity and stress at yield data for some amorphous chemical family classes



VINOFLEX-COMPOUND G 627

PVC

Characteristic density 23oC

Creep modulus 1h

Creep modulus 1000h

Date of last update

Deg. of light transmission

Density

Density of melt

Dielectric strength

Dissipation factor 1MHz

Dissipation factor 50Hz

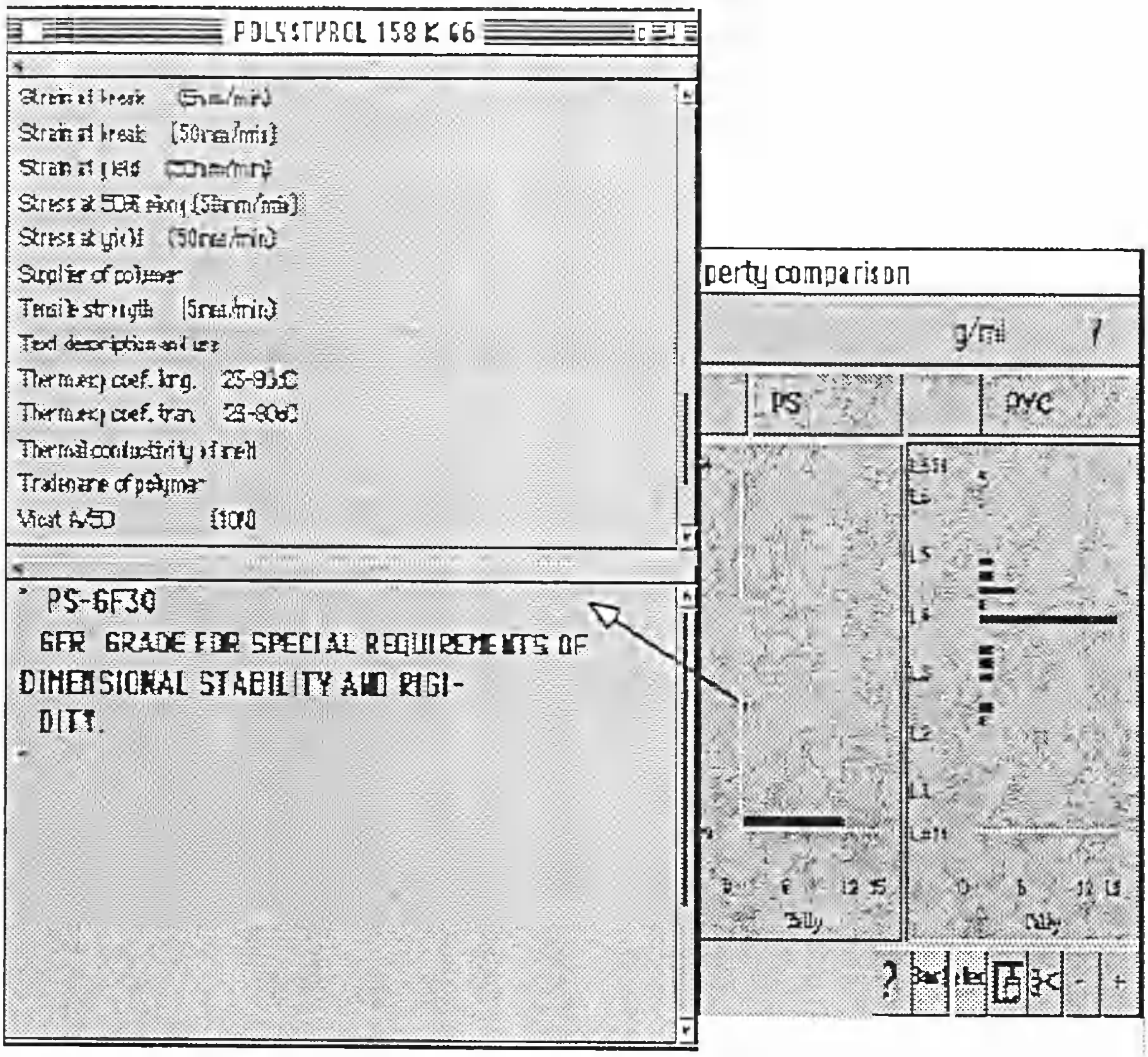
Eff. thermal diffusivity

PVC-U-MOULDING COMPOUND WITH FILLER

PLASTICISER FREE PVC COMPOUND FOR CABLE DUCTING AND OTHER TECHNICAL

PROFILES VINOFLEX COMPOUND G 627 IS LEAD STABILISED.

Plate 10 The grade behind the high density value on the PVC histogram



POLYSTYROL 158 K 66

Strain at break (5mm/min)
Strain at break (50mm/min)
Strain at yield (50mm/min)
Stress at 50% elong (50mm/min)
Stress at yield (50mm/min)
Supplier of polymer
Tensile strength (5mm/min)
Text description and use
Therm.exp coef. lng. 23-80oC
Therm.exp coef. tran. 23-80oC
Thermal conductivity of melt
Tradename of polymer
Vicat A/50 (100)

PS-GF30
GFR GRADE FOR SPECIAL REQUIREMENTS OF DIMENSIONAL STABILITY AND RIGIDITY.

Plate 11 The grade behind the high density value on the polystyrene histogram

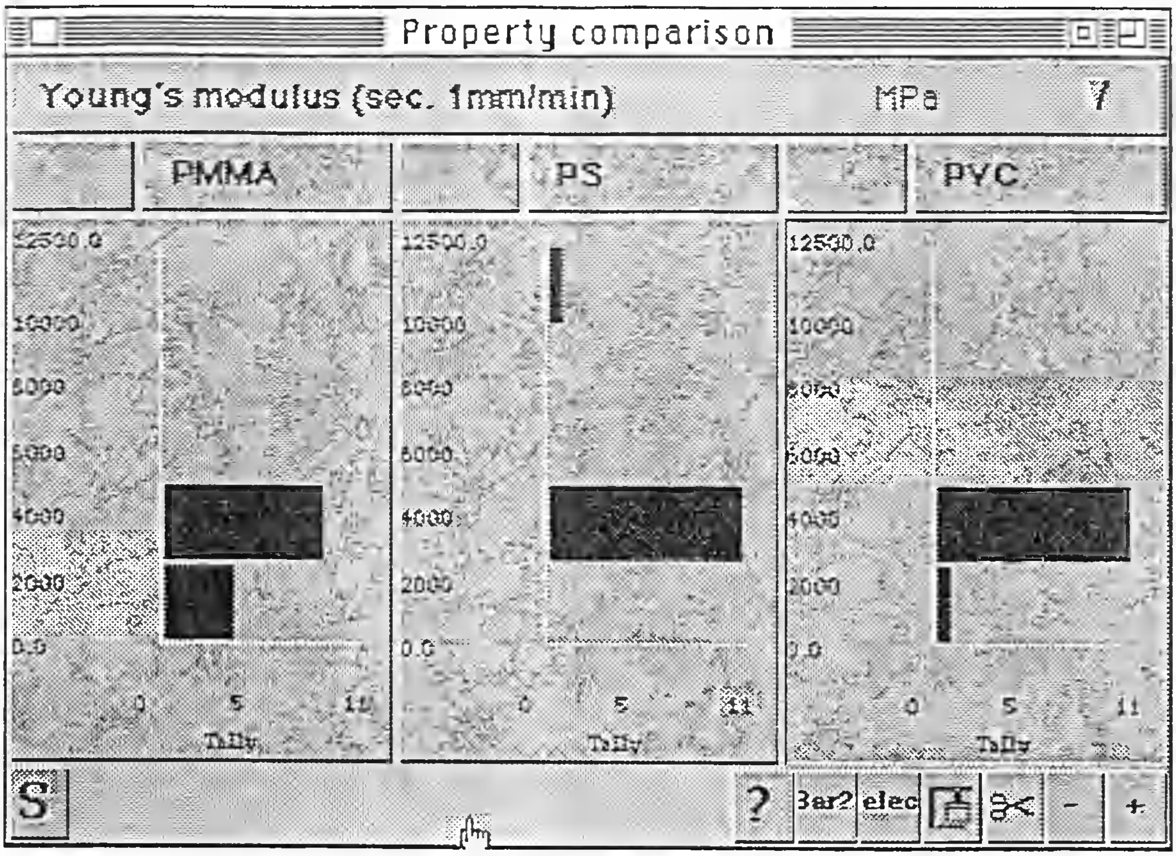
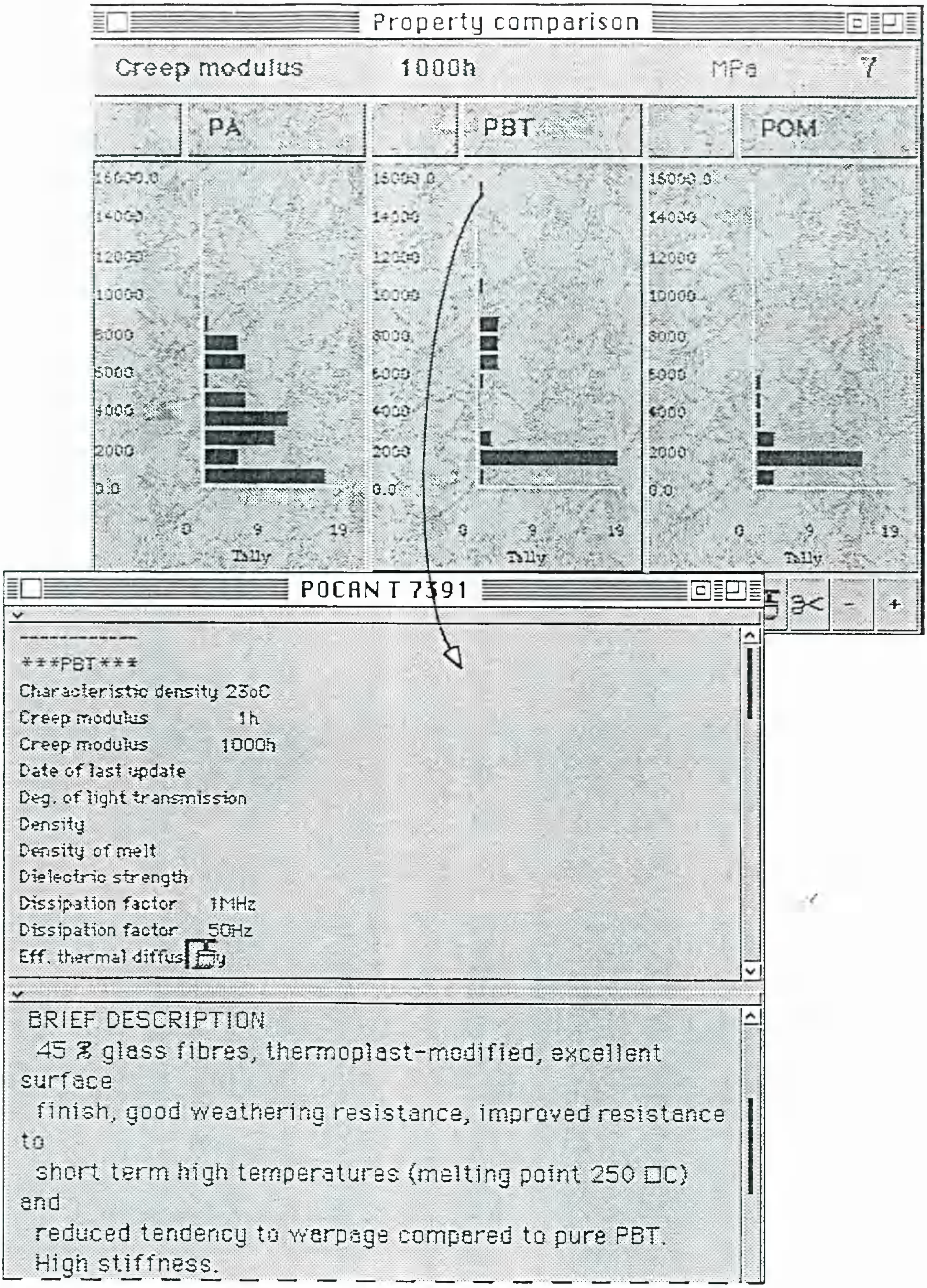


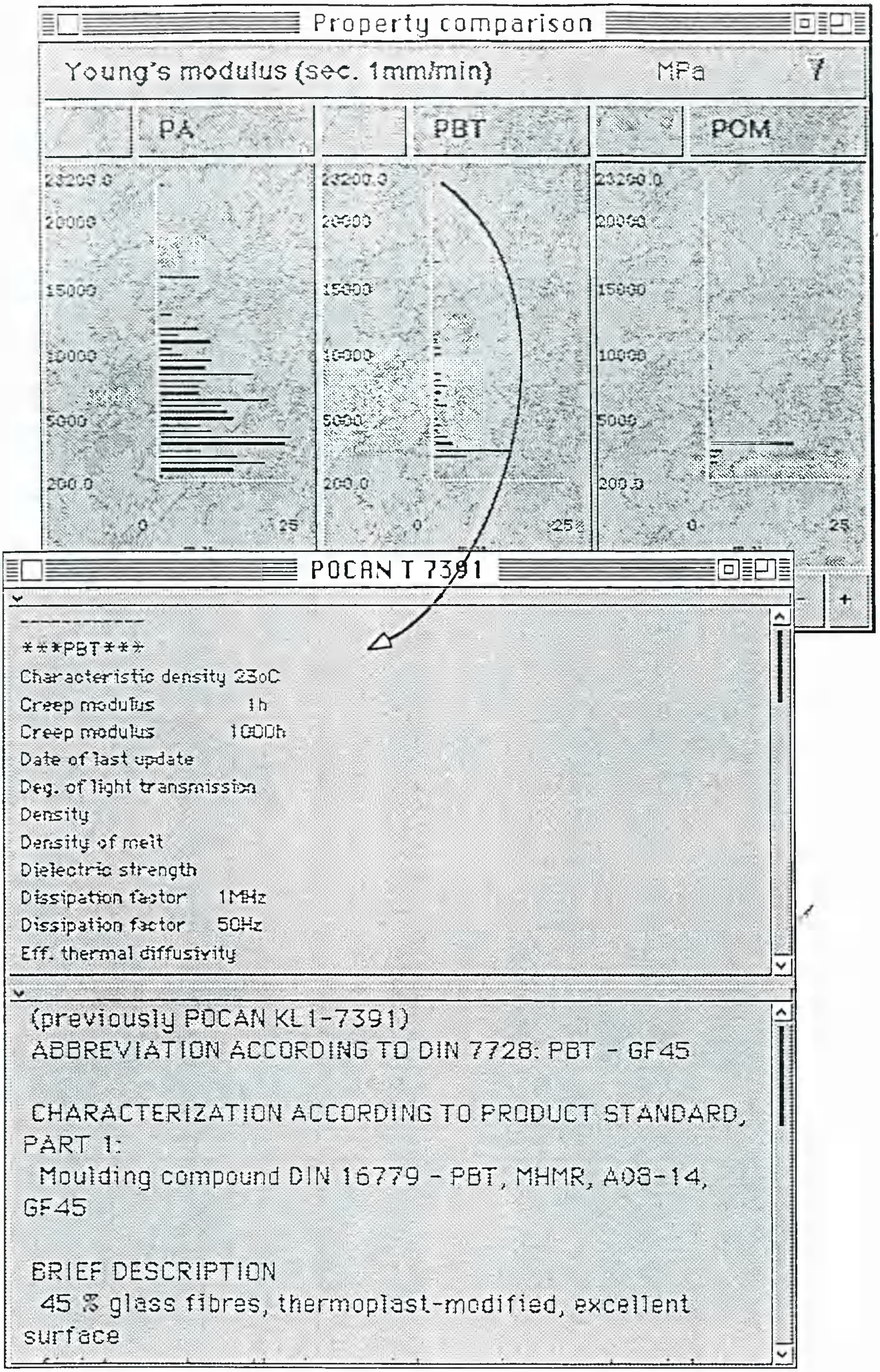
Plate 12 Young's modulus for some amorphous chemical family classes



PBT
Characteristic density 23oC
Creep modulus 1h
Creep modulus 1000h
Date of last update
Deg. of light transmission
Density
Density of melt
Dielectric strength
Dissipation factor 1MHz
Dissipation factor 50Hz
Eff. thermal diffus[illegible]y

BRIEF DESCRIPTION
45 % glass fibres, thermoplast-modified, excellent surface finish, good weathering resistance, improved resistance to short term high temperatures (melting point 250 □C) and reduced tendency to warpage compared to pure PBT. High stiffness.

Plate 13 Creep modulus data for some partly crystalline chemical family classes showing the PBT grade with the high value



PBT
Characteristic density 23oC
Creep modulus 1h
Creep modulus 1000h
Date of last update
Deg. of light transmission
Density
Density of melt
Dielectric strength
Dissipation factor 1MHz
Dissipation factor 50Hz
Eff. thermal diffusivity

(previously POCAN KL1-7391)
ABBREVIATION ACCORDING TO DIN 7728: PBT - GF45

CHARACTERIZATION ACCORDING TO PRODUCT STANDARD, PART 1:
Moulding compound DIN 16779 - PBT, MHMR, A08-14, GF45

BRIEF DESCRIPTION
45 % glass fibres, thermoplast-modified, excellent surface

Plate 14 Young's modulus for some partly crystalline family classes showing the PBT grade with a high value.

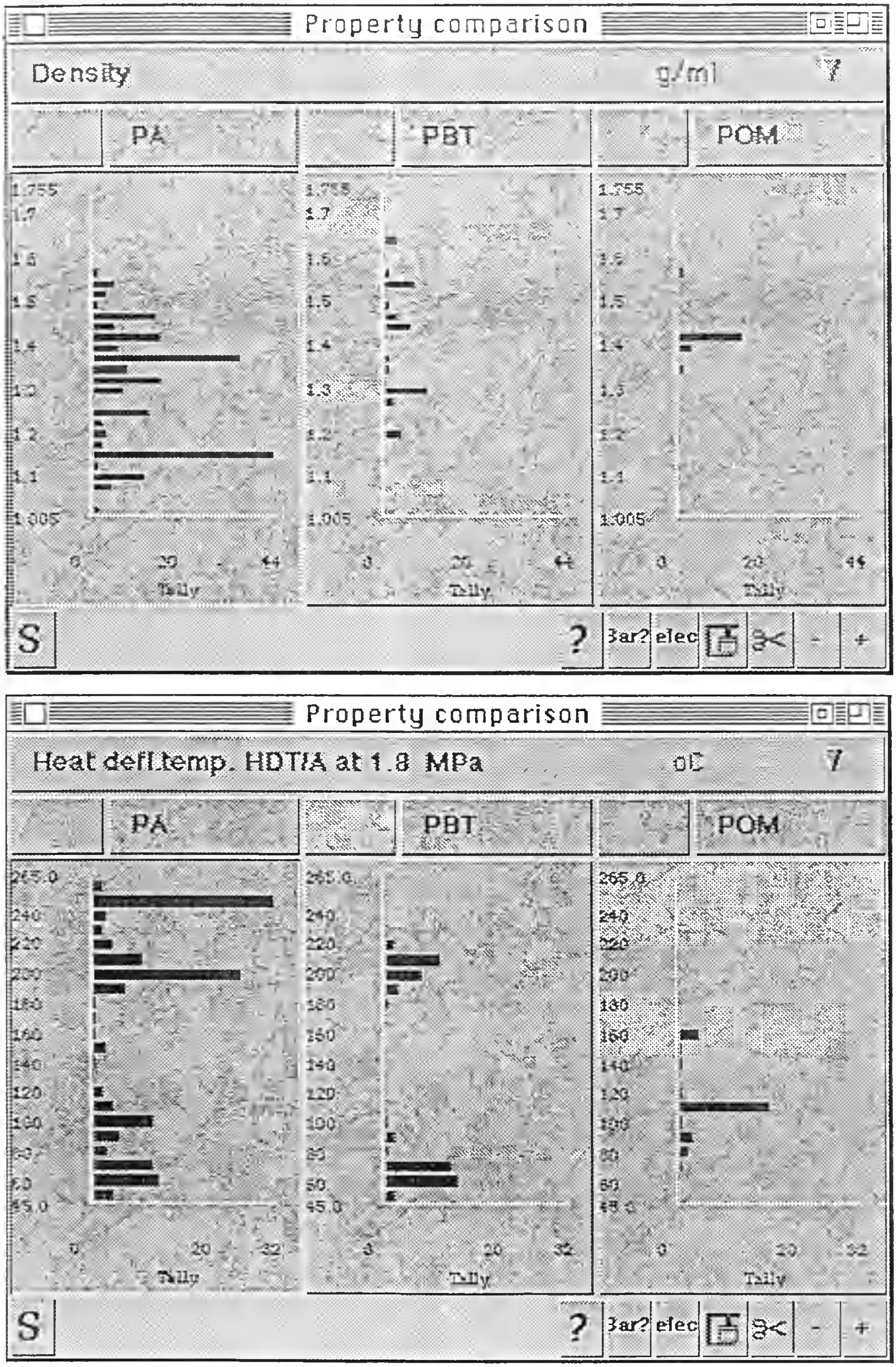


Plate 15 Density and heat deflection temperature data for some partly crystalline chemical family classes

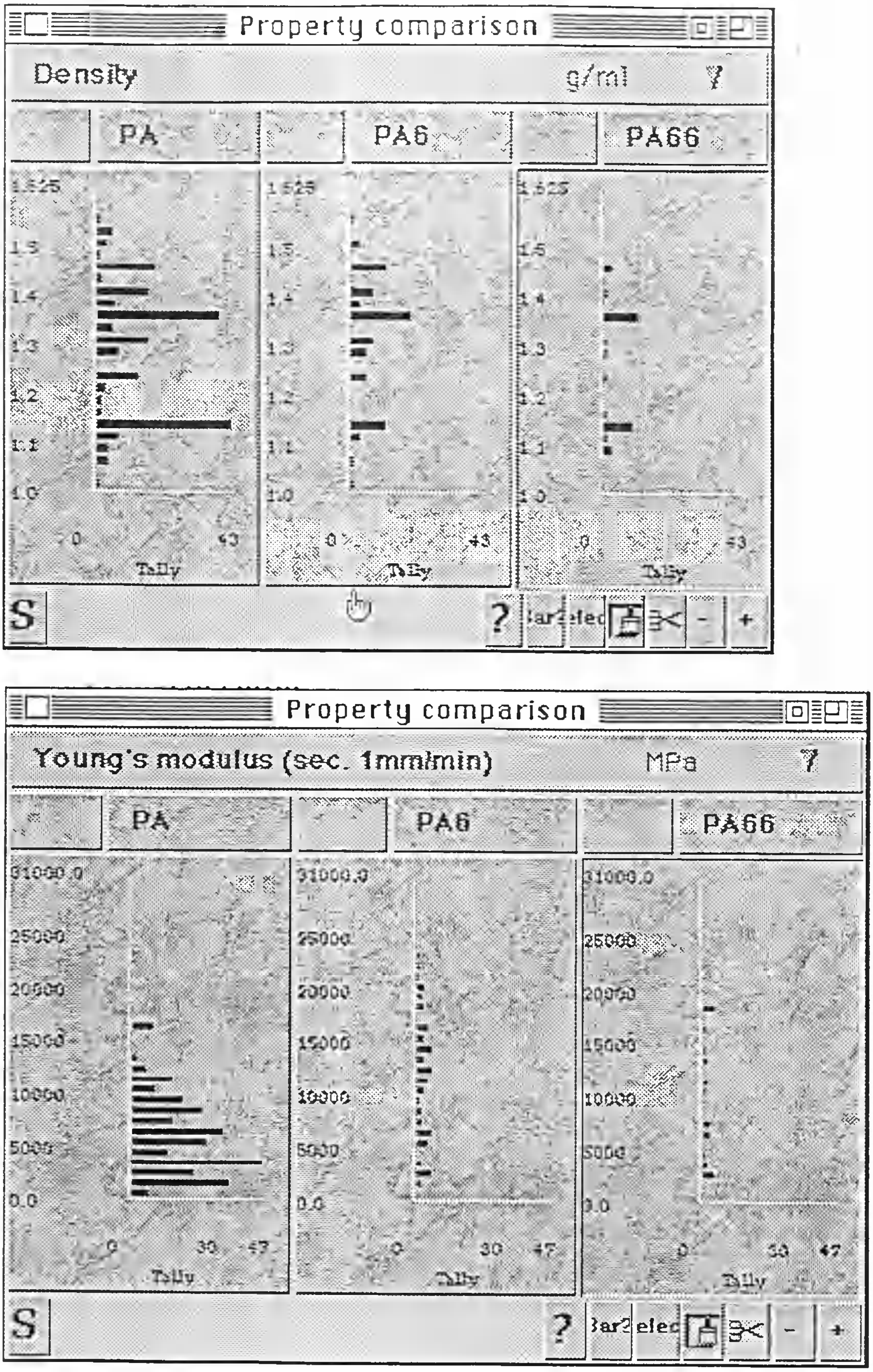


Plate 16 Density and Young's modulus data for NYLON (PA) and its subclasses

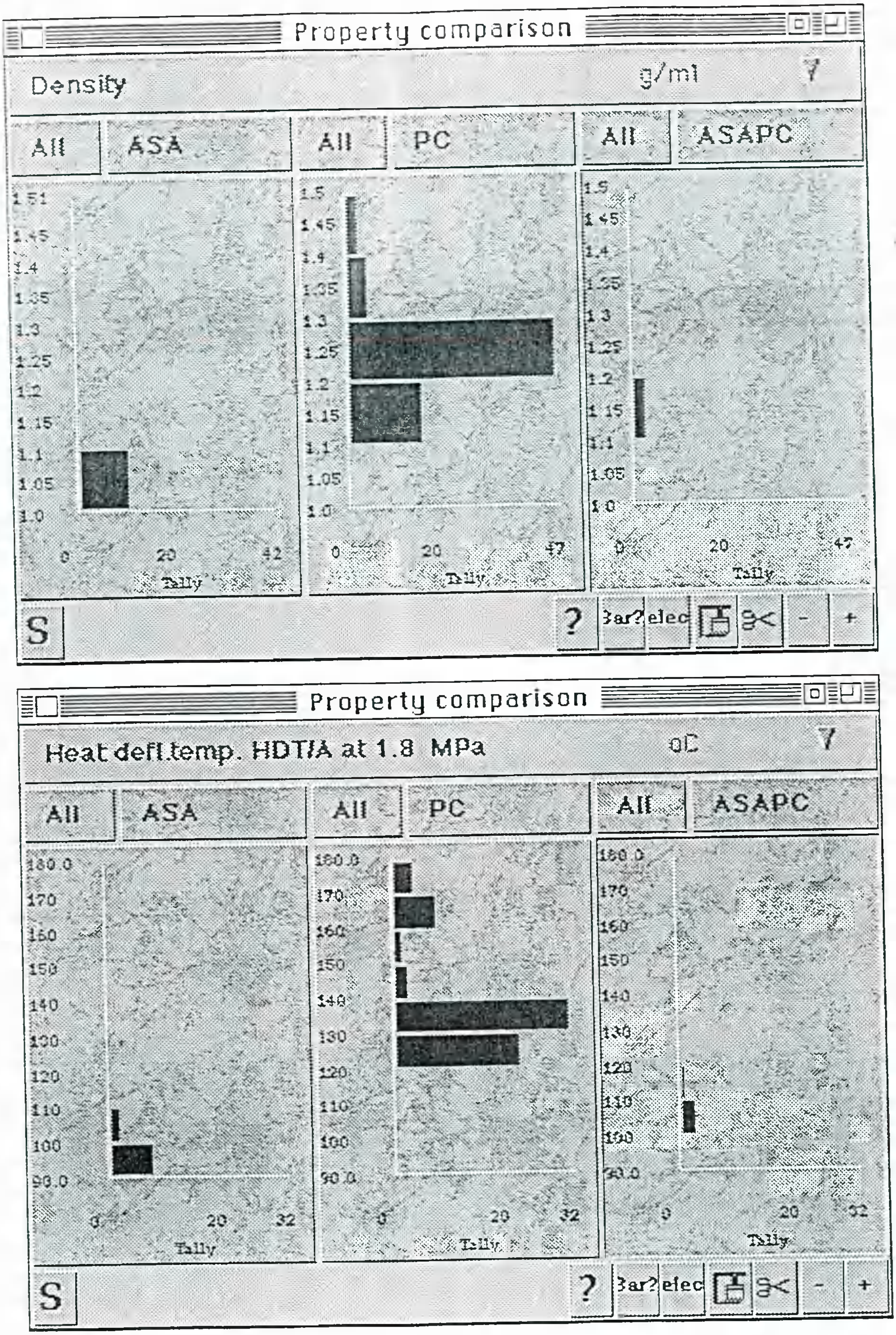


Plate 17 Density and heat deflection data for the copolymer ASAPC and the polymers made from its constituent monomers: ASA and PC

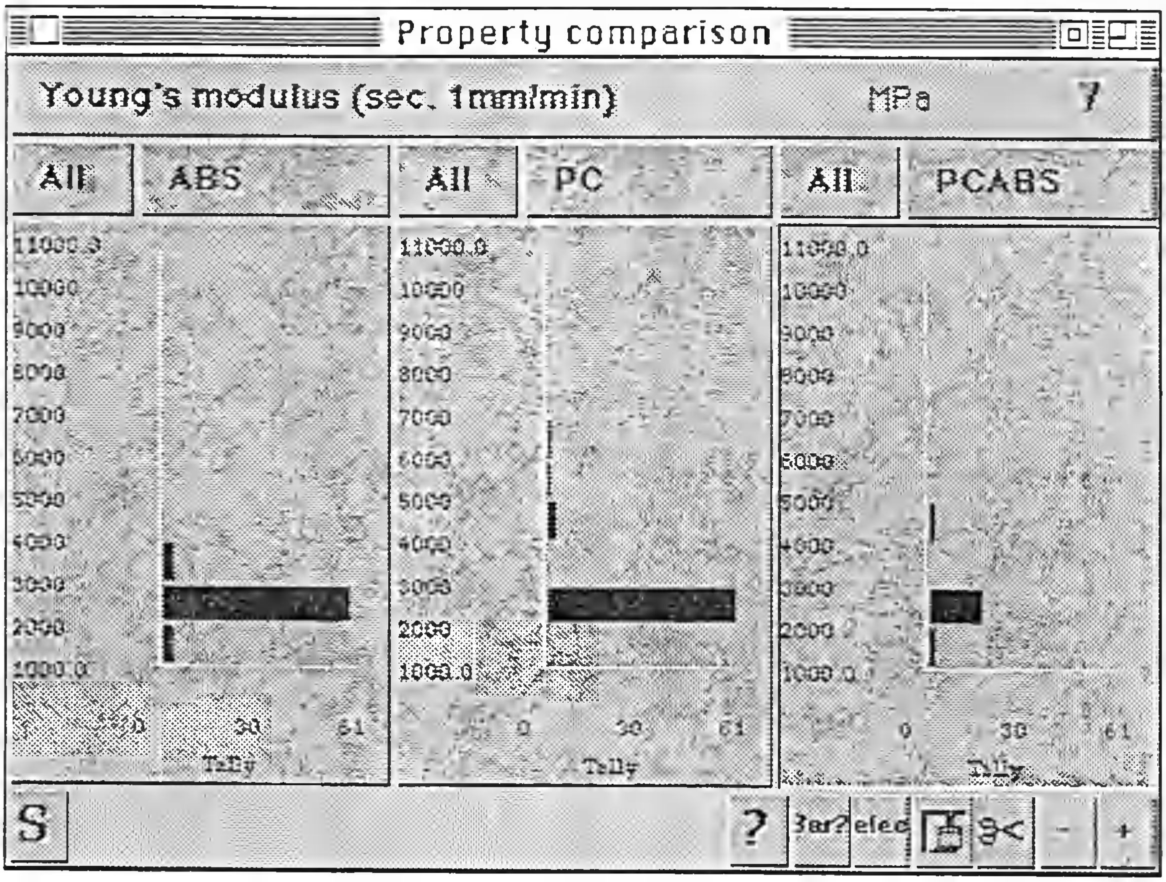
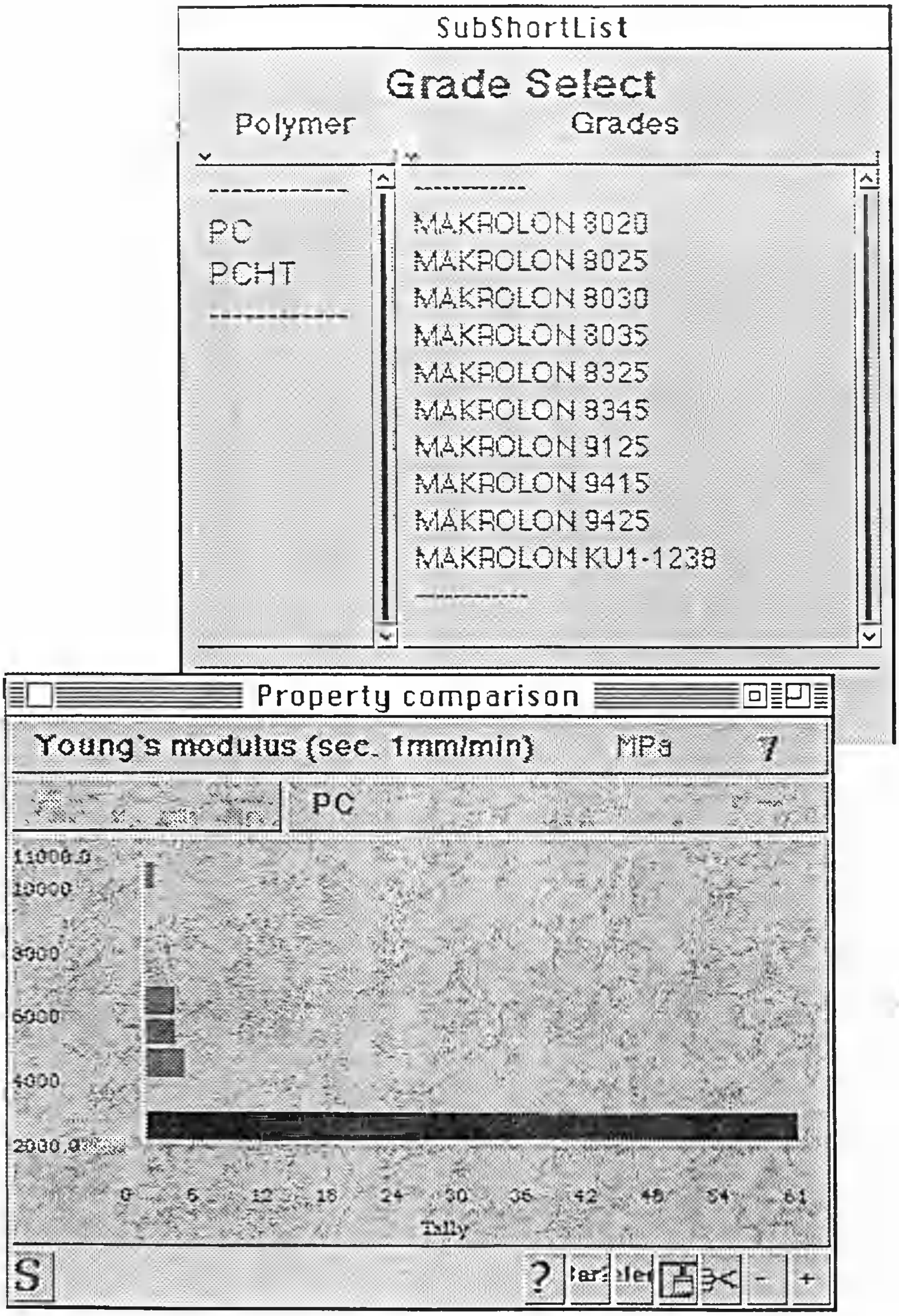


Plate 18 Young's modulus data for the copolymer PCABS and the polymers PC and ABS



SubShortList

Grade Select

Polymer

- PC
- PCHT

Grades

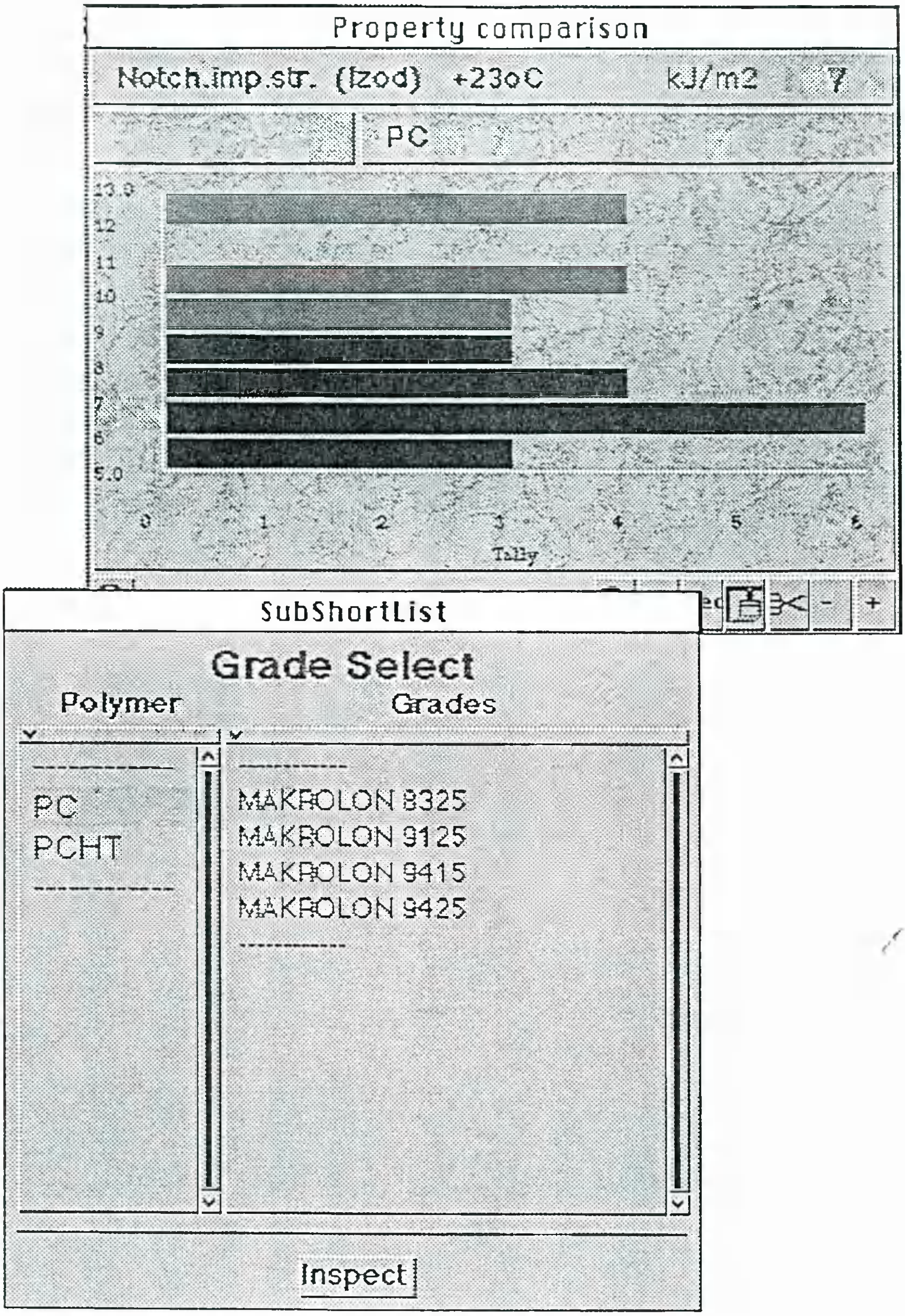
- MAKROLON 8020
- MAKROLON 8025
- MAKROLON 8030
- MAKROLON 8035
- MAKROLON 8325
- MAKROLON 8345
- MAKROLON 9125
- MAKROLON 9415
- MAKROLON 9425
- MAKROLON KU1-1238

Property comparison

Young's modulus (sec. 1mm/min) MPa

PC

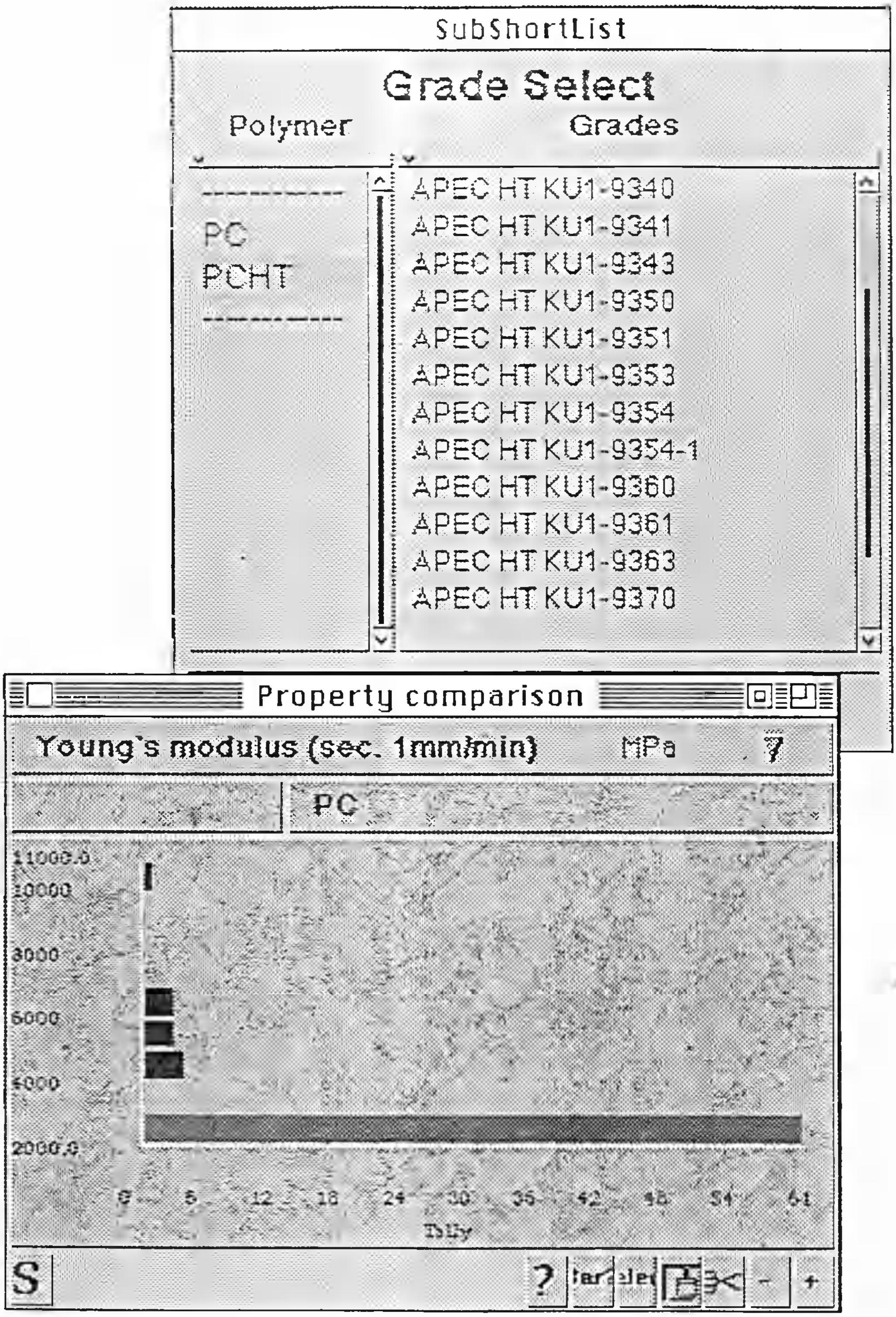
Plate 19 Investigation of Pugh's Rule: grades of PC with high values of Young's modulus



Polymer:
- PC
- PCHT

Grades:
- MAKROLON 8325
- MAKROLON 9125
- MAKROLON 9415
- MAKROLON 9425

Plate 20 Investigation of Pugh's Rule: grades of PC with high values of notched impact strength



SubShortList

Grade Select

Polymer

- ----------
- PC
- PCHT
- ----------

Grades

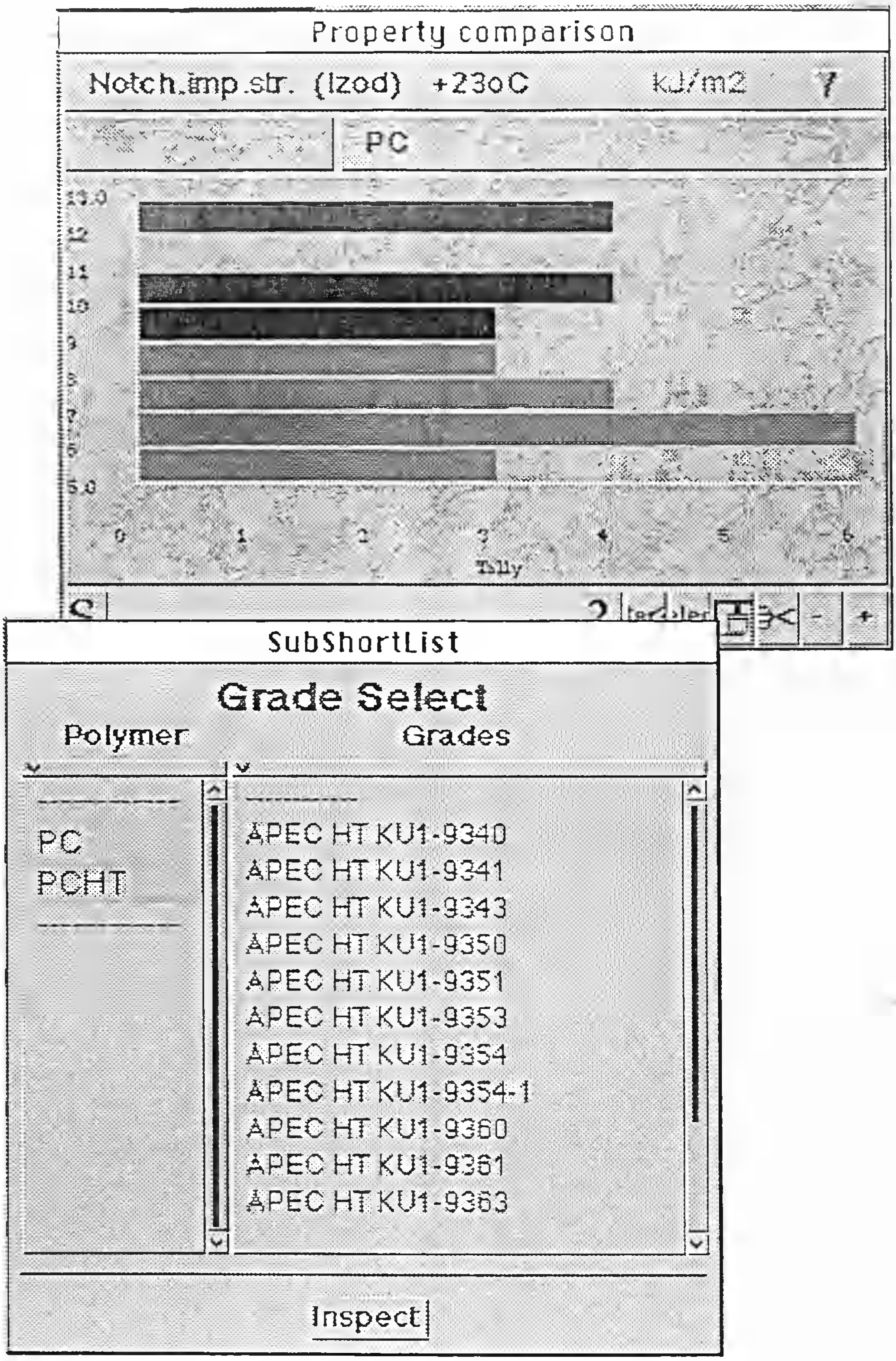
- APEC HT KU1-9340
- APEC HT KU1-9341
- APEC HT KU1-9343
- APEC HT KU1-9350
- APEC HT KU1-9351
- APEC HT KU1-9353
- APEC HT KU1-9354
- APEC HT KU1-9354-1
- APEC HT KU1-9360
- APEC HT KU1-9361
- APEC HT KU1-9363
- APEC HT KU1-9370

Property comparison

Young's modulus (sec. 1mm/min) MPa

PC

Plate 21 Investigation of Pugh's Rule: grades of PC with low values of Young's modulus



PC
PCHT

APEC HT KU1-9340
APEC HT KU1-9341
APEC HT KU1-9343
APEC HT KU1-9350
APEC HT KU1-9351
APEC HT KU1-9353
APEC HT KU1-9354
APEC HT KU1-9354-1
APEC HT KU1-9360
APEC HT KU1-9361
APEC HT KU1-9363

Plate 22 Investigation of Pugh's Rule: grades of PC with low values of notched impact strength

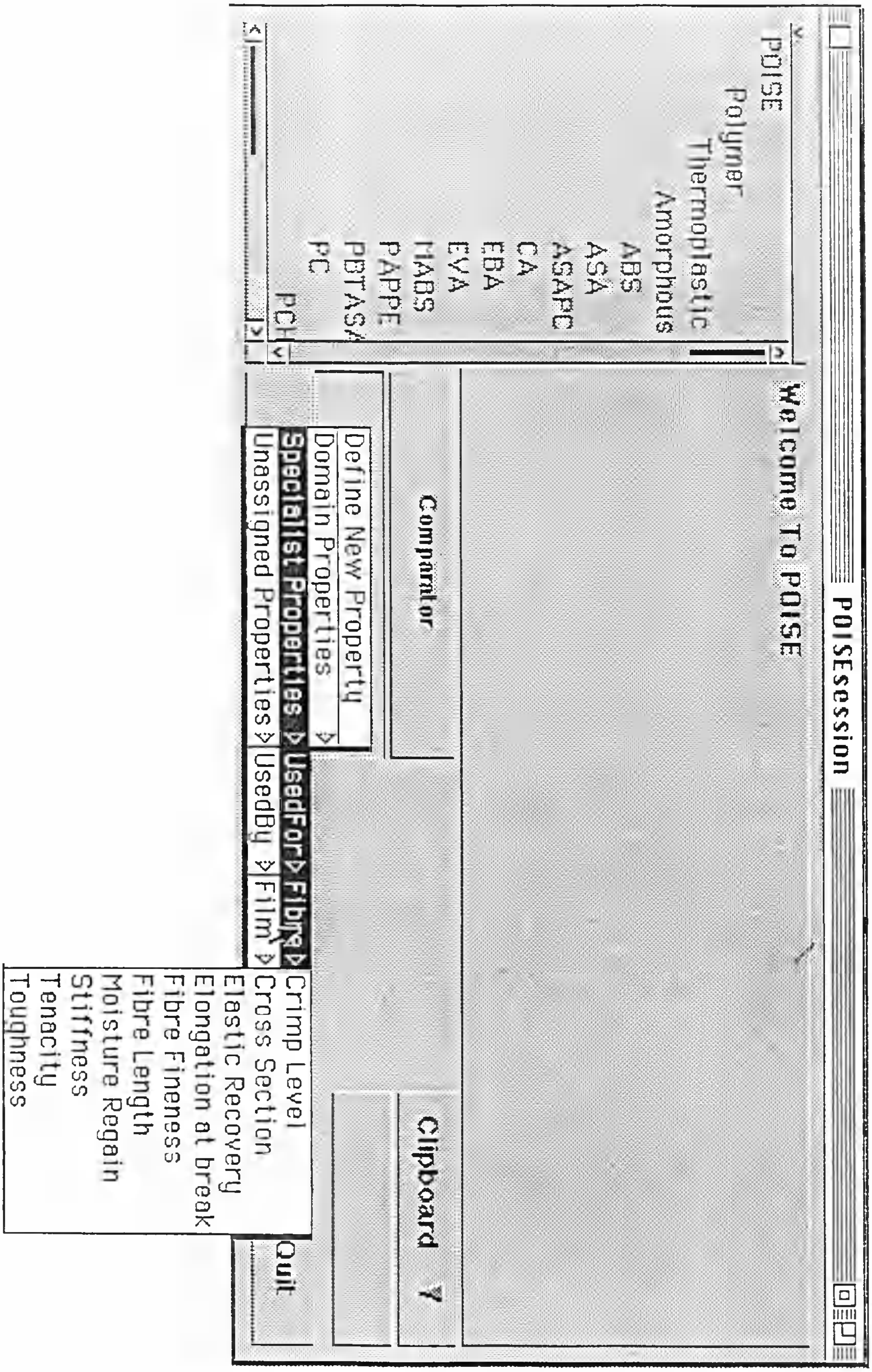
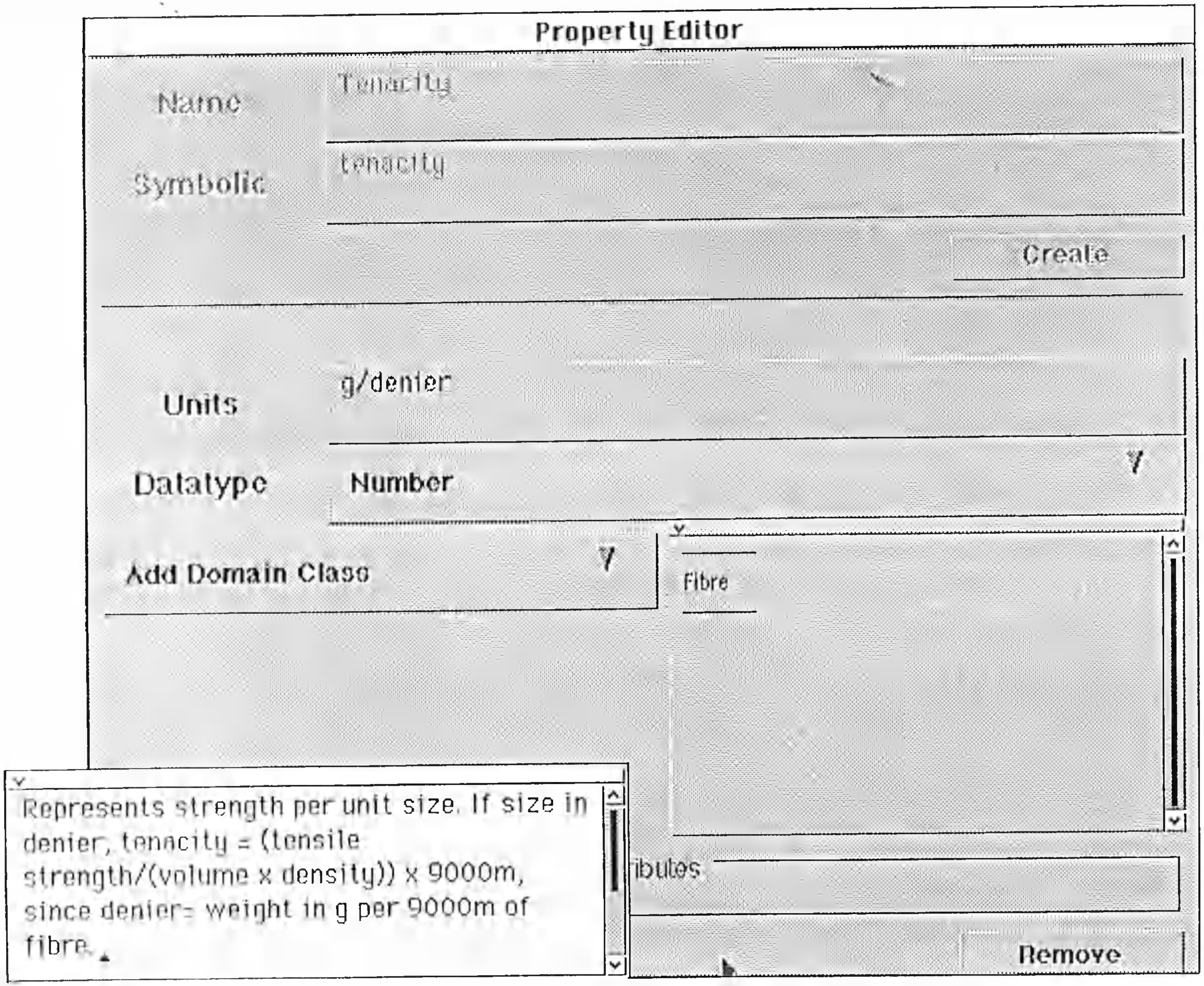


Plate 23 The specialist property menu: fibre properties



Name Tenacity

Symbolic tenacity

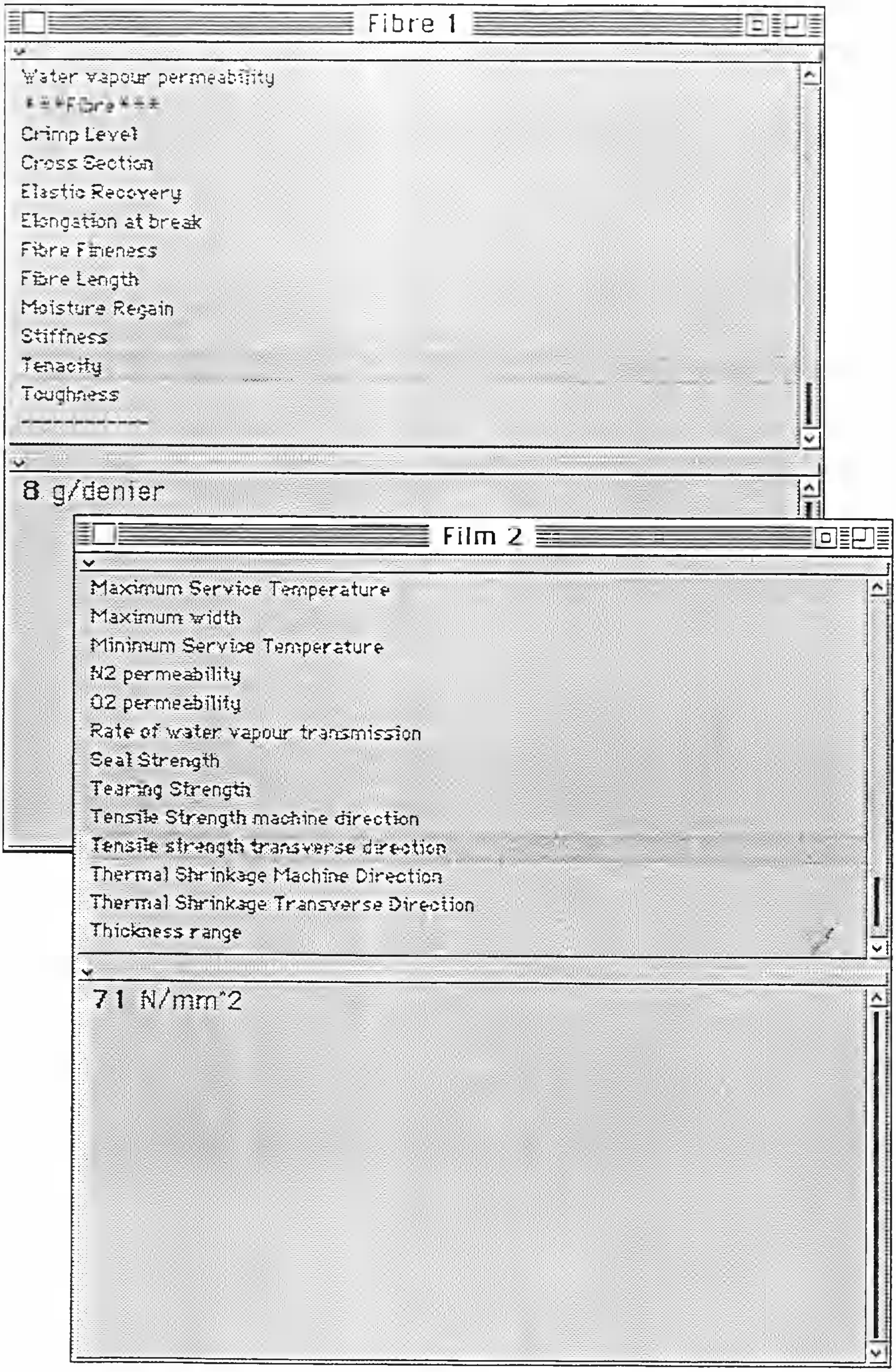
Units g/denier

Datatype Number

Fibre

Represents strength per unit size. If size in denier, tenacity = (tensile strength/(volume x density)) x 9000m, since denier= weight in g per 9000m of fibre.

Plate 24 Property Editor window on the fibre property tenacity with comment



Water vapour permeability
Fibre
Crimp Level
Cross Section
Elastic Recovery
Elongation at break
Fibre Fineness
Fibre Length
Moisture Regain
Stiffness
Tenacity
Toughness
----

8 g/denier

Maximum Service Temperature
Maximum width
Minimum Service Temperature
N2 permeability
O2 permeability
Rate of water vapour transmission
Seal Strength
Tearing Strength
Tensile Strength machine direction
Tensile strength transverse direction
Thermal Shrinkage Machine Direction
Thermal Shrinkage Transverse Direction
Thickness range

71 N/mm^2

Plate 25 Example film and fibre grades

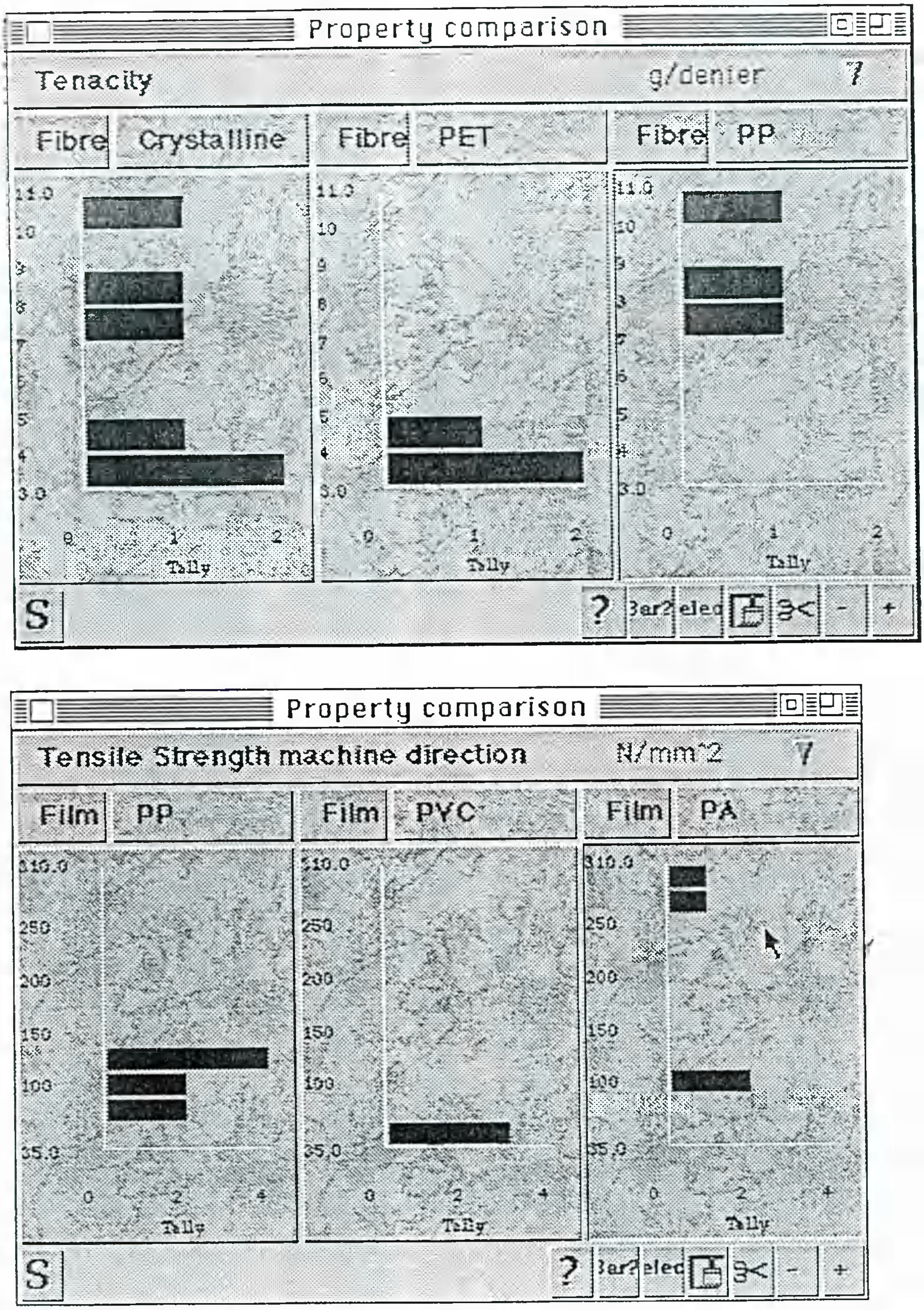
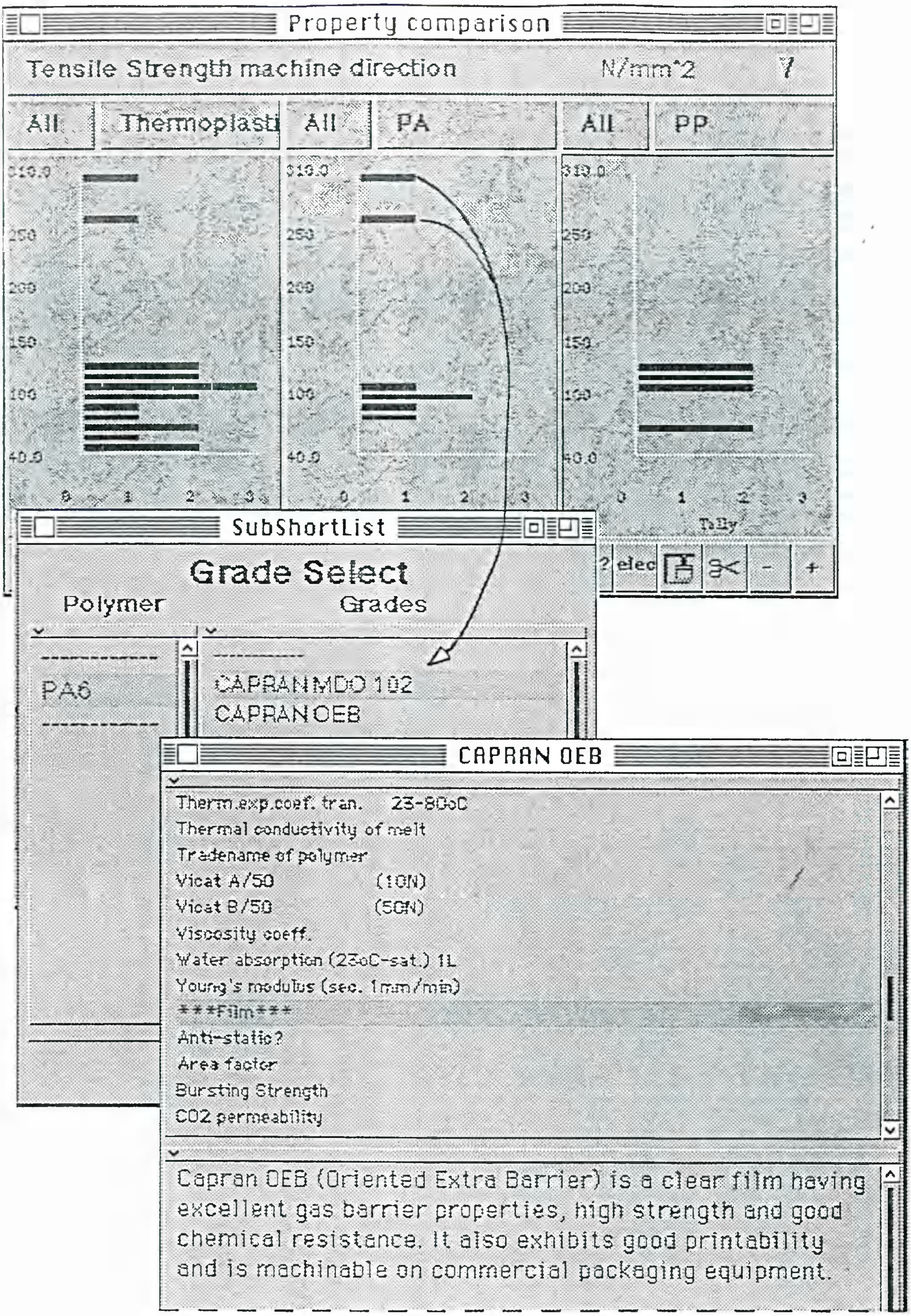


Plate 26 Comparison of tenacity data for fibre grades of Partly Crystalline, PET and PP; and of tensile strength, machine direction data, for the film grades of PP, PVC and PA

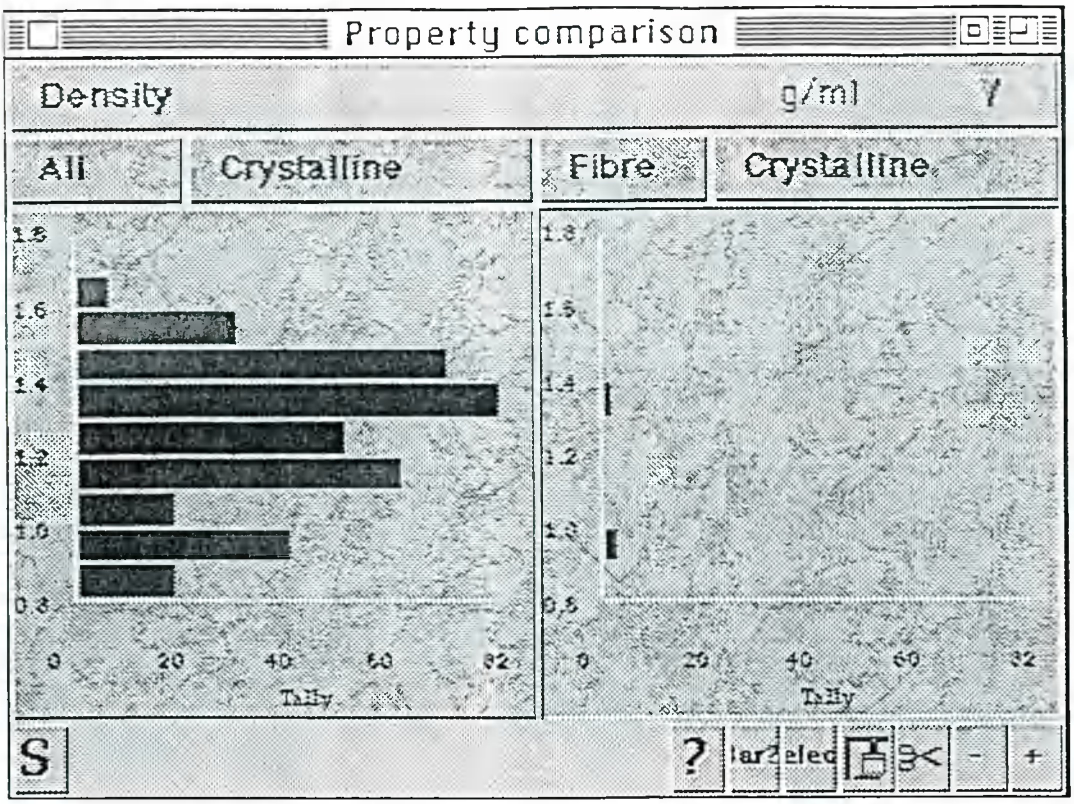


CAPRAN MDO 102
CAPRAN OEB

Therm.exp.coef. tran. 23-80oC
Thermal conductivity of melt
Tradename of polymer
Vicat A/50 (10N)
Vicat B/50 (50N)
Viscosity coeff.
Water absorption (23oC-sat.) 1L
Young's modulus (sec. 1mm/min)
Film
Anti-static?
Area factor
Bursting Strength
CO2 permeability

Capran OEB (Oriented Extra Barrier) is a clear film having excellent gas barrier properties, high strength and good chemical resistance. It also exhibits good printability and is machinable on commercial packaging equipment.

Plate 27 Comparison of tensile strength, machine direction data for all grades of Thermoplastic, PA and PP: selected bars show the property has picked out film grades



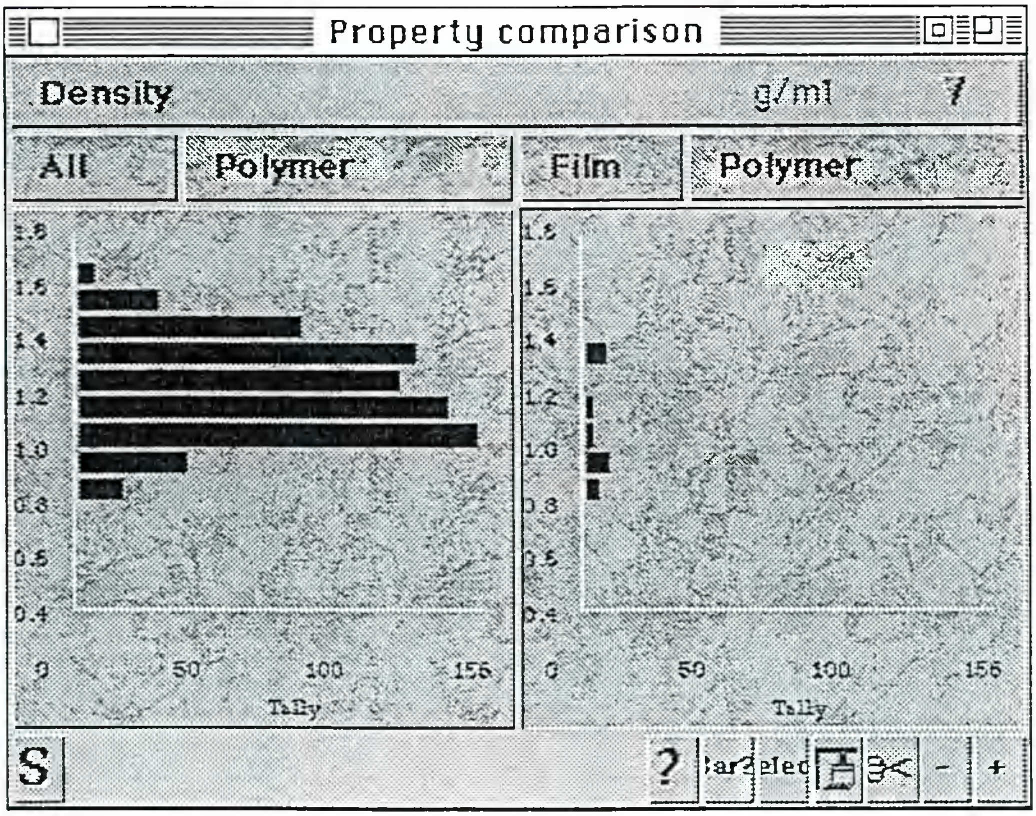
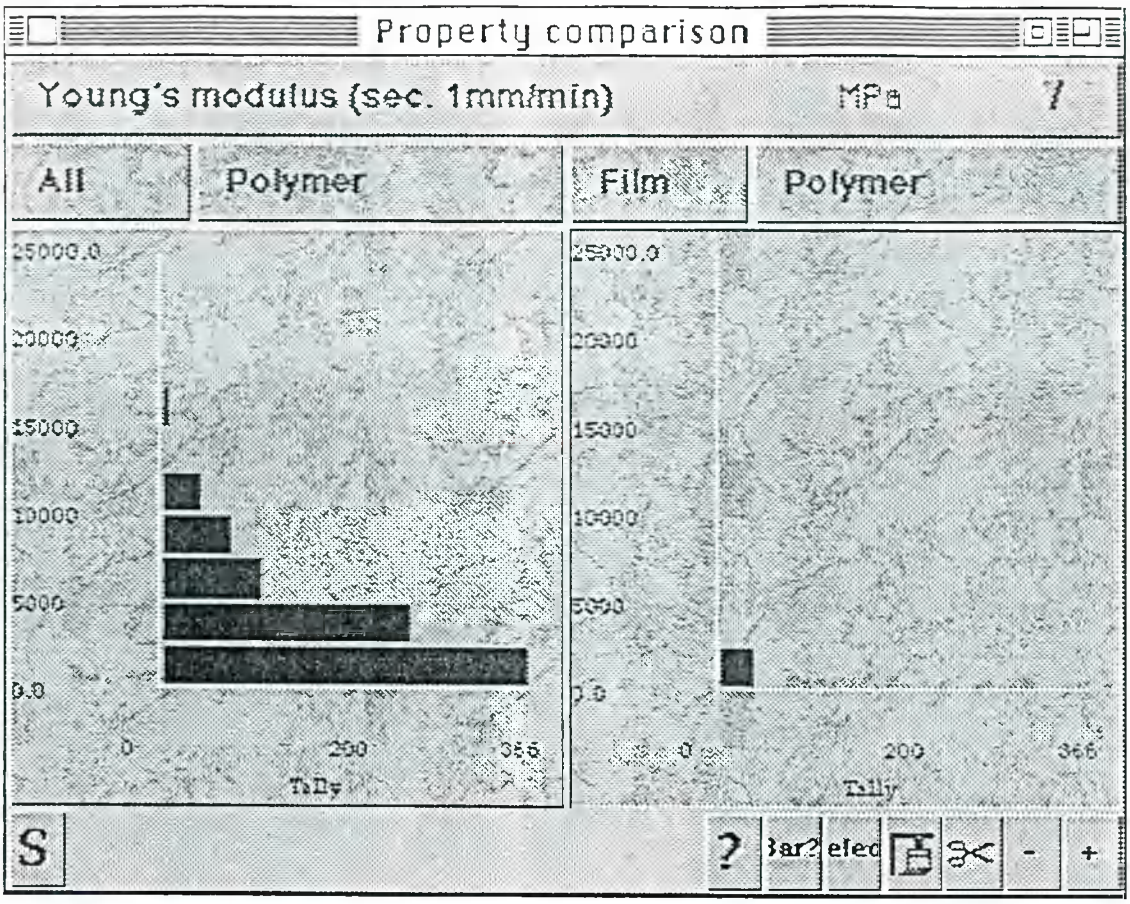


Plate 28 Density data for all Partly Crystalline grades compared with fibre Partly Crystalline grades only; repeated for all Polymer grades and film Polymer grades



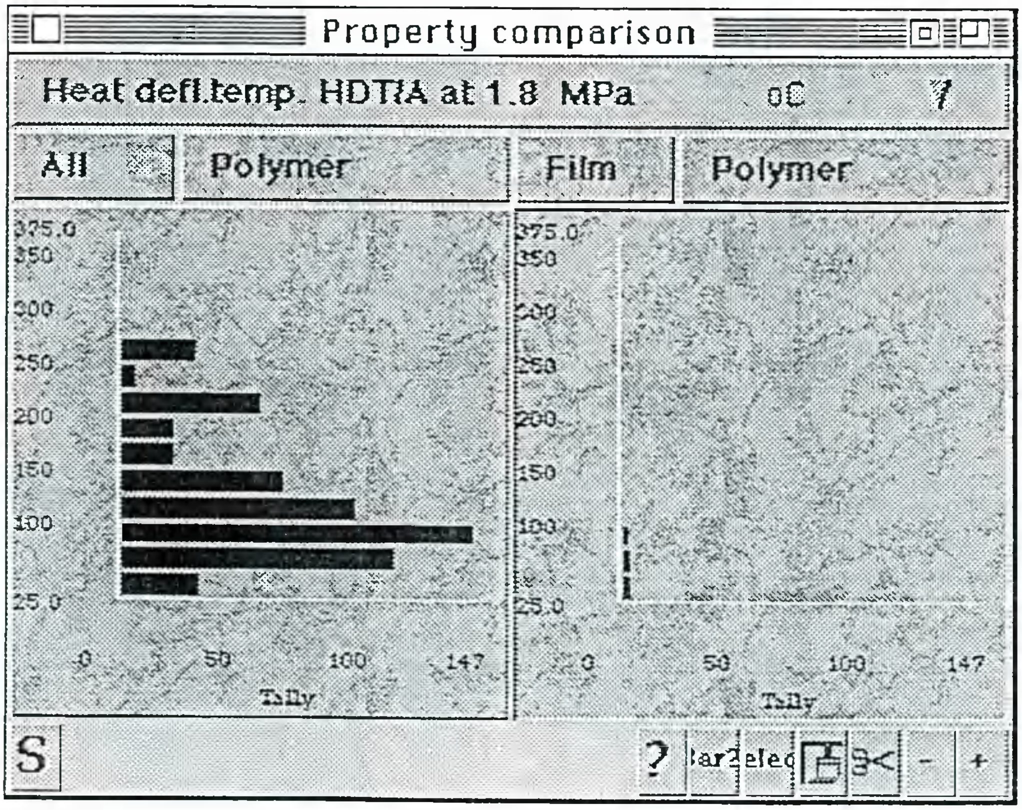


Plate 29 All polymers compared with film grades of the Polymer class for Young's modulus and heat deflection temperature

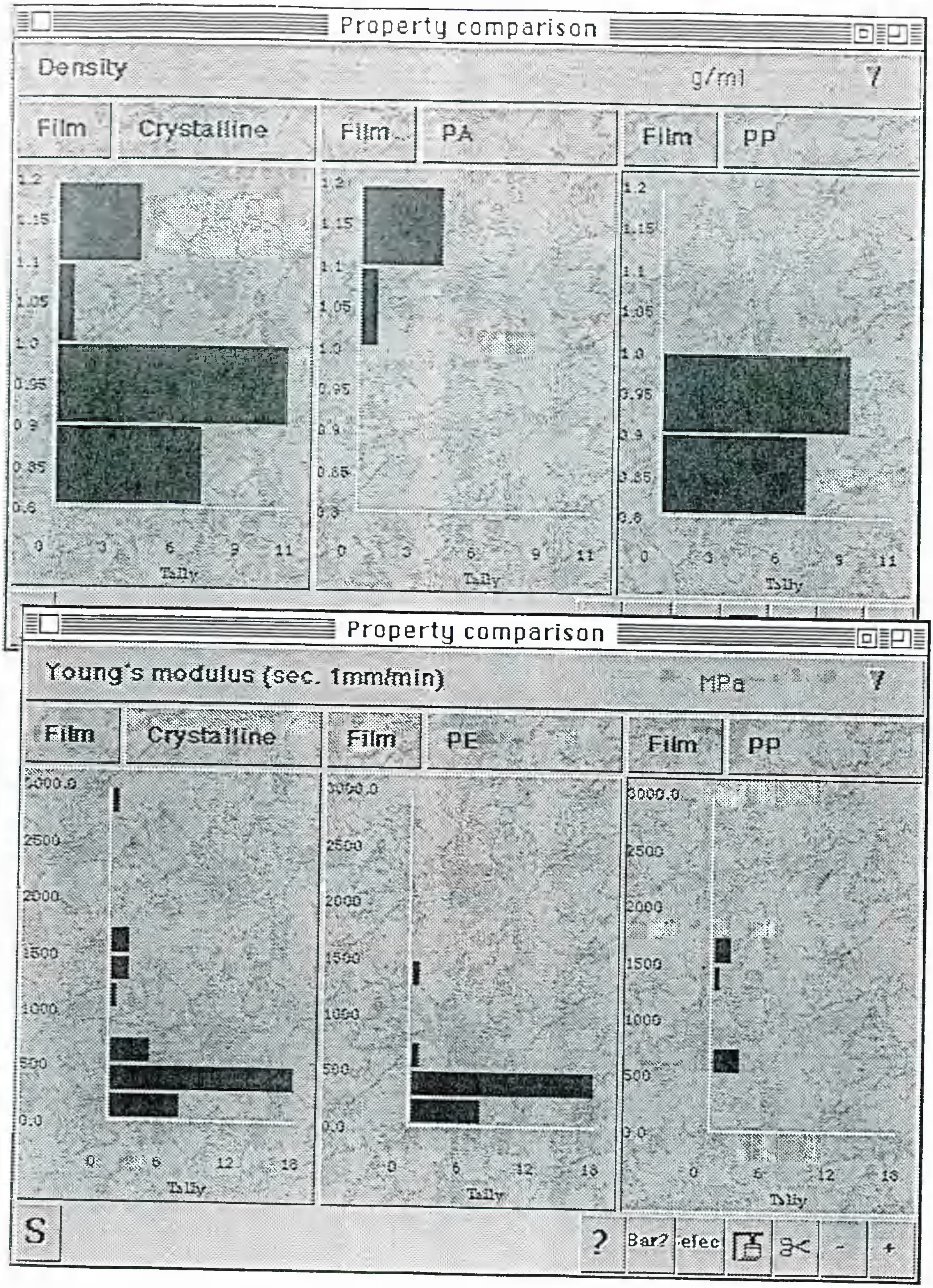
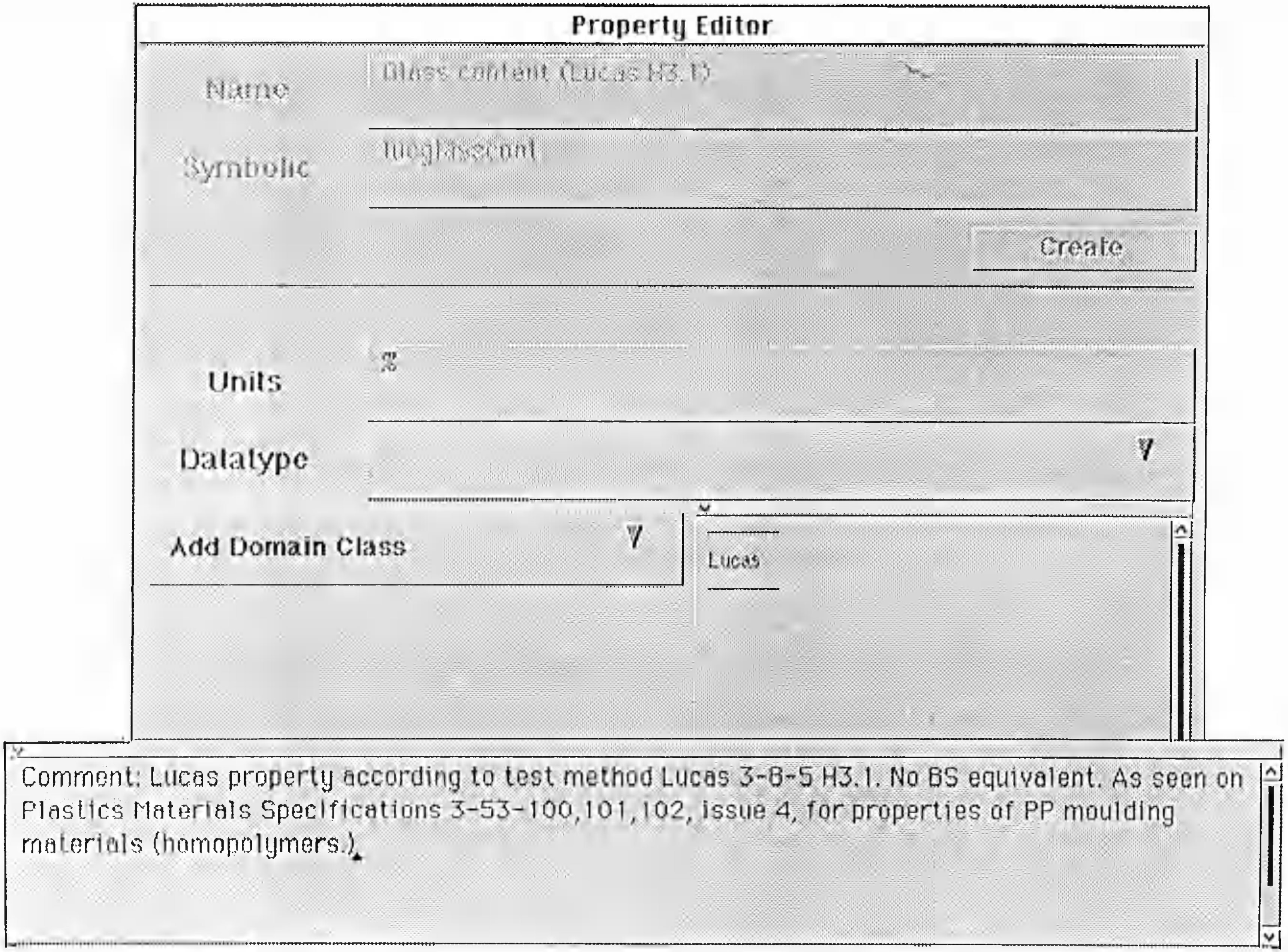


Plate 30 Density and Young's modulus data for the film grades of some Partly Crystalline classes



Name: Glass content (Lucas H3.1)

Symbolic: lucglasscont

Units: %

Datatype:

Add Domain Class: Lucas

Comment: Lucas property according to test method Lucas 3-8-5 H3.1. No BS equivalent. As seen on Plastics Materials Specifications 3-53-100,101,102, issue 4, for properties of PP moulding materials (homopolymers.)

Plate 31 Property editor window for the Lucas property glass content

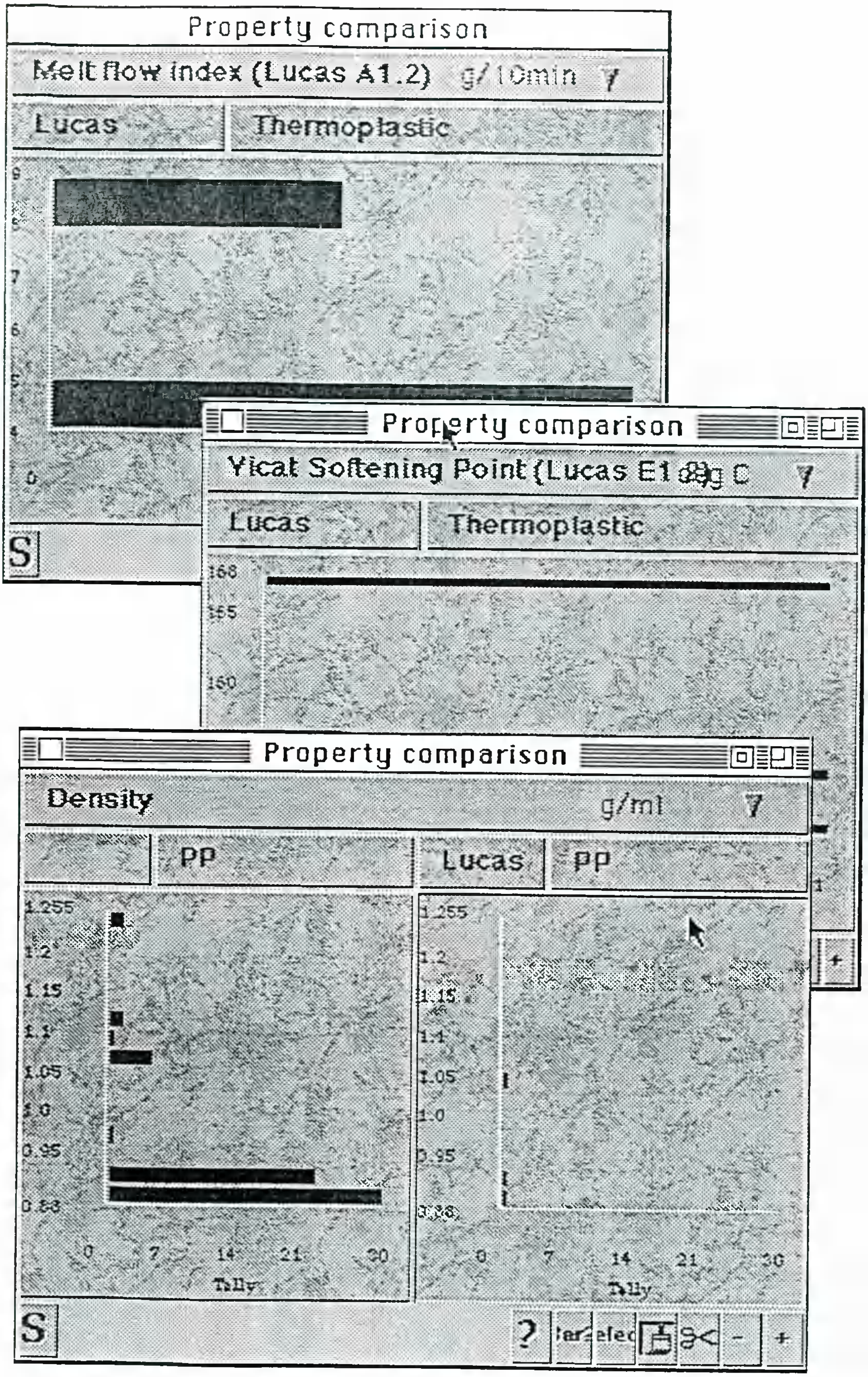


Plate 32 Illustration of two Lucas properties for the class Thermoplastic; also, comparison of density data for all of the PP class and just the Lucas grades of the PP class