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CHARACTERIZATION OF FINITE LENGTH COMPOSITES: PART V. MODELLING OF STIFFNESS

(Technical Report)

The authors and contributing members dedicate this paper to their colleague and friend,
Professor Gerhard Zachmann

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Characterization of finite length fibre composites. Part V: Modelling of stiffness (Technical Report)

Abstract: This characterization of a range of glass and carbon fibre reinforced polypropylene and polyamide injection moldings forms part of a wider IUPAC Working Party IV.2.1 study of these materials. In this part of the work we summarise observations of stiffness and microstructural characterization with the aim of linking these features via an micromechanical model. The model makes a number of simplifying assumptions in order to be tractable and is based on calculating the stiffness of a number of "imaginary" layers through the thickness of the molding, with each layer having a singular fibre orientation. The stiffness of the molding is then determined by an appropriate summation of the stiffness of these layers. The agreement between observed and 'modelled' stiffness is reasonable within the context of the assumptions necessary for tractability.

1. INTRODUCTION

Injection molded fibre reinforced thermoplastics can be prepared from extrusion and pultrusion compounded feedstocks. It is now well established that pultruded feedstock produces longer fibres in the molded artefact (ref. 1) often by an order of magnitude. The characteristics of the traditional injection molding process are however similar in both cases. The moulding will be anisotropic in the plane and heterogeneous through the thickness (ref. 2). The in-plane anisotropy can be modified during processing by the injection molding methods reported by Allan and Bevis (ref. 3). In their invention, the melt is pulsed in such a manner as to change the orientation of "core" fibres in order to obtain alignment in the direction of mold-fill. Their process is known as the multiple live-feed process.

The microstructure of injection molding is often relatively complex. This applies to both traditional and multiple live-feed methods. In fact, many materials scientists do not refer to injection moldings as materials but rather as 'structures'. This reflects the varied and complex nature of their character. Naturally, this complicates any description of the properties of the injection moldings. In particular, if the moldings are truly 'structures' then there is an implication that each structure requires experimental characcterization of its mechanical properties because a description of the material properties is redundant.

One way of overcoming this dilemma could emerge if there were a quantitative understanding between the measured properties of a molding and the observations of its microstructure. Exploring this possibility is the main aim of this paper and three stages are involved.

(i) It is necessary to measure the characteristics of the microstructure. In principle this involves a measurement of fibre length distribution, fibre content and the fibre orientation function. It is implicit that fibre dimensions and fibre/matrix stiffnesses are known.

(ii) It will be necessary to measure the stiffness of the mouldings. Naturally, for anisotropic moldings it would not be expected that this mechanical characterization is a simple discrete function. It will depend upon the direction and mode of applied stress in the molding and inevitably these properties will have an associated distribution function.

(iii) In order to relate the measured microstructure with the measured properties there will be a model or theory. For example, be comparing a measured property with a calculated property it will be easy to establish whether the understanding between structure and properties is effective. Inevitably, such a simple success criterion is elusive, as we shall see. Therefore prediction is replaced by modelling in order to judge our understanding. (This will be discussed more fully in due course).

In exploring the relationship between microstructure and properties we intend to conduct to conduct the work with both traditional and multiple live-feed moldings. Moreover, the materials will have two different fibre systems (glass and carbon) and two different matrix materials (polyamide 6,6 and polypropylene). It is hoped that such choice will permit a wider generalisation of our work.

Finally, the conduct of the work is also unusual in that many laboratories have contributed to this project under the umbrella of an IUPAC working party (Working Party IV.2.1). The project is indeed multiple in that particular studies have focused on the processing of the materials (refs. 4-6), other contributions on mechanical properties (ref. 5) and others on the structural characterization (ref. 7). This removes a requirement in this paper of providing all the detailed structural and mechanical measurements since these are reported elsewhere. Nevertheless, the important and relevant observations which have been detailed in the other publications will be summarized.

In this stage of the work the following Laboratories have contributed:

Laboratory 1: ICI plc (D R Moore, R S Bailey, G von Bradsky, R S Prediger)
Laboratory 2: Shell Research Arnhem (A Cervenka)
Laboratory 3: Rhone-Poulenc (Y Giraud)
Laboratory 4: HULS AG (H Motz)
Laboratory 5: National Research Council Canada (T Vu-Khanh)
Laboratory 6: Brunel University (M J Bevis, P S Allan)
Laboratory 7: BP Chemicals (M J Cawood, A Gray with contributions from the IRC at Leeds University)

2. DESCRIPTION OF SAMPLES

Three different long fibre discontinuous materials were injection molded in the form of plaques for this IUPAC project. Full details of the materials and their preparation are reported elsewhere (ref. 4). The materials were all fibre reinforced with either Kevlar, glass or carbon fibres; the matrix materials also differed and included polypropylene and polyamide 6,6. In this paper only the composites with glass and carbon fibre reinforcement are considered. The composites were compounded by a pultrusion method and were then processed by injection molding. (All materials were experimental grades of "Verton" supplied (at that time) by ICI PLC and incorporated a notional mass fraction of 40% of fibre reinforcement). Pultrusion compounding enabled a granule feedstock for injection molding to be prepared with control of the length of the continuous fibre reinforcement. The fibre length in the granule was either 5 mm or 10 mm.

In addition. two types of injection molding methodology were used. A standard procedure and a multiple live-feed procedure (ref. 3). Although these details are more fully described elsewhere, in essence the aim was for the multiple live-feed procedure to more fully align the fibre in the direction of mold fill, whilst the expectation was for the conventional molding process to achieve the more traditional "skin-core" structure through the thickness of the molding (i.e. the fibres in the "skin" would be aligned in the direction of mold fill, whilst the fibres in the "core" would be aligned transverse to the direction of mold fill). Naturally, this is a tentative description of fibre orientation, included here merely for purposes of describing the materials.

The composites for study can therefore be described with the following nomenclature:

- Multiple live-feed moldings, which are designated "DYNAMIC" moldings.
- Conventional injection moldings, which are designated "STATIC" moldings

Fibre lengths in the pultruded granule (the feedstock for injection molding) are designated 5 or 10 (which describes the length in mm of the fibre in the granule).

The fibre type is either carbon, designated c or glass designated g.

The matrix material is either polypropylene, designated PP or polyamide 6,6 designated PA.

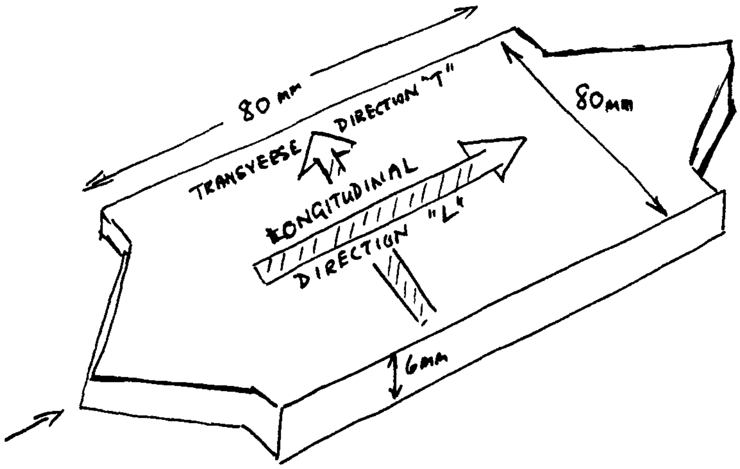
Ten different materials were used in the study:

PA/c 10 DYNAMIC and PA/c 10 STATIC

PA/g 5 DYNAMIC and PA/g 5 STATIC; PA/g 10 DYNAMIC and PA/g 10 STATIC

PP/g 5 DYNAMIC and PP/g 5 STATIC; PP/g 10 DYNAMIC and PP/g 10 STATIC

The plaque moldings were nominal 6 mm thick and Fig. 1 shows their geometry and dimensions. The conventional molding process (STATIC employed a single side fan gate, whilst the multiple live-feed molding process (DYNAMIC) employed a fan gate at each end of the mold.



Second gate used for multiple live feed moulding

Gate for conventional injection moulding

Fig. 1 Molding used for the work

3. OBSERVATION OF THE MICROSTRUCTURE

A full description of the microstructure of these moldings is documented in another publication (ref. 7). Three characteristics of the microstructure are described, namely fibre orientation distribution (FOB), fibre content and fibre length analysis. In practice, it is easier to be quantitative about the fibre content and fibre length distribution than it is about the fibre orientation functions. Reference 7 conducts a review of the problems and discusses some practical solutions.

In terms of the fibre orientation distribution, a number of qualitative observations emerged (ref. 7):

- PA/g and PP/g systems behave similarly with well defined skin/core structures.
- PA/c system appears more random in structure.
- In all cases, the DYNAMIC molding process provides improved alignment of fibres in the direction of mold fill resulting in a smaller core region.

In addition, a number of quantitative observations can be made:

- Image Analysis allows direct access to in-plane and out-of-plane fibre angles.
- For STATIC moldings, PP/g systems contain defined skin/core regions with little out-of-plane orientation.
- For STATIC moldings, the PA/c system has a significantly greater out-of-plane orientation distribution.
- Comparison of samples from DYNAMIC and STATIC moldings confirms the greater alignment of fibres through the thickness of the specimen for the DYNAMIC mode.

For the size and shape of the mold used in this work, it is quite apparent that the usual amount of lamellar flow that can be associated with large area injection molded component is not occurring. This of course makes a simple identification of the "skin-core" type structure through the thickness of the molding difficult. Nevertheless, an attempt has been made from the microstructural observations to describe an "imaginary" layered structure through the thickness where each layer has a single angle of fibre orientation, since this is required for the modelling activities which will be described later. Tables 4 and 5 in Appendix summarize these microstructures through the thickness, together with a summary of the fibre content measurements and fibre length distributions.

4. STIFFNESS OBSERVATIONS

A full account of all various mechanical property measurements is reported by Glas (ref. 5) and Cervenka (ref. 6) complementing this work with studies of wafers cut through the thickness of the moldings. These publications enabled a summary of appropriate measurements to be extracted for the purpose of summarising stiffness in the context of modelling. Such stiffness measurements were made at 23 °C by three different Laboratories employing flexural and tensile methods. The contributing Laboratories used various forms of universal testing machines where constant rate of deformation inputs were used at as nominal crosshead speed of 0.016 mm/s. There was no intention of employing standard test conditions and therefore each Laboratory used its current practice for achieving the measurement of modulus. Consequently, the data base of moduli values varied according to the location and number of specimens tested. It was certainly observed that modulus varied according to position of test specimen from the plaque molding.

It is particularly important to distinguish between moduli derived by tensile and flexural methods. In the tensile test a uniform force is applied across the complete thickness section of the specimen. In the flexural test the maximum force is applied to the mold surface region of the specimen and at some location (near the centre of the specimen) there will exist a neutral axis where the applied force is zero. This inevitably leads to a modulus by tension being a different engineering property from that measured by flexure.

In addition, the direction of applied force could be aligned with the direction of mold fill (designated L for longitudinal) or at right angle to the direction of mold fill (designated T for transverse). Accordingly, Table 1 summarises the various moduli measurements. The values summarised in this table relate to average values at some point near the centre of the molding. They do not reflect the variation in modulus at different locations in the mold.

All measurements on the polyamide 6,6 moldings relate to specimens stored nominally under dry conditions.

It can be observed in all cases for the 'L' direction that the DYNAMIC molding exhibits a higher modulus than that for STATIC molding; this relates to modulus by both tension and flexure. In addition, there is little difference in modulus for the different lengths of fibre in the granule used as the feedstock for injection molding (i.e. there is little difference between those of 5 mm and 10 mm fibre lengths). As expected, there is a large difference between moduli obtained in tension and flexure.

5. RELATING MICROSTRUCTURE TO STIFFNESS BY MODELS

5.1 The micromechanical model

In principle, it should be possible to use the microstructural observations to predict the stiffness measurements. This would not only demonstrate a full understanding of the deformational behaviour of the composites but would also be a powerful design tool. In practice, such an approach can be achieved although prediction is limited by an incomplete description of the microstructure as verified by the properties varying at different locations within the moldings. It is possible however to establish a micromechanical model that is adequate at describing the broad trends in the deformational behaviour of the composites. We describe this approach as a modelling activity, rather than a predictive activity because it lacks fine resolution of the properties.

The are a number of different approaches to establishing a micromechanical model aimed at calculating modulus. The principal strategy of the model is common but progresses to different points of detail and assumption. The main theme of the model is as follows:

(i) The discontinuous fibre reinforced molding is assumed to be composed of a number of laminae of equal thickness. Each lamina contains a common fibre volume fraction v_F and a common fibre length distribution. The lamina can be defined as having a unique in-plane fibre orientation relative to the direction Θ of the applied stress. The modulus of each lamina is given by $E_i(\Theta_i)$ with I varying from 1 to n (the number of laminae).

The modulus of the composite molding is therefore the sum of these lamina moduli. For tensile and flexural deformations the procedure for conducting this summation will be different, but in general can be given by (ref. 8):

$$E_c = \frac{\sum_{i=1}^{n} W_i E_i(\Theta_i)}{\sum_{i=1}^{n} W_i} \tag{1}$$

Material	Tensile modulus Longit. / GPa	Tensile modulus Transv / GPa	Flex. modulus Longit. / GPa	Flex. modulus Transv. / GPa	Laboratory
PA/c 10 DYNAMIC	28-32	12-13			5
			13	5.6	1
PA/c 10 STATIC	13-20	20-27			5
			8.8	12.1	1
PA/g 5 DYNAMIC	11	6.2			5
			10	5.9	3
			9	4.5	1
PA/g 5 STATIC	8.8	11.9			5
			6.6	6.9	3
			8	6	1
PA/g 10 DYNAMIC	12.5	6.1			5
			9.7	5.7	3
			9.1	4.8	1
PA/g 10 STATIC	8.9	11.1			5
			7.4	7.2	3
			8.1	6.1	1
PP/g 5 DYNAMIC	13.6	4.6			5
			8.8	3.5	3
			7.3	2.8	1
PP/g 5 STATIC	5				5
			4.9	5.1	3
			5.6	4.5	1
PP/g 10 DYNAMIC	13.8	4.2			5
			8.6	3.3	3
			7.3	2.9	1
PP/g 10 STATIC	5.9	7.9			5
			4.8	5.1	3
			6.1	4.9	1

For the tensile case:

$W_i = 1$

and for the flexure case:

$$W_i = \left[\left(i - \frac{n}{2}\right)^3 - \left(i - 1 - \frac{n}{2}\right)^3\right] \tag{2}$$

where I=1 and i=n correspond to the two outer layers.

ii) The next step is to calculate the modulus of each lamina: When the fibres are aligned along the direction of applied stress (Θ=0 °) or at right angles to the direction of applied stress (Θ=90 °) then this can be achieved in a straight forward manner:

$$E(0)=\eta_l E_f v_f+(1-v_f)E_m \tag{3}$$

$$\frac{1}{E(90)}=\frac{1-v_f}{E_m}+\frac{v_f}{E_f} \tag{4}$$

The suffices *f* and *m* relate to properties for fibre and matrix.

The term η_L relates to the efficiency of reinforcement of the fibre and can be described by Cox's shear lag model (ref. 9) as:

$$\eta_l=\left\{1-\frac{\tanh\frac{\beta l}{2}}{\frac{\beta l}{2}}\right\} \tag{5}$$

where l can be an average fibre length or a fibre length distribution function. The term β relates to the fibre radius, mass fraction of a reinforcement and the matrix and fibre Young's moduli.

When the fibre orientation within a lamina is neither 0 or 90 ° a more complex expression is required for the definition of the lamina modulus. This is formerly derived elsewhere (ref. 11) and is based on classical laminate theory. Two important expressions emerge from the analysis which we summarize here in terms of the engineering constants that are obtained experimentally (rather than in terms of the elastic constants utilised in laminate theory). For example, when the stress on the lamina is longitudinal the modulus is defined from the following expression:

$$\frac{1}{E_x}=\frac{1}{E_1}\cos^4\Theta+\left(\frac{1}{G_{12}}-\frac{2\nu_{12}}{E_1}\right)\sin^2\Theta\cos^2\Theta+\frac{1}{E_2}\sin^4\Theta \tag{6}$$

The various engineering constants for the lamina are those usual in classical laminate theory of composites and are fully described by, for example Jones in ref. 12. (Of course, the anisotropic engineering properties (eg G_{12} and ν_{12} etc) can rigorously only apply to homogeneous anisotropic laminar materials, but they are retained here for clarity of definition ie so that the stress and strain directions relative to the fibre orientation are defined.

iii) The output from this model is a value for composite modulus for either stress aligned along the mold fill direction (ie modulus measured in the longitudinal direction) or stress aligned at right angles to the mold fill direction (ie transverse modulus). These can be determined for both tensile and flexural loading. These moduli can then be compared with those obtained by experiment.

This model makes a key assumption about the orientation of the fibres. It assumes that the fibres are all in-plane in the lamina. Other models accommodate out-of-plane fibre orientations as well as in plane orientations. Such out-of-plane fibre orientations will not be accommodated in the modelling work in this paper.

Two Laboratories conducted stiffness modelling work. Laboratory 1 used their own software package and determined modulus for flexural deformations. Laboratory 2 used software based on the University of Delaware work (ref. 13) and determined modulus for tensile deformations. In this case, the use of equation 1 was modified in order to accommodate laminar interactions.

5.2 Comparison between modulus by measurement and modelling

Table 2 summarises the comparisons of modulus by measurement and by modelling from the calculations of Laboratory 1, where the deformations relate to flexural loading. The basis of modulus determinations from the model are summarised in Appendix 1. The agreement between model and measurement is close without being precise. However, the absence of accommodation of the out-of-plane fibre orientations for these moldings can lead only to approximations from the model.

Table 3 summarises a similar set of results for comparisons between modulus by measurement and model from Laboratory 2 relating to tensile loading. The parameters used in this model are also summarised in Appendix 1.

All the data are presented graphically as plots of measured modulus versus modelled modulus in Figs. 2 - 5. In all these Figures the dotted line indicates the expectation of a perfect fit between the two moduli. Figures 2 and 3 relate to modulus by flexure and the modelling by Laboratory 1; figures 4 and 5 relate to modulus in tension with the modelling by Laboratory 2. Where a range of measured values exists, then a simple average modulus has been used.

The best fit is seen to be for modulus by flexure for the longitudinal case (DYNAMIC and STATIC moldings are mixed in this plot). In this case, the fibre alignment dominating the modulus value relates to alignment in the direction of applied stress, for which complications such as out-of-plane fibres have less significance.

Table 2 Comparison of modulus by flexural deformation from measurement and modelling (laboratory 1)

Material	Exper. modulus Longit. / GPa	Exper. modulus Transv. / GPa	Calculated modulus Longit. / GPa	Calculated modulus Transv. / GPa
PA/c 10 DYNAMIC	13	5.6	13	4
PA/c 10 STATIC	8.8	12.1	10	13.6
PA/g 10 DYNAMIC	9.1-9.7	4.8-5.7	10	3.6
PA/g 10 STATIC	7.4-8.1	6.1-7.2	10	3.7
PP/g 10 DYNAMIC	7.3-8.6	2.9-3.3	6.1	1.9
PP/g 10 STATIC	4.8-6.1	4.9-5.0	6.7	2.1

Table 3 Comparison of modulus by tensile deformation from measurement and modelling (laboratory 2)

Material	Exper. modulus Longit. / GPa	Exper. modulus Transv. / GPa	Calculated modulus Longit. / GPa	Calculated modulus Transv. / GPa
PA/c 10 DYNAMIC	28-32	12-13	22.4	9.7
PA/c 10 STATIC	13-20	20-27	11.8	19.4
PA/g 10 DYNAMIC	12.5	6.1	12.5	5.0
PA/g 10 STATIC	8.9	11.1	6.5	11.1
PP/g 10 DYNAMIC	13.8	4.2	10.5	3.0
PP/g 10 STATIC	5.9	7.9	4.1	6.8

5.3 Discussion of the modelling procedures

In order to make the modelling procedures tractable it has been necessary to make a number of simplifying assumptions. Each of these assumptions minimises the predictive skills involved in using the micromechanical model but nevertheless do not distract from the actual process of "modelling".

The main assumption used in modelling is to assume that the fibre orientation functions can be described by in-plane orientations for the fibres. This assumption is perhaps reasonable for the glass fibre composites but is less so for the carbon fibre systems where much larger out-of-plane fibre orientations have been observed (ref. 7).

A second simplifying assumption in the modelling invokes the belief that the through thickness structure in the molding can be modelled in terms of a skin-core morphology. It is noted in the observations of the microstructure that such a structure is barely noticeable for the carbon fibre composites and not completely apparent for the glass fibre systems (ref. 7).

It is difficult to condense the quantitative observations about the fibre orientation distributions, the fibre contents and the fibre length distributions to a single set of consensus observations necessary for the idealised requirements of the model.

A third assumption involves the adoption of a plane of symmetry about a centre line through the thickness of the molding. However, the work by Cervenka et al (ref. 6) shows that this is nor rigorously accurate.

Finally, it is quite apparent that the averaged observations of modulus cannot be confined to a single value for the needs of the model. This is quite apart from the undetailed but real variations of measured modulus for specimens from different parts of the moldings.

It is therefore unquestionable that the calculated moduli are not predictions but estimates of modulus. It could be argued as a consequence of this that any similarity between measured and modelled modulus can only be approximate. In part, this can only be so because of the lack of laminar flow for these particularly thick but small volume moldings. This is reflected in the good fit between measurement and "model" in Fig. 2 and the poorer fir in Figs. 3-5. However, there is a more optimistic argument that recognizes some similarity between measured and modelled moduli. If this argument is based on the themes set out in this work, then it suggests that at least the description of the microstructure embodied here is what is necessary for design predictability for these types of structures, provided that a molding is considered where laminar flow can be achieved.

6. CONCLUDING COMMENTS

We have attempted to describe the way in which the microstructure and stiffness of discontinuous fibre composites can be articulated and linked. The determination and description of modulus for such moldings is not straightforward. The moldings need to be considered as structures rather than homogeneous materials where traditional simple property measurements can be used to describe stiffness.

It is possible to utilise micromechanical models as a predictive tool for describing the stiffness characteristics. In order to achieve this there is a requirement to have knowledge about the fibre length distribution and the fibre orientation through the structure. We have shown that even with some simplifying assumptions such model can create a similarity between measurements and modelling. However, if this procedure is to be more accurate then the number of these assumptions will need to be reduced.

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Appendix I. Summary of data used for modelling modulus

Section 5 describes the calculation of modulus from the micromechanical model. In order to achieve these calculations a number of inputs are necessary to the software packages that have been used to determine the moduli. This Appendix summarizes these inputs which arise from knowledge of the elastic properties of the fibres and matrix materials together with consensus data emanating from the observations of the microstructure which are discussed in section 3, but which are described more fully in ref. 7.

Elastic properties of the fibres and matrix materials are as follows:

Modulus of fibres / GPa: 76 (glass), 230 (carbon)

Modulus of matrix materials / GPa: 2.8 (PA), 1.5 (PP)

Lateral contraction ratios for fibres: 0.33 (g), 0.28 (c)

Lateral contraction ratios for matrices: 0.4 (PA), 0.33 (PP)

Fibre radius / μm: 8.5 (g), 4 (c)

The remaining input relates to the microstructure which needs to be specific to each molding. This is summarized in Tables 4 and 5. It should be noted that "skin 1" relates to the top surface of the molding and that the molding is assumed to be symmetric about its central thickness.

Table 4 Microstructural data used for modelling PP/g AND PA/g

	PP/g 10 DYNAMIC	PP/g 10 STATIC	PA/g 10 DYNAMIC	PA/g 10 STATIC
Number average fibre length / mm	2.5	2.5	1.4	2.2
Fibre volume fraction	0.19	0.19	0.22	0.22
% of molding thickness being core		38		17
Number of laminae used in model	12	12	12	12
Fibre orientation				
skin 1	30	30	30	30
2	10	10	10	10
3	10	10	10	10
4	30	30	20	20
5			30	30
core 1	20	70	20	80
2	20	80		

Table 5 Microstructural data used for modelling PA/c

	PA/c 10 DYNAMIC	PA/c 10 STATIC
Number average fibre length / mm	0.24	0.27
Fibre volume fraction	0.3	0.3
% of molding thickness being core	70	70
Number of laminae used in model	4	14
Fibre orientation		
skin 1	20	20
2		20
core 1	20	80
2		80
3		90
4		90
5		90

Figure 2 Modulus by Flexure
Longitudinal Laboratory 1

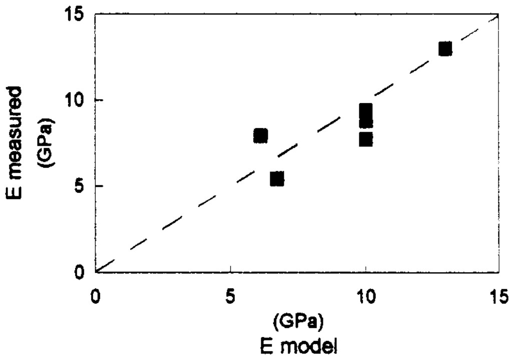

Figure 3 Modulus by Flexure
Transverse Laboratory 1

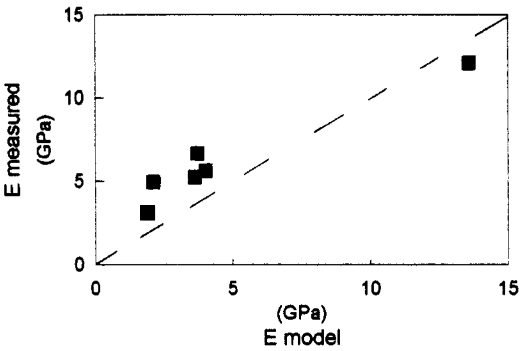

Figure 4 Modulus by Tension
Longitudinal Laboratory 2

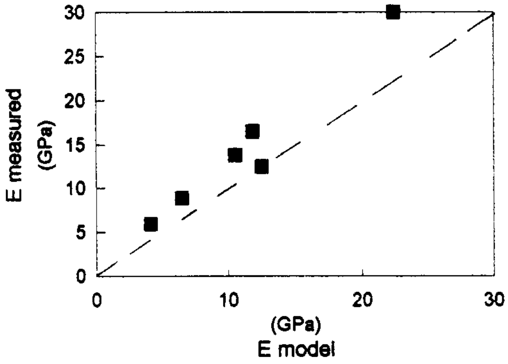

Figure 5 Modulus by Tension
Transverse Laboratory 2