ADVANCED MATERIALS

Materials Processing—a Key Factor

Injection and Extrusion Molding
Process Optimization
Computer Aided Design
Liquid Crystal Polymers

By Walter Michaeli *

1. Introduction

New polymers, computer-integrated manufacturing and quality requirements ask for a daily new, and never ending attempt to answer the question of how to optimize processing. The answer is very complex and requires fundamental knowledge of how, for a given polymer, the structure of a product correlates to its processing conditions since this influences crucially its final properties and performance.

Processing conditions are often dependent on the specific design of the processing equipment, the quality of the control systems, handling and pretreatment, for example, drying and compounding, and on environmental conditions. Moreover, the change of one parameter during processing can affect final product properties. Therefore, it is necessary to study the individual influences on a given material. However, before optimizing material processing it is first essential to optimize the plastics part design. It is the objective of many R & D departments in industry and academia to define rules, models, and software packages according to which a part is to be designed and processed. This has to be combined with the innovative potential of those who create new polymers.

In view of the increasingly more complex requirements put on part properties, computer-aided processes for part and tool design have become generally established in planning departments, and the necessary software packages are steadily improving. This will help to avoid a poor design and will lead to better processing and improved quality. Let me give some examples: As advanced composites with infinite fibers are formed during processing, the possibility of affecting product properties at this stage is increased. Voids and air entrapments have a tremendous influence on the mechanical properties of such a composite. This can be shown impressively by applying an interlaminar shear load, since the voids are mainly formed between the fiber and the matrix[1] and have a negative influence on the bonding. The strong influence of the void content on the interlaminar shear strength during dynamic loading is demonstrated in Figure 1.

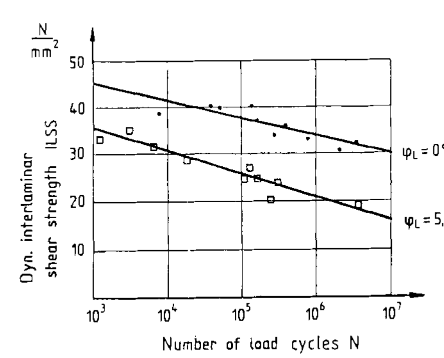

Fig. 1. The influence of void content φ_L on the mechanical properties of an FRP laminate, a composite material.

Another very important factor in part design and processing is the fiber orientation. Deviations from the given fiber orientation, e.g. of only 5°, may lead to a drop in strength of about 40% for a fiber content of 60 vol-% (Figure 2).[2] This gives an idea of the importance of the reproducible laydown of fibers during material processing. There are many other key factors in material processing. To discuss them all is impossible but it is my intention to cover the most essential parameters used to set up process models, which give the key to separate and estimate the effect of single processing conditions on future products.

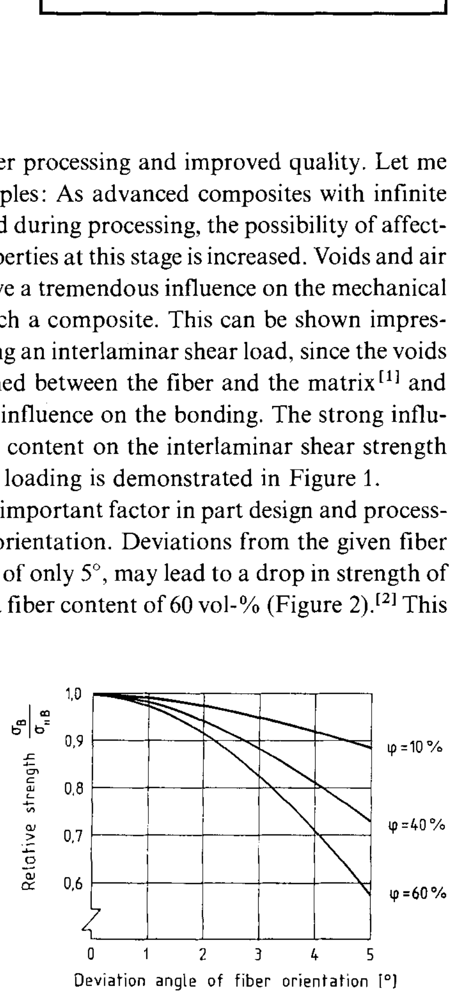

Fig. 2. The influence of fiber orientation on the mechanical properties of composite parts. φ = Filament volume ratio.

Manufacturing philosophy is that the final properties of a plastic part made from a well defined polymer should be independent of the production process used, in as much that it is the inner structure/morphology, crystallinity, fiber dispersion and distribution, orientation, and internal stress pattern, which determine the properties. However, if we analyze the processing of thermoplastic materials, we find that the structure formed is a function of thermal and mechanical

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influences. The absolute values of structural characteristics, like orientation or crystallinity, vary for different processes or products but can always be derived from the specific process conditions. Therefore, we have to analyze a process in terms of single steps for which the processing parameters are defined, and for which the internal properties (structure) and final properties are then determined.[3] This is depicted in Figure 3.

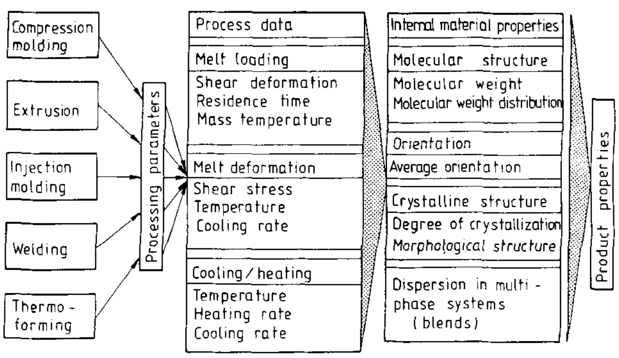

Fig. 3. Production process to part properties.

Process data are independent of molding- and processing equipment and are derived or calculated from the processing conditions and the specific geometrical boundary conditions of the equipment.

The material is more loaded (e.g. sheared, heated) during compression molding than during extrusion and therefore we expect alterations on the molecular level. A comparison of extrusion and injection molding gives a similar set of process data, but the pressure level and the shearing forces in injection molding are significantly higher than in extrusion.[3] The structural parameters (like orientation or boundary layers) are less distinct in extrusion. Similar cooling gradients exist, but due to the melt flow during the packing phase, high deformation rates at fairly low melt temperatures influence the internal structure. The morphology and internal stress patterns can be correlated for both processes to the cooling, pressure, and deformation conditions. A detailed analysis of these factors allows us to better understand materials processing.

2.1. Component (Part) Properties

To illustrate how properties, e.g. mechanical properties, are influenced by the internal morphology consider the following examples.[3] Figure 4 gives the thermal coefficient of expansion as a function of the degree of stretching λ (which correlates to orientation)[4] for different materials. Figure 5 shows for polypropylene (PP) how the Young's modulus E_0 and the tensile stress σ_s are influenced by crystallinity,[5] which is a function of the cooling and material deformation conditions during processing.

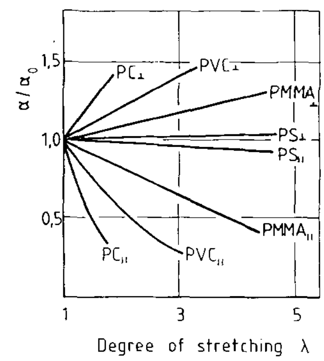

Fig. 4. Thermal expansion coefficient as a function of the degree of stretching.

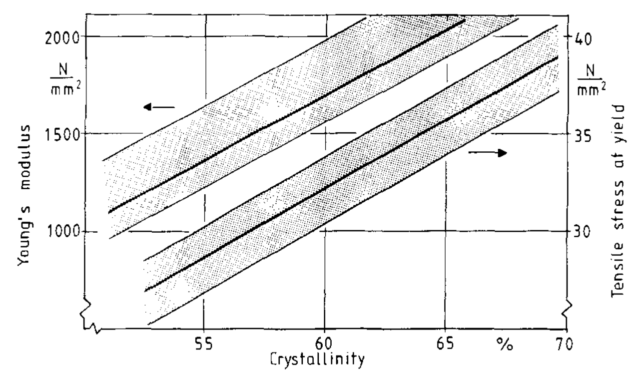

Fig. 5. Young's modulus and tensile stress (for polypropylene) as a function of crystallinity.

2.2. Influence of Melt Loading on Part Properties

The state of a thermoplastic material[3] while being processed and molded into a plastic part is defined by:

- melt loading (degradation)
- melt deformation (orientation) and
- cooling conditions

A certain molecular weight is necessary to achieve product properties like impact and corrosion resistance or dimensional stability under mechanical loading. Molecular weight and flow properties can be correlated, and also give a good correlation to degradation when the melt is loaded.[3] Figure 6[3] describes the effect of melt loading on the melt vis-

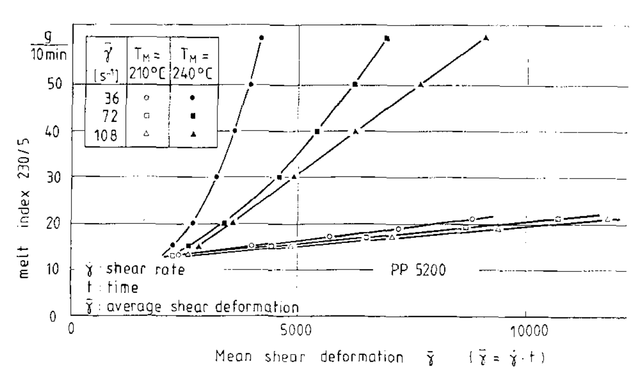

Fig. 6. Melt loading of polypropylene (PP).

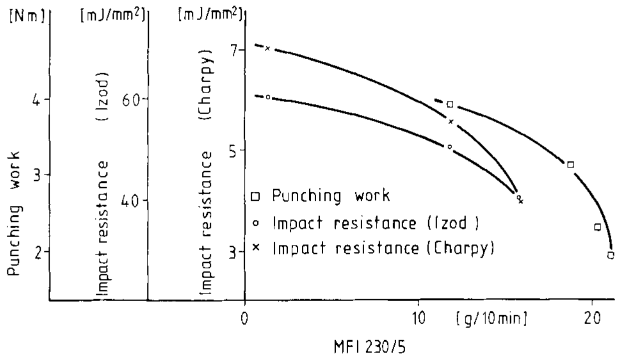

Fig. 7. Change in impact strength according to melt flow index (MFI).

cosity (melt index) as a function of mass temperature and shear deformation during extrusion. The significance of the mass temperature can clearly be seen. These experiments were made in extrusion but injection molding shows the same tendencies. Tensile tests often do not reveal the significance of the degradation, but impact resistance tests show how significantly chain scission influences performance (Fig. 7).[13]

3. Modeling of Part Design and Processing

If we wish to follow a straight line from the initial idea to the final product we have to structure our approach. The world-wide tendency to use software packages to guide us from the idea to the product is perhaps the strongest driving force bringing structure and unity to our approach. All steps from the idea to the final product have to be defined and have to be under control. This may sound simple to some or like utopia to others, but it is an essential objective.

The first step is to define the requirements the part has to fulfill (Fig. 8), and to select the right material.[6] Several software houses, and a large number of raw material manufacturers offer data banks for polymer materials, some even enabling the potential user to store his own proprietary knowledge and call it up as required.

The next step is the first layout of the geometry of the part. CAD-Macros defining and generating specific design elements of parts like snap-fit joints, gears, screw joints, rib reinforcements etc. are a most valuable tool and help to avoid poor designs. All design rules for the part will be automatically generated and observed. Fairly simple programs applying the basic rules of mechanics help to predimension a part. Here non-linear viscoelastic stress-strain relationships can be taken into consideration. The use of Finite Elements Methods (FEM) is commonplace in cases where the critical molding situation cannot be analyzed closely enough using empirical methods, or where complex or critical loads are involved. During mechanical analysis and structure optimization using FEM computer programs, the generally inhomogeneous, anisotropic and non-linear material behavior of plastics can be numerically approximated.

The next step is to check a design against accepted design rules (Figure 8). A software package for injection molded parts has been developed at our institute which examines the part geometry for material accumulations, draft angles and undercuts, checks the demoldability of a part and even defines the parting lines of a mold.[6]

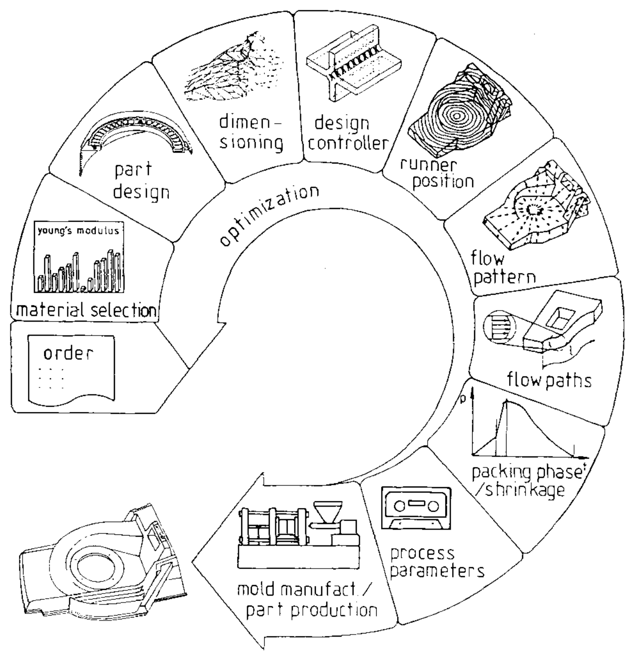

Fig. 8. Part and mold development.

At first sight, these rules and computer programs may appear to be trivial and obvious to the experienced designer. However, the automatic control of the geometry provides an additional check and helps to reduce costs by avoiding problems during materials processing. Such systems still have to be developed for advanced composites, where they will be especially important. The logical consequence of using a computer-guided approach in part design is also to use the computer to simulate processing and detect possible problems before going to the factory floor. The processing conditions can also be optimized in order to get the most out of the material with optimum economy.

Our institute has developed such a program system, called CADFORM-CADMOULD,[6] which incorporates programs

- for calculating the temporal melt front advance, which gives information about weld-lines, air entrapments, and the pressure distribution during the mold filling phase (Figure 9)
- for calculating the shear rates, shear stresses and melt temperatures along freely selected flow paths
- for analysis of the holding pressure phase and estimation of the shrinkage

- for determining the most favorable machine operating point and its dependence on operating parameters; say, to find better processing conditions
- for predicting the orientation pattern

This information is important to help design the mold and to minimize processing problems. In injection molding and extrusion, such programs for the rheological, thermal, and mechanical mold design are frequently and successfully used. Models for reactive materials processing are under development.

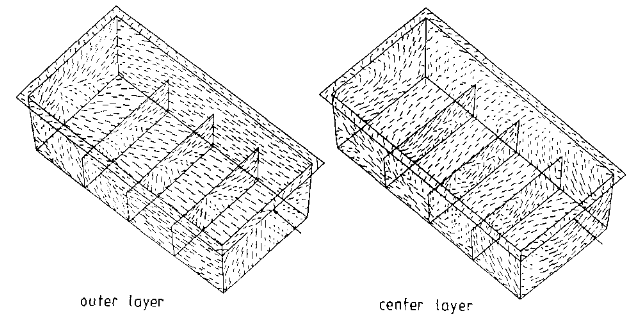

Fig. 10. Computed orientation of fibers.

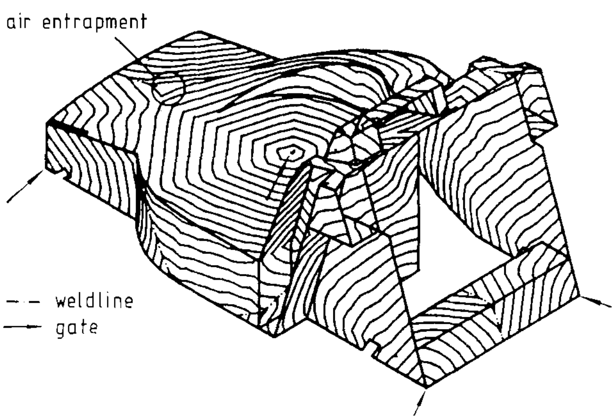

Fig. 9. Filling pattern of a complex part.

Modeling also provides the data to run the equipment, and it is no longer regarded as magic in advanced injection molding, to generate the best machine settings using a computer simulation, and to transfer these data directly to the control cabinet of the machine via the central and machine computers.[7, 8] It is very important to realize that next to reproducibility, proper transfer of information is a key factor in material processing, as is the choice of the most suitable equipment. If one knows, for example, the pressure drop in a cavity of an injection mold, one can predict the necessary clamping force and select the right machine. Such machine selection algorithms which are oriented towards optimum materials processing are to some extent already in existence.[9]

3.1. Processing and Properties of Short-Fiber Reinforced Polymers

If we want to make a part out of a short-fiber reinforced thermoplastic material we want to predict its mechanical properties and see how process variations will affect quality. Many independent investigations have found a symmetrical set-up of layers with different main fiber orientations in injection molded parts. The center layer is about 15% of the cross-section, the sheared layers about two-times 37.5% and the boundary layers about two-times 5%. This distribution varies little with injection rate, mass and mold wall temperature, or packing pressure for common wall thicknesses of the molding,[10] and holds true for almost all injection molded parts.

However, we have to keep in mind that there is always a distribution in fiber length and orientation angle, relative to the main orientation direction if we want to predict mechanical part performance. With the models described we can predict the fiber orientation according to the flow pattern during the filling of the cavity. The main orientation directions of the fibers are shown in Figure 10 for the center (core) and outer layers. We see the orientation in flow direction next to the wall and the perpendicular fiber arrangement in the central area.

The designer of a molding, and finally the customer, are in general interested in the overall mechanical properties of a part, and not only in the fiber orientation. Of special interest here, is the anisotropic elastic material behavior at each point of the molding. If this is known one can calculate the overall mechanical properties.[10]

3.2. Processing of Liquid Crystal Polymers

Modeling is a key factor in the processing of liquid crystal polymers (LCP). These new, self-reinforcing materials are very sensitive to their processing conditions. They show mechanical properties similar to steel and ceramics in the main orientation directions, but show little strength or stiffness transverse to the molecular chains. The orientation model shown in Figure 10 can also be found in these polymers (Fig. 11).[11] An attempt to predict their mechanical properties in the same way as for the short-fiber reinforced materials mentioned previously is presently being examined in our Institute.

There is still one problematic area in processing LCP's. The problem relates to those points where two flow fronts come into contact and form a weld-line. Figure 12 shows how two melt fronts will align parallel to each other.[12] This configuration results in poor mechanical performance, but it is possible to overcome this weakness to some extent by controlling the flow, through mold design and filling condi-

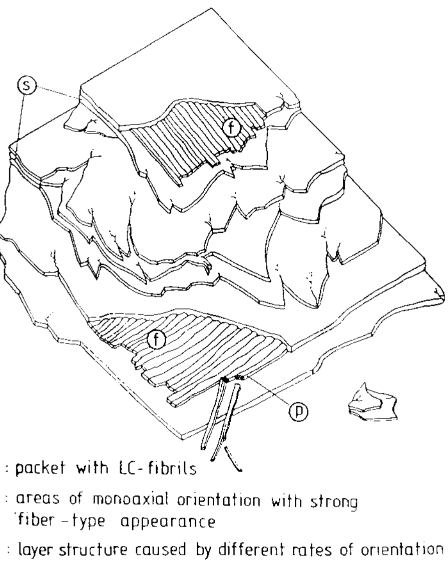

Fig. 11. Model of the "plywood-like structure" of liquid crystal polymers in moldings.

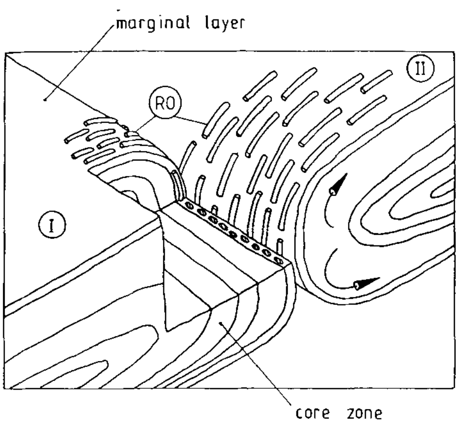

Fig. 12. Welding line in liquid crystal polymer molding. RO: Orientations in the marginal layers. I, II: Partial streams of the melt.

tions. Due to the anisotropic material properties, the analysis of the mold filling in conjunction with the calculation of the orientation pattern, is essential in order to exploit the high mechanical potential of this highly interesting group of polymers.

3.3. Processing of Composites

Advanced composites with endless fibers are relatively new materials with which many engineers and designers have little experience. Comprehensive rules, models, and design methods for composite parts have not been available to designers who are used to working with conventional materials. Today, however, composite parts are gaining importance in general mechanical engineering, especially in the design of rapidly moving parts which have to have a low weight. Designers now must deal with an added set of rules[13]:

- Anisotropic material properties. A part is stiff and strong in the fiber direction but weaker and more compliant in the perpendicular direction.
- Material properties are influenced by processing conditions. For example, the fiber content is influenced by the tension in the filament, the pressure in the parts, and by resin flow.
- Different material failure modes, e.g., if the interlaminar shear strength is exceeded, delamination occurs.

Therefore systematic sets of rules have emerged to aid the designer in laying out a composite part. The special rules that apply to fiber reinforced composites are now being incorporated into a computer aided design (CAD) and engineering (CAE) software program called CADFIBER. With this program, one can make predictions on part properties within reasonable time frames, reducing expensive and time consuming trial and error experiments to a minimum. When completely developed and implemented, CADFIBER will be able to design a part and simulate on minicomputers the processing of that part. The software program is composed of four main modules: materials data bank, construction and dimensioning, process simulation, and quality assurance.

4. Self-Optimization in Materials Processing

In materials processing, be it in product design, equipment design or in process adjustment and control, we are always striving for perfection. Optimization strategies which structure and direct our approach to our final goal are very helpful and of increasing importance. We are experimenting with the so called "evolution strategy" according to *Rechenberg*,[14] which is well suited for optimizing flow channels. We are also applying this strategy to optimize the parameters of electric controllers on-line during processing, and for adjusting injection molding machines. The initial results are very encouraging and will lead to new dimensions in answering questions concerning the optimization of materials processing.

In this paper the necessity to be assisted by the computer has been stressed. Although computerization is an essential factor in materials processing, we are aware that man, who analyzes and acts, is still *the* key factor. I have described an engineering point of view of materials processing. A chemist or a physicist might have another approach and may interpret things differently. That is good, since it is always best to look at things with different eyes. Let us put our expertise, knowledge and will together and face the challenge of future materials processing.

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The Kevlar Story—an Advanced Materials Case Study

Process Development
High Performance Fibers
High Impact Composites
Rigid-Rod Polymers

By David Tanner, James A. Fitzgerald, and Brian R. Phillips*

1. Introduction

The Kevlar story is an excellent example of the innovation process where a laboratory discovery is placed into commercial production. It started in the early 1960's with an identified need. In 1965, this led to an important scientific discovery. At this time the research and development phase was entered and in 1972 a 1 000 000 lb per year market development plant was built. By 1982 full commercialization was reached with a 45 000 000 lb/yr. plant. During this period several tough hurdles were encountered. To overcome these obstacles a multi-disciplinary approach was almost always required.

2. The Need for a Heat Resistant Stiff Fiber

The invention of Nylon and subsequent textile fibers provided powerful vision and direction for the research effort aimed at 'super' fibers. In the early 1960's Du Pont was driven by two goals, a fiber with the heat-resistance of asbestos and the stiffness of glass. A fiber of this type could be visualized to fill many market needs. Experimental work indicated that the route to such a material lay with stiff chain aromatic polyamides. These materials, however, had evaded the scientist by virtue of their extreme insolubility and intractability.

3. The Discovery of a Rigid Rod Spinnable Polymer

In 1965 *Stephanie Kwolek,* a research scientist at the Du Pont Experimental Station in Wilmington, made a major discovery. She found that *p*-aminobenzoic acid could be polymerized and solubilized under special conditions to yield a rigid-rod spinnable polymer. Initially, when these polymer solutions were first made, it was not believed that they would spin into fibers since the solution was opaque and could not be clarified by heating or filtration. This implied that there was inert matter dispersed in the spin dope which would plug the spinneret holes. However, the fibers spun well. We now know that this capacity was due to the formation of polymer

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