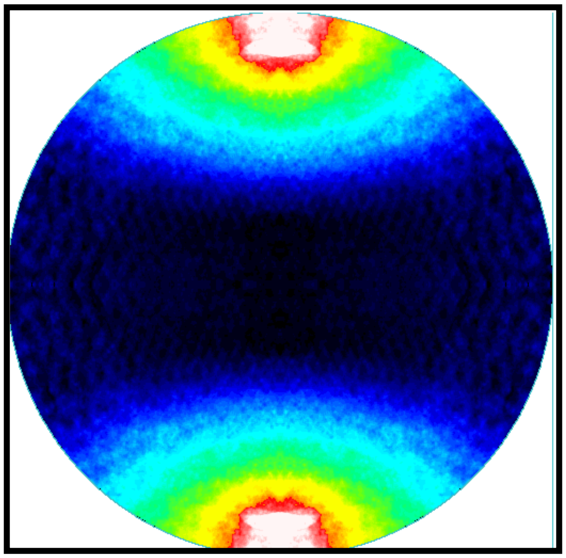
Application Note PT-002

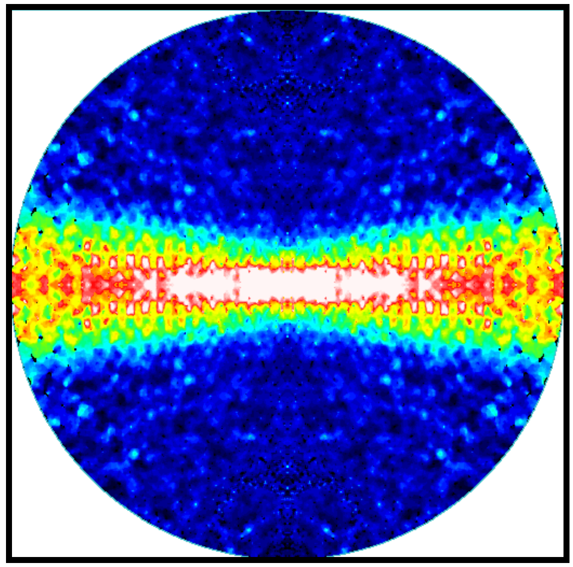
Orientation / Texture Polyethylene films

Polyethylene (PE) film is one of the most commonly used polymeric products and orientation measurements of this material are of great interest. Biaxial orientation of a polymer sheet is closely related to its mechanical and performance properties. The material properties of the blown or drawn PE films vary with different processing parameters. The production process may induce special orientation of the crystallites within the sheet's processing directions which are referred to as the axial (machine direction M) of the film, the lateral (transverse direction T – perpendicular to the machine direction), and normal (N) direction to the film. The processing parameters of the polymer sheet usually induce a biaxially oriented film. The orientation distribution of crystallites or "texture" of the films can be determined by x-ray diffraction pole figures. The texture is a measurement of the orientation of the crystallites with respect to these processing parameters (M, T and N).

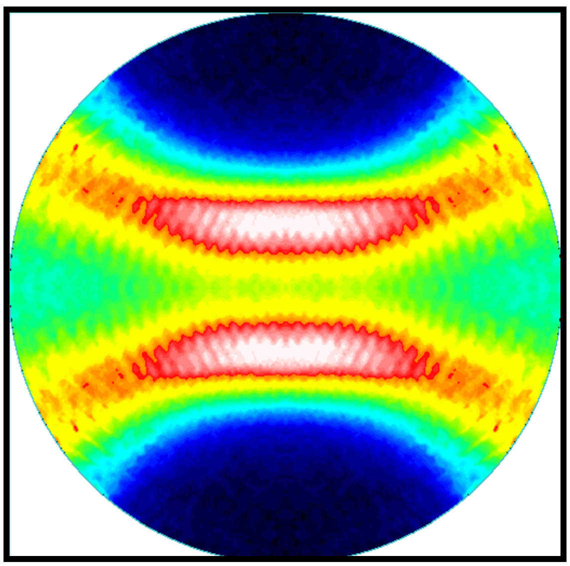
A pole figure is a stereographic projection which represents the distribution of diffraction plane normals (proportional to the volume fraction of crystallites oriented in a particular direction) as a function of direction to three orthogonal directions. Pole figures are most efficiently collected using a 2D detector which observes a large section of the Debye ring(s). After a set of pole figures are measured (for PE films this would include the (110), (200) and (020) reflections, the direction and magnitude of the texture can be displayed in a number of ways. For films, the most commonly used representation of the direction and quantification of texture strength include the Herman's Orientation Function, the Stein triangle, and the White-Spruiell function. An example of a set of pole figures collected on a low density PE film, and an explanation of the quantification by each method follows.



PE (200) Pole Figure

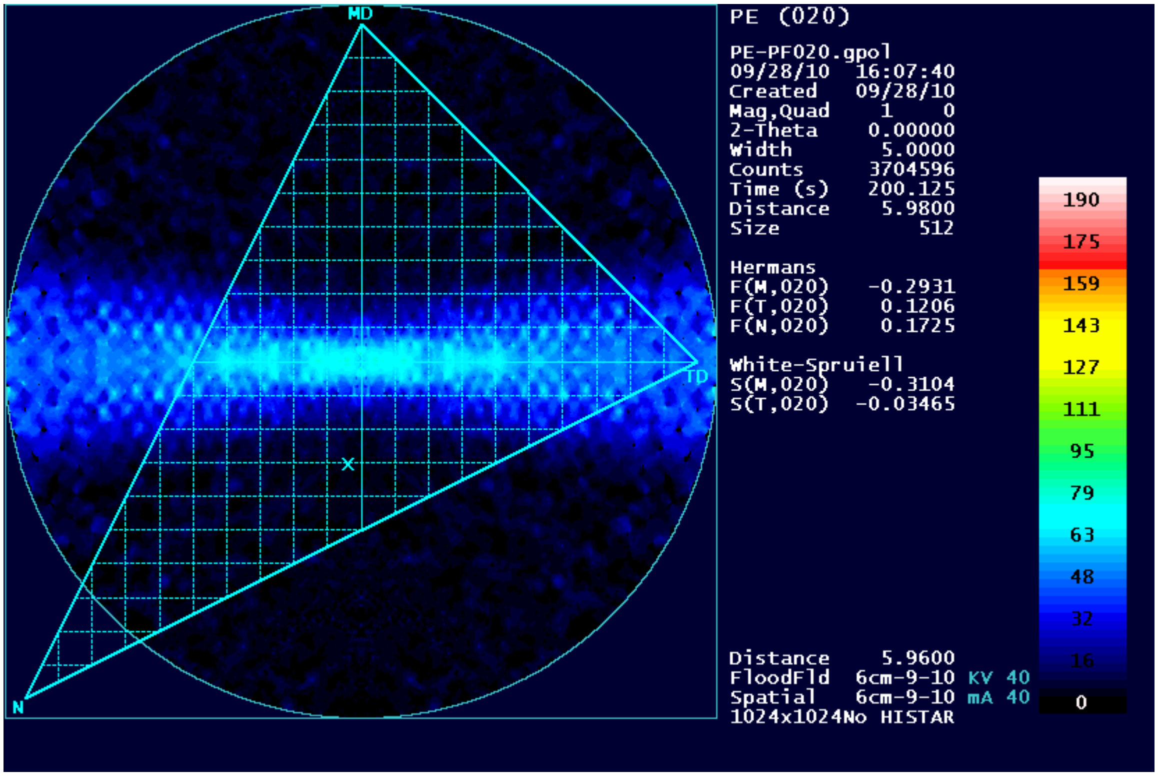


PE (020) Pole Figure

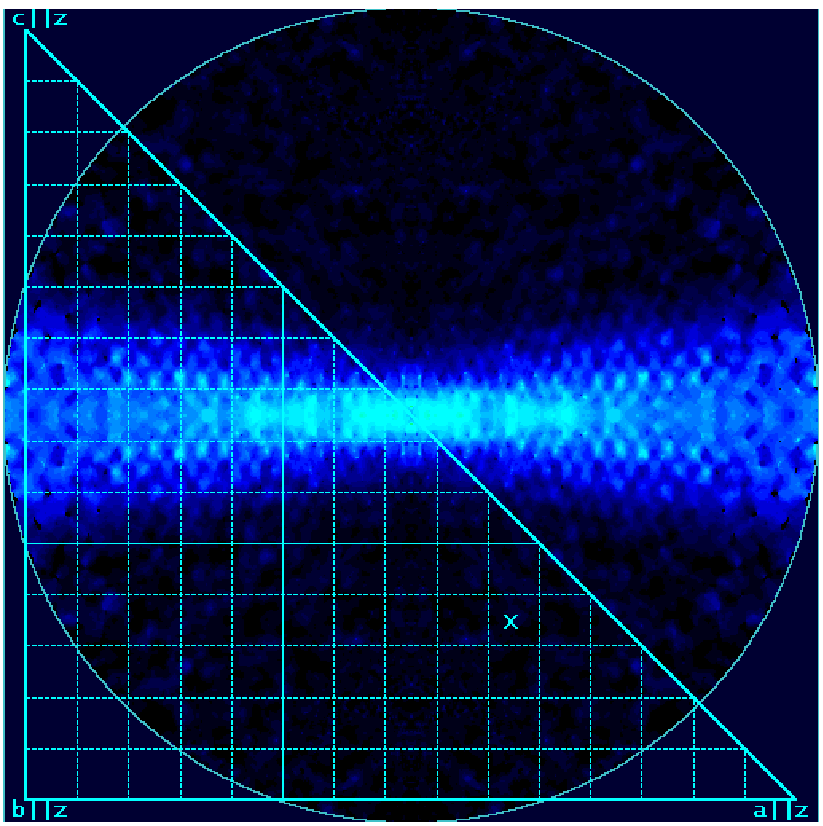


PE (110) Pole Figure

For all pole figures shown above, the machine direction M points up (vertical) and transverse direction (T) is in the horizontal plane. The view is down the normal (N) axis.

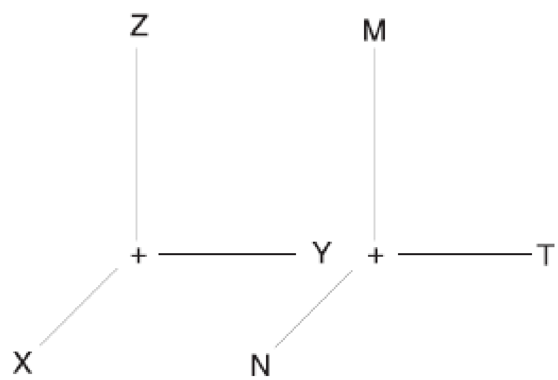


Hermans Orientation and White-Spruiell function



Stein Triangle

A widely used analytical representation of unit cells in a specimen is based on the second order moment of a specific unit cell direction (hkl) with respect to a specific direction in the specimen (M). These second moment functions are used to define an orientation index for a one-dimensional structure (fiber) and an index for a two-dimensional structure (film). These indices are directly related to certain physical properties such as birefringence. Calculation of orientation indices requires evaluation of the angle between a specific crystallographic direction and a processing direction. Both the sample and the pole projection must be defined as below, and are best implemented for crystallographic axes which are orthogonal.



For materials oriented uniaxially about a single processing direction (such as would be the case for spun fibers), one usually calculates Hermans' orientation indices for each crystallographic axis with respect to that processing axis. Herman's orientation indices are defined by:

$$F(X,x)=\frac{3\langle\cos^2 a\rangle-1}{2}$$

where:
X = processing direction, i.e. MD, TD, N
x = crystallographic direction
a = angle between above
<...> = averaged over entire pole figure

Typically, Herman's indices are plotted on a Stein triangle. The three apexes of the triangle correspond to the crystallographic axis (a, b, c) being parallel to the z-axis of the sample. The edges of the triangle represent the orientation of a crystallographic axis being perpendicular to the z-axis. A condition of no orientation is the origin.
White-Spruiell orientation indices are useful on polymer films, where orientations occur with some degree of biaxial character. White-Spruiell orientation indices are usually displayed on an isosceles triangle. The three apexes of the triangle correspond to perfect orientation along a particular direction, whereas the center of the triangle corresponds to isotropic orientation.

Table 1: Some limiting cases of orientation and their second moments and orientation indices.

Orientation	Angle c,z	$\langle \cos^2 c,z \rangle$	Fc,z
Chain axis is parallel to the fiber axis	0	1	+1.0
Chain axis perpen-dicular to the fiber axis	90	0	-0.5
Chain axis oriented a random	random	1/3	0.0
Equal bimodal orien-tation of chains	0 or 90	1/3	0.0

S(MD,x) = 2<cos2 a>MD,x + <cos2 a>TD,x - 1
S(TD,x) = 2<cos2 a>TD,x + <cos2 a>MD,x – 1

In certain cases the reflection from the hkl plane will be too week in intensity to give useful data. In such cases, one must interpolate the desired second-moment from second-moments of two or more other hkl poles for which data is obtainable. For our orthogonal case, the expression of second-moments for orthogonal relationships:

<cos2 a,z> + <cos2 b,z> + <cos2 c,z> = 1 (eq 1)

From which it follows:

Fa,z + Fb,z + Fc,z = 0 (eq 2)

Second-moment for an hk0 pole can be interpolated using:

<cos2 hk0,z> = e2 <cos2 a,z> + f2 <cos2 b,z> (eq 3)

Where e and f are the direction cosines between the a- and b-axes with the hk0 plane. Stein triangles are plotted using Fa,z and Fc,z Herman's indices. These are directly calculated from h00 and 00l poles. Alternately, one can obtain these two values from h00 and 0k0 poles or 0k0 and 00l poles. Otherwise, it gets more complicated. One needs the crystal lattice and at least three poles, such as 110, 210, and 001. By applying equation 3 above, one can derive the Herman's indices.