## 090608 Final XRD

1) Hiltner and Baer [1] have coextruded polymer films with thin layers containing single polymer crystals that can act as a barrier to gas transport. Explain what the following micrographs and schematic show concerning these thin polymer layers. Compare the crystalline morphology in these films to that seen in the recrystallized bleach jugs studied in the DOC/SAXS labs as well as to the PHB spherulites studied in the light scattering lab.



[1] Wang H.; Keum, J. K.; Hiltner, A.; Baer, E.; Freeman, B.; Rozanski, A.; Galeski, A. *Science* **323**, 757-760 (and supplement) (2009).

## 2. From the following pole figures [1] what can be said concerning the crystallographic orientation in the films of Hiltner and Baer?



**Fig. 3.** Pole figures of normals to the (120) and (032) planes of the PEO monoclinic αystals (27). The extrusion direction is vertical and the transverse direction is horizontal. The normal direction is in the center of the pole figure. **(A)** The PEO control film. **(B)** An EAA/PEO film with 50/50 composition, 33 alternating layers, and nominal PEO layer thickness of 3.6 μm. **(C)** An EAA/PEO

film with 70/30 composition, 1025 alternating layers, and nominal PEO layer thickness of 110 nm. Orientation of the (120) planes is perpendicular to the layer plane, and orientation of the (032) planes is at 67°. (**D**) An EAA/PEO film with 90/10 composition, 1025 alternating layers, and nominal PEO layer thickness of 20 nm.

3.70

3.24

2.77

2.31

1.84

1.38

0.91

0.45

3.70

3.24

2.77

2.31

1.84

1.38

0.91

0.45

3. Explain the following 2D SAXS patterns [1]. Describe how these patterns were obtained (sketch the instrument and sample orientation). Explain the morphology that gives rise to the features are that are indicated by arrows in the patterns. What does 0.25 nm<sup>-1</sup> refer to? What do ND and ED refer to?



4. Why is  $Iq^2$  used on the y-axis rather than I(q) in the following plots? These patterns were obtained from the 2D patterns in question 3. Explain why the meridian and equator curves differ (how are these curves obtained from the figure in question 3 and why would two pie slices be averaged along the horizon (equator) and vertically (meridian)?)



5. What can be said about orientation from the following XRD patterns [1]? Is there a difference in orientation between the polyethylene-co-acrylic acid (EAA) and the polyethylene oxide (PEO) layers? PEO layer thickness:  $3.6 \mu m = A$ ; 110 nm = B; 20 nm = C. How do these patterns differ from the powder diffraction pattern of a metal? How could the Hermans Orientation function be used to analyze this data?



6) Derive Bragg's Law using the specular analogy (using the fact that the incident and exiting beams have the same angle with the crystal plane.

7) Derive Bragg's Law using the momentum change of an elastic collision of a photon with a crystal plane. (Consider that a photon is a perfectly elastic ball that is incident on a surface. Calculate the energy change  $\Delta E$  and the momentum change  $\Delta p$  in terms of the wavelength.)

8) Sketch the diffraction pattern from a crystal, amorphous or liquid, and from an ideal gas. Explain the differences, e.g. what is the structural difference between a liquid and a gas, and between a liquid and a crystal.

9) Describe Vergard's Law for phase analysis and how it was applied to the composition of brass in our lab.