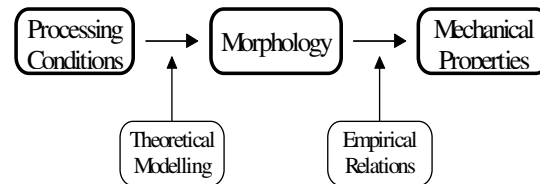


Modeling analysis

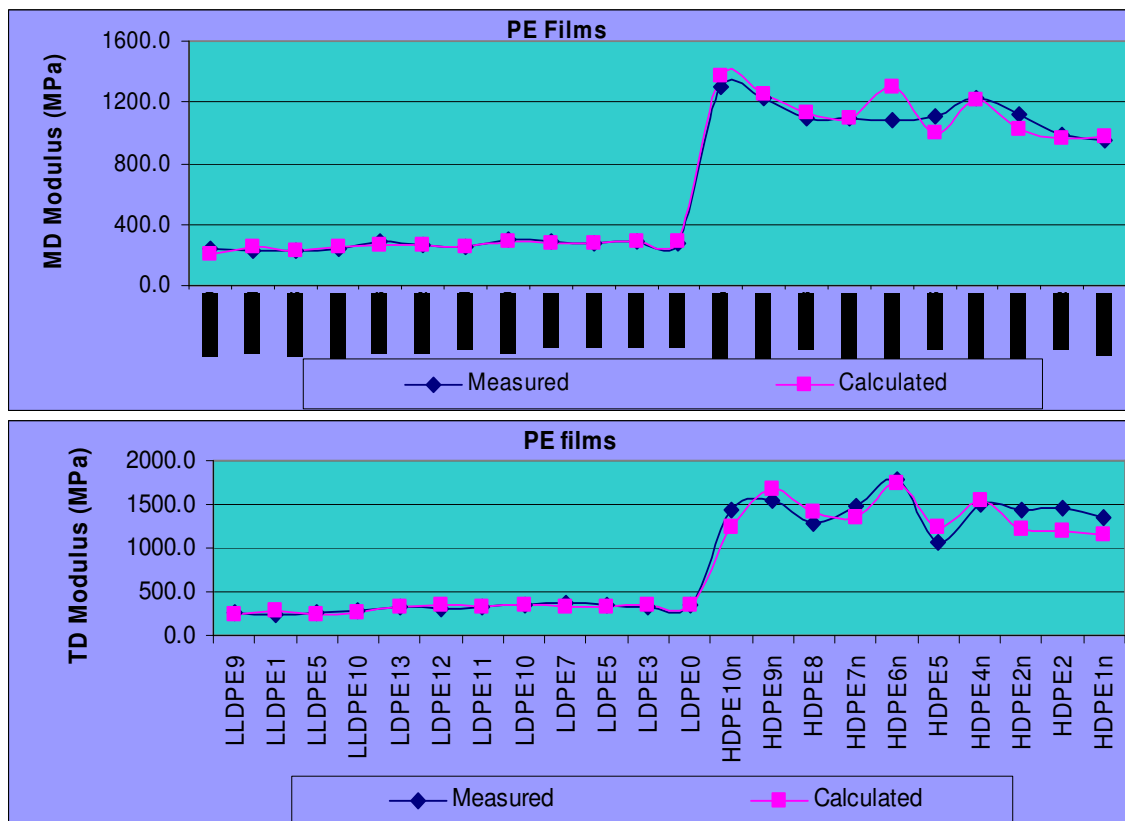
- ☐ Define the problem
 - ☐ Development of the model
 - ☐ Analyze the structure parameters
 - ☐ Specify independent and dependant variables
 - ☐ Measure variables
 - ☐ Crystalline content and lamellar thickness measurements
 - ☐ Orientation determination and morphological study of the blown film by Wide & small angle X-ray diffraction
- ☐ Formulate the mathematical model
- ☐ Evaluate the model
- Empirical modeling (statistical design of experiments and multivariate modeling)
- Fundamental/structure modeling



Basic concept for modeling

Modeling analysis

Evaluation of the model



Modeling analysis

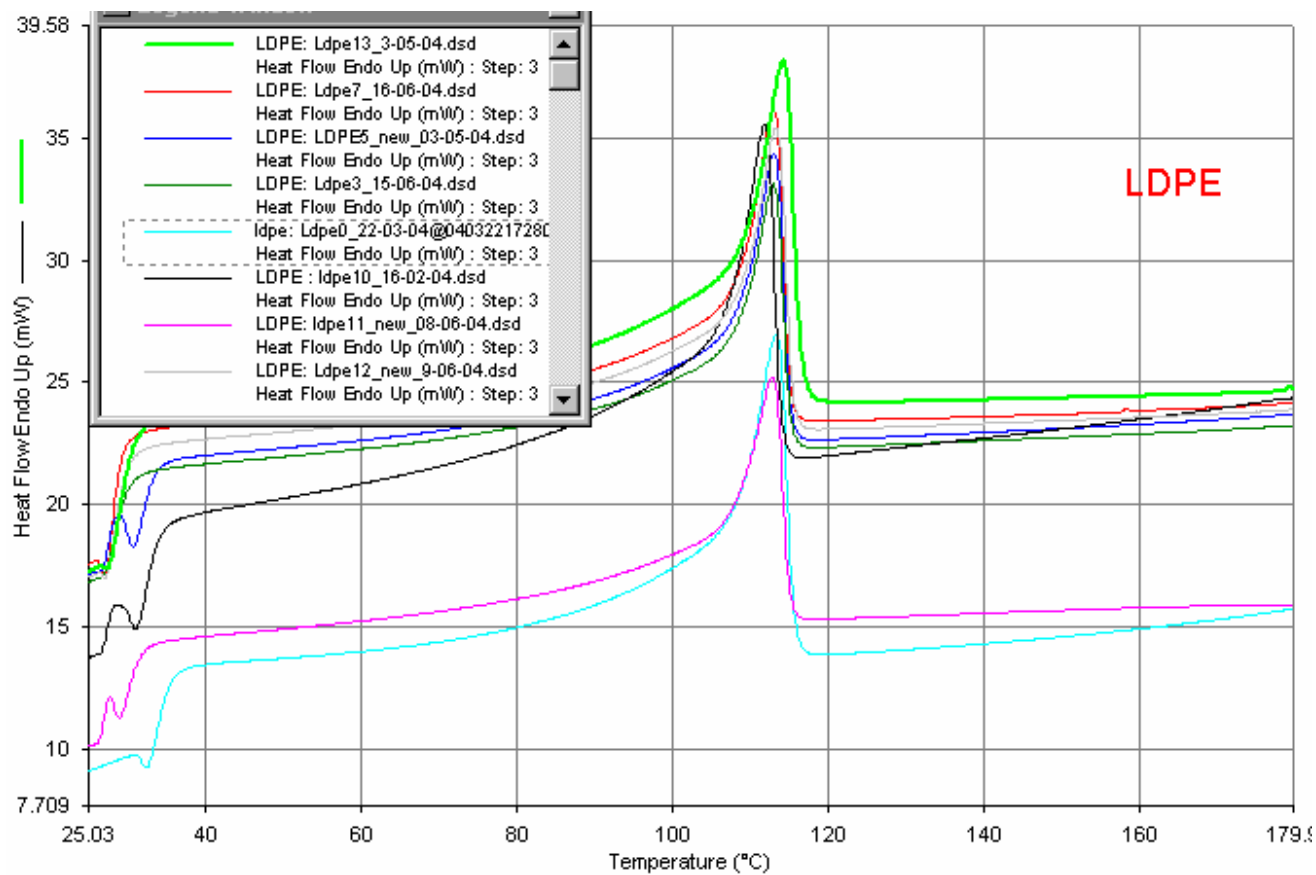
Analyze the structure parameters

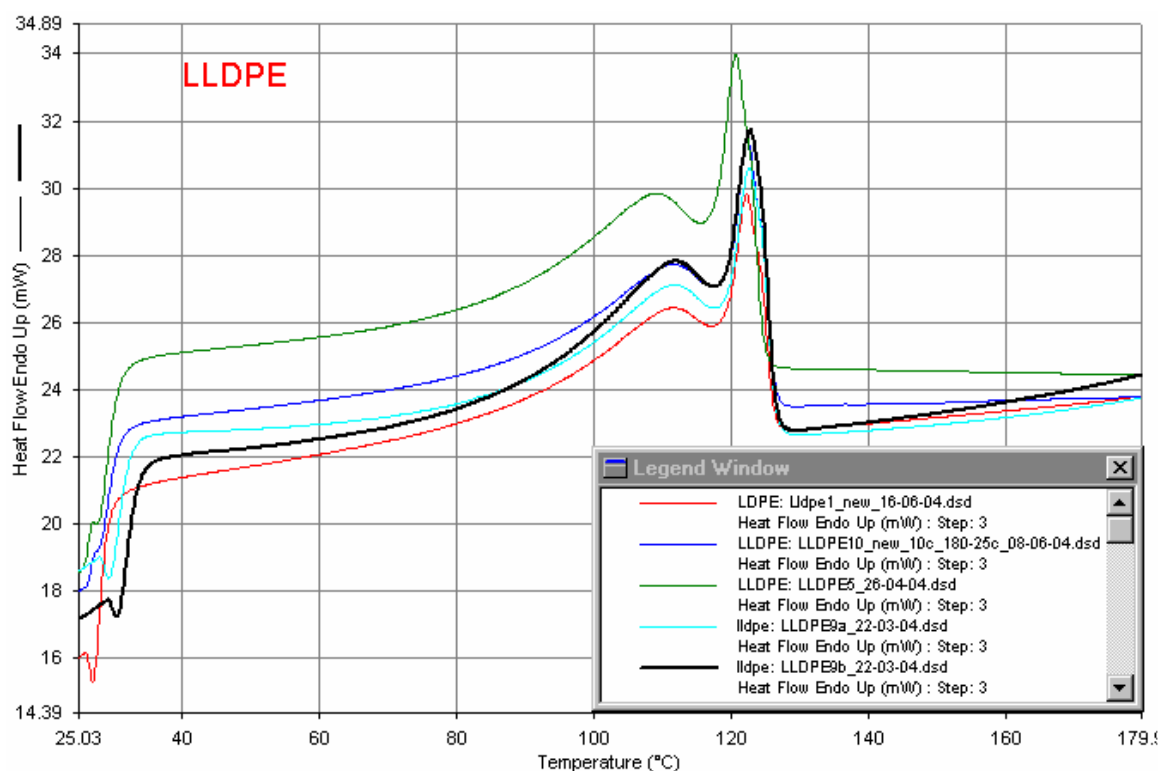
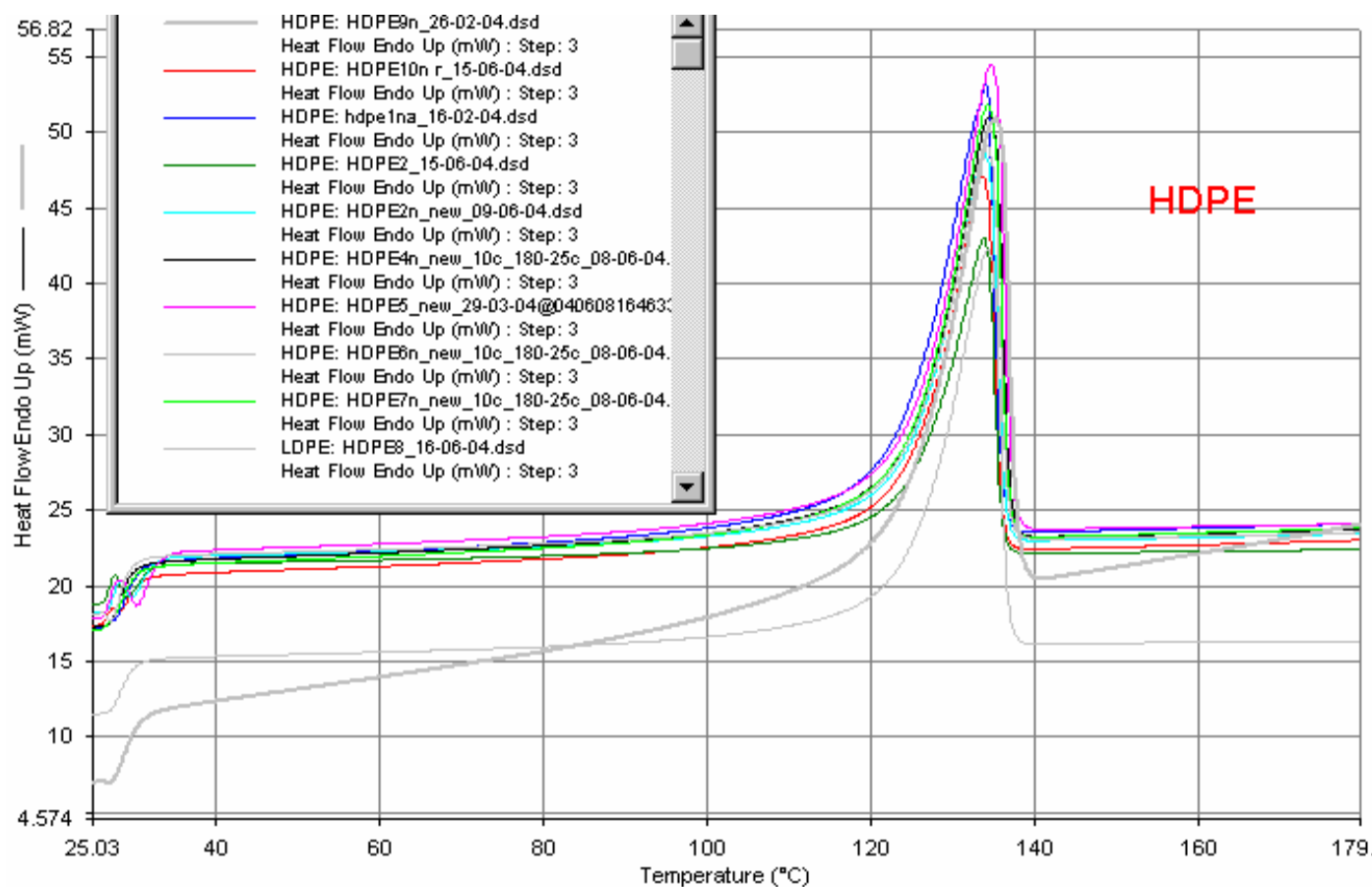
Crystalline content and lamellar thickness measurements

$$\ell = 414.2 \cdot 0.627 / (259.7034 - T_f)$$

**Orientation determination and morphological study
of the blown film by Wide & small angle X-ray diffraction**

$$\Lambda_{(hkl)}^* = \frac{K\lambda}{\beta_{(hkl)} \cos \theta} \quad l = L - D \text{ (nm)}$$



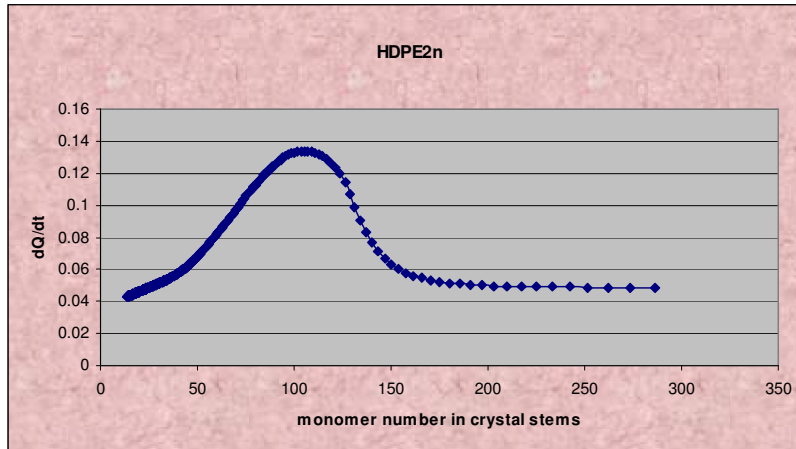


$$n = 2 \cdot \sigma_e \cdot T_f^\circ / (\Delta H^\circ \cdot (T_f^\circ - T_f))$$

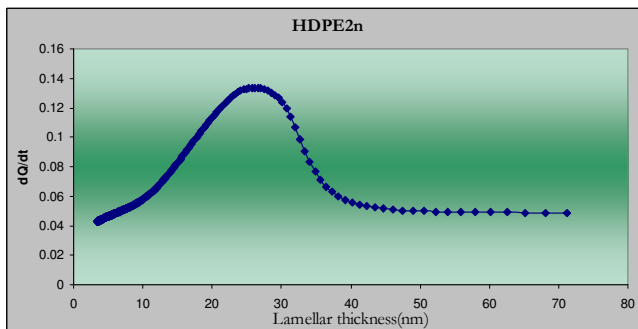
$$\sigma_e = 10.2 \text{ kJ/mol}$$

$$\Delta H^\circ = 8.106 \text{ kJ/mol}$$

$$T_f = 145.5^\circ\text{C}$$



Experimental: Measured Properties



$$l = 2 \cdot \sigma_e \cdot T_f^\circ / (\Delta H^\circ \cdot \rho_c \cdot (T_f^\circ - T_f))$$

$$\sigma_e = 90 \text{ erg/cm}^2 \text{ (basal surface free energy)}$$

$$\Delta H^\circ = 289 \text{ J/gr} \quad \text{(Heat of fusion of 100% crystalline)}$$

$$\rho_c = 0.995 \text{ gr/cm}^3 \quad \text{(The density of the crystalline phase)}$$

$$T_f^\circ = 418.7^\circ\text{K} \quad \text{(Melt temperature of 100% crystalline)}$$

$$(dM/M)(1/dL) = f(L) \quad \text{Alberola model}$$

$$(dM/M)(1/dL) = (dE/dT) \cdot (T_f^\circ - T)^2 / (2 \cdot \sigma_e \cdot T_f^\circ \cdot X_c \cdot m_c)$$

X_c is the percent of crystallinity

m_c is the weight of sample in DSC analysis

dE/dT is the required energy to melt the mass crystalline dM

$$dM/M = (dE/dT) \cdot dT / (\Delta H_f^\circ \cdot \rho_c \cdot X_c \cdot m_c)$$

