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Supporting information for article:

Determining paracrystallinity in mixed-tacticity polyhydroxybutyrates

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Supplementary information

1. Verbatim BG MN structure file code to simulate microstrain and paracrystalline order.

```
anisolin(3):sqrt(sqr(h/A)*#1+sqr(k/B)*#2+sqr(l/C)*#3)/sk //
PARAM=exph=1_1^2 PARAM=expk=1_1^2 PARAM=expl=1_1^2 //
exp=anisolin(exph,expk,expl) //
B2=k1*sqr(B1)+power(k2*power(sqr(pi)*sqrt(sqr(h)+sqr(k)+sqr(l)),exp-1),exp)*sqr(sk) //
```

Here, h, k, l are the Miller indices, A, B, C the lattice parameters, $exph, expk, expl$ are the directional values of the exponent p , $B2$ is β_{hkl}^2 , the square of the broadening of individual reflections, $k1=1$ the weighting factor for Gaussian-like broadening, $B1$ the broadening due to crystallite size (proportional to $1/\bar{L}$), $\sqrt{sqr(h)+sqr(k)+sqr(l)}$ the scattering order n , sk the scattering vector n/d , and π . $k2=ANISO=ANISOSQR$ is v^2 , using a predefined tensor. In BG MN, the total sample function is then calculated by the product of one Lorentzian and one squared Lorentzian, whose half-width at half-maximum scale parameters are $B1$ for the former, and $B2$ for the latter; BG MN Manual Equations (5.15) to (5.18). (Bergmann & Taut, 2005)

2. Disorder function for the second kind

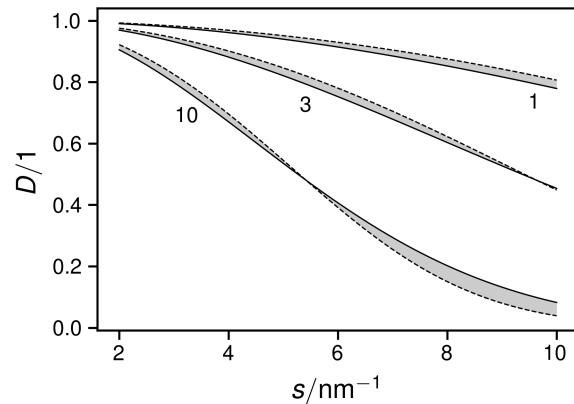


Fig. S1. Plots of disorder functions $D = \exp(-B(\sin \theta/\lambda)^2)$, (full lines: Thermal motions, disorder of the first kind) and $D_{II} = \exp(-A(\sin \theta/\lambda)^2) \cdot 2/(1 + \exp(-A(\sin \theta/\lambda)^2))$, (dashed lines: Structural disorder, of the second kind) with $A = \pi/2 \cdot B$ and differences shaded grey, for $B = [10, 3, 1]$.

3. Results from Vonk's method

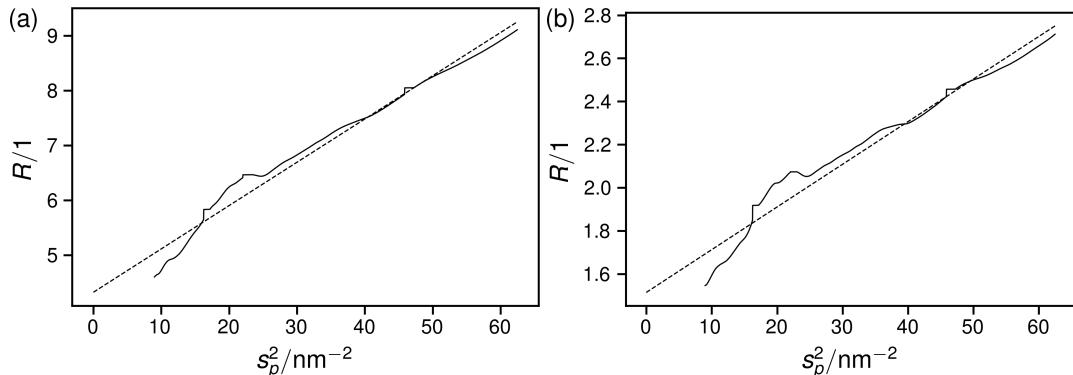


Fig. S2. Exemplary plots of R (full lines) and a squared second-degree polynomial (dashed curve) over s_p^2 for (a) $f_{\text{meso}} = 0.64$ and (b) $f_{\text{meso}} = 1$, to visualize Vonk's method (according to Figure 1 and Equations (1-7) in cited article).(Vonk, 1973)

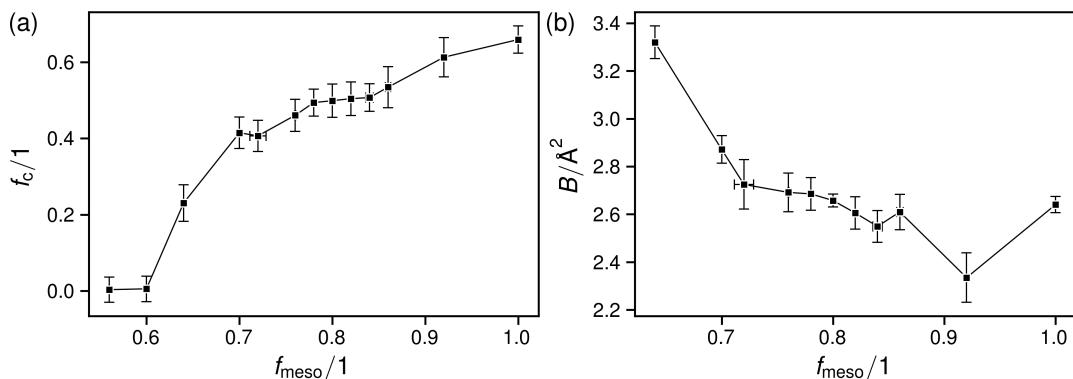


Fig. S3. (a) Bulk crystalline phase contents and (b) thermal factors determined by Vonk's method.(Vonk, 1973)