Supporting Information

Quantitative Adjustment to the Molecular Energy Parameter in the Lake-Thomas Theory of Polymer Fracture Energy

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Calculation of $W$ and $U$. In order to estimate $W$, the modified Freely Jointed Chain (m-FJC) was chosen to represent the full range of polymer elasticity up to break (eq. 2).1,2 A plot of eq. 2 is shown in Figure S1a, in which $L_0 = 21 \text{ nm}$, $f_c = 7 \text{ pN}$, and $f_s = 12 \text{ nN}$.3 Since an accurate inverse function of eq. 2 is not available, we calculated $W$ (red shaded region in Figure S1b) by:

$$W = f_{\text{break}}R_{\text{break}} - \int_{0}^{f_{\text{break}}} Rdf$$  \hspace{1cm} (S1)

where $\int_{0}^{f_{\text{break}}} Rdf$ is the gray area in Figure S1b. Based on a typical breaking force of C-C bond ($f_{\text{break}} = 4.5 \text{ nN}$)4,5 and the parameters shown above, $R_{\text{break}} \approx 28.8 \text{ nm}$ was given by eq. 2.
and $\int_0^{f_{\text{break}}} R \, df \approx 111 \, nN \cdot nm$ was obtained by integrating eq. 2 to $f_{\text{break}} = 4.5 \, nN$.

Therefore, $W$ is estimated to be $18.5 \, nN \cdot nm$. This value was divided by the number of bonds $n = 175$ ($N = 35$, each Kuhn segment $b = 0.6 \, nm$ is assumed to contain five main chain bonds) to give $U \approx 64 \, kJ \cdot mol^{-1}$.

**Figure S1.** (a) The end-to-end distance $R$ of a polymer chain is plotted as a function of the force $f$ based on eq. 2, where $L_0 = 21 \, nm$, $f_c = 7 \, pN$, and $f_S = 12 \, nN$. (b) Schematic illustration for the estimation of $W$.

**REFERENCES:**


