Supporting Information for "Effect of polymer-nanoparticle interaction on strain localization in polymer nanopillars"

1. Structure functions parameters and cut off distance determination

To calculate softness, we need to first define the parameters used to characterize particles' local structures. As stated in main text, we have two groups of structure functions, G_R and G_A. For the G_R group, we have two parameters: L and μ. Here we take $L = 0.05$ for all these structure functions, and we have $\mu \in \{0.9, 0.95, 1.0, \ldots, 2.35\}$. R_{cut} of this group can be calculated through:

$$R_{cut} = \mu + L * \ln(1/\epsilon_R)$$

We choose $\epsilon_R = 0.01$, so for the G_R group here, $R_{cut} \approx 2.5\ \sigma$.

For the G_A group, there are three parameters: ξ, ζ, and λ. In this study, we have $\xi \in \{1.75, 1.2, 2.0\}$, $\zeta \in \{1, 2, 4, 16\}$, and $\lambda \in \{1, -1\}$. We had 10 combinations of these parameters: $\{1.75, 1, 1\}$, $\{1.75, 2, 1\}$, $\{1.75, 4, 1\}$, $\{1.75, 16, 1\}$, $\{1.2, 1, 1\}$, $\{1.2, 2, 1\}$, $\{2.0, 1, -1\}$, $\{2.0, 2, -1\}$, $\{2.0, 4, -1\}$, $\{2.0, 16, -1\}$. R_{cut} of this group can be calculated through:

$$R_{cut} = \begin{cases} \xi \cdot \sqrt{2 \cdot \log(1/\epsilon_A)/3}, when\ \lambda = 1 \\ \xi \cdot \sqrt{2 \cdot \log(1/\epsilon_A)/2}, when\ \lambda = -1 \end{cases}$$

We choose $\epsilon_A = 0.05$, so for the G_A group, $R_{cut} \approx 2.5\ \sigma$. Thus, our structure functions have a cut off radius approximately $2.5\ \sigma$.

2. Approximation of treating nanoparticle sites as polymer monomers

To further verify our protocol, we change cut off distance of structure functions. The aim of changing the cutoff distance is to explore whether including more or fewer nanoparticle monomers has any effects on the training performance and the softness distribution in radial direction. Two new hyperplanes are trained in the bulk system, using two groups of structure functions with a shorter cutoff distance $R_{cut,1} \approx 1.5\ \sigma$ and a larger cutoff distance $R_{cut,2} \approx 3.5\ \sigma$ respectively.

These hyperplanes are applied into the same polymer nanopillars with a nanoparticle, $R_p = 4.0\ \sigma$, through same process described in main text, to calculate the softness. There are two reasons of using the 4σ-nanoparticle system. The first is that systems with smaller nanoparticle have clearer turning points between different regions, which can be proved by the **Fig. 7** in main text. Another reason is that using nanoparticle with this size can guarantee that the larger cutoff distance will enclose the most but also not the entire nanoparticle during the softness calculation, which can be regarded as the extreme condition with our approximation in this study. To simplify the work, here we only calculate the softness in systems with three different interactions, where $\varepsilon_{pn} = 0.2, 1.0,$ and 3.0 respectively.

The accuracy of prediction in all cases are above 90%, which is defined as the rearranged particles labeled as soft, indicating a good learning performance. The distributions of softness in systems with three interactions are presented in **Fig. 1**. We can see that in the near-nanoparticle region, no matter we try to include more or fewer monomers in the nanoparticle, the averaged softness distributions always have a similar shape. Thus, it is reasonable to treat the nanoparticle monomers as the polymer monomers in this study. This also exclude the possibility that the width of near-nanoparticle region (~$2.5\ \sigma$) in softness distribution is due to the structure functions' cut off distance (R_{cut}).

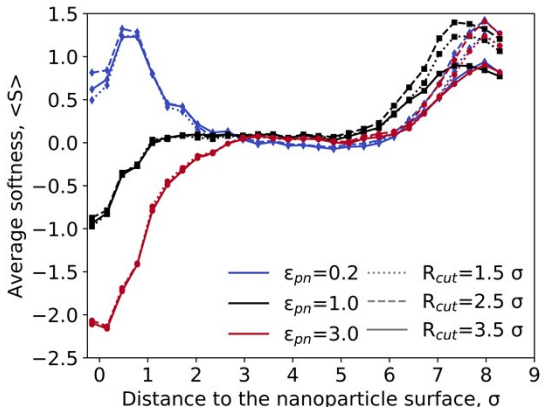

Fig. S1 Softness distribution calculated with hyperplanes generated from structure functions with different cutoff distance (denoted by line style). Tests have been done for three different polymer-NP interactions ($\varepsilon_{pn} = 0.2, 1.0,$ and 3.0, denoted by color). In these testing pillars, all the NPs have a same radius, $R_p = 4.0\ \sigma$.