

Supporting Information for

Impact of interfacial properties on the viscoelastic relaxation of hard-soft block copolymers
using Finite Element Analysis

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1. Significance Ranking of Interphase Property on overall Responses

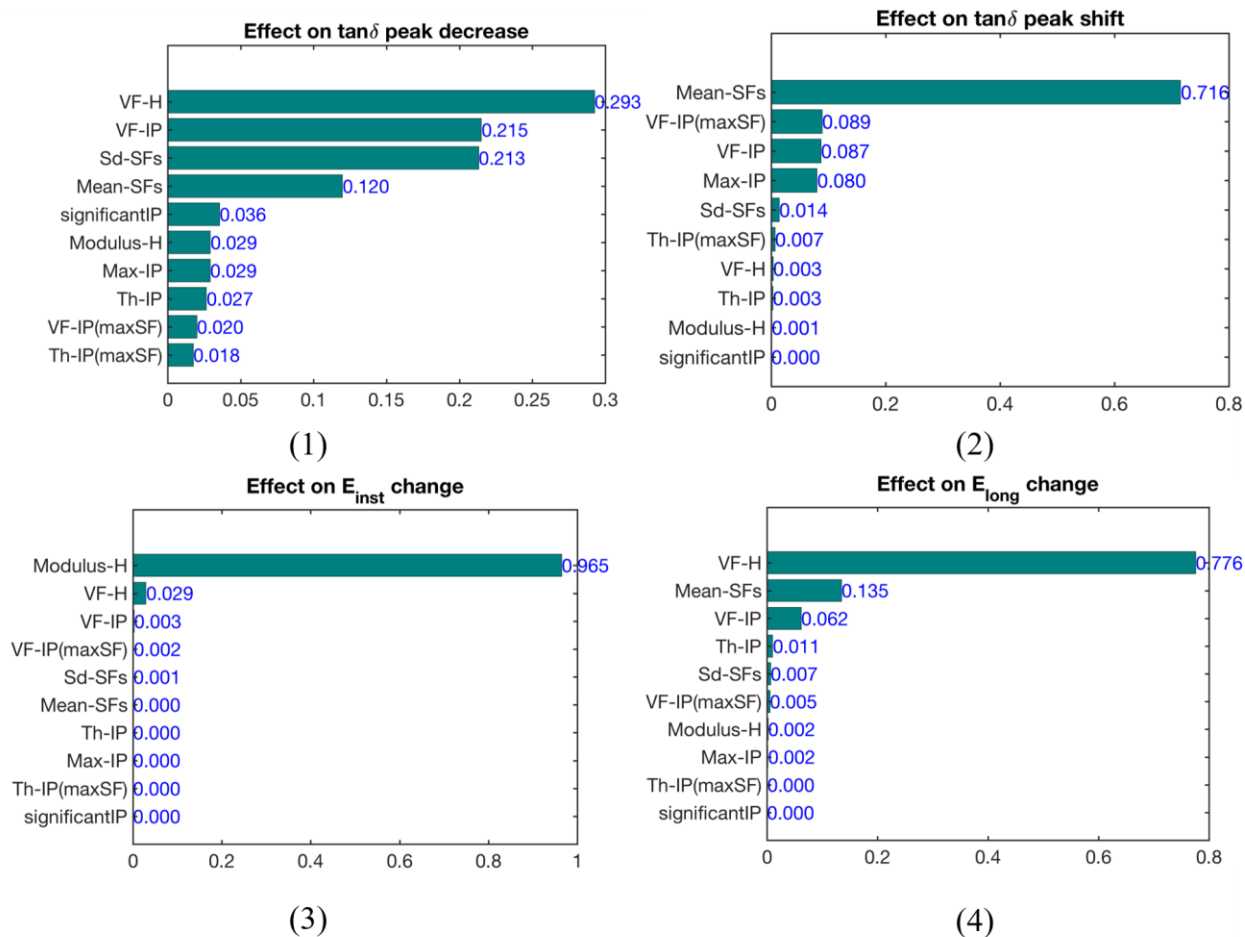


Figure S1 Detailed values of the significance ranking of ten structural and property features on $\tan \delta$ peak decrease, $\tan \delta$ peak shift, instantaneous modulus and long-term modulus.

2. Correlation Function of 2D Binarized Image vs. 3D Reconstructed Structures

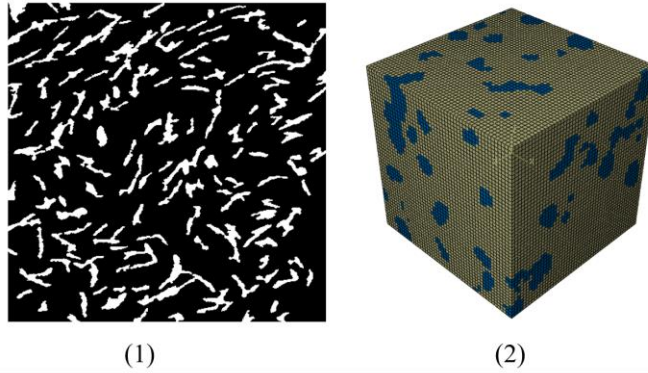


Figure S2 (1) 2D binarized image 441nm×441 nm, (2) 3D reconstructed image 50nm×50nm

Utilizing the method in Ref ¹, we reconstruct the 3D microstructure (Figure S2-(2)) based on the 2D binarized one (Figure S2-(1)). In order to make reliable comparison between the interphase effects on viscoelastic behavior of these two types of structures, we use correlation functions to validate the equivalence of the 2D microstructures and the 3D reconstructions.

Mathematically, correlation functions quantify the conditional probability of finding two randomly chosen points in the same phase. Statistical correlation functions can be utilized for mathematical description of the morphology of microstructure and quantitatively connecting the macroscopic properties of a heterogeneous image to its complex microstructure ²⁻⁴. Since the 3D reconstruction is based on the two-point correlation functions extracted from the 2D microstructure ¹, we present another correlation function, linear path correlation function of both cases together with their two point correlation functions.

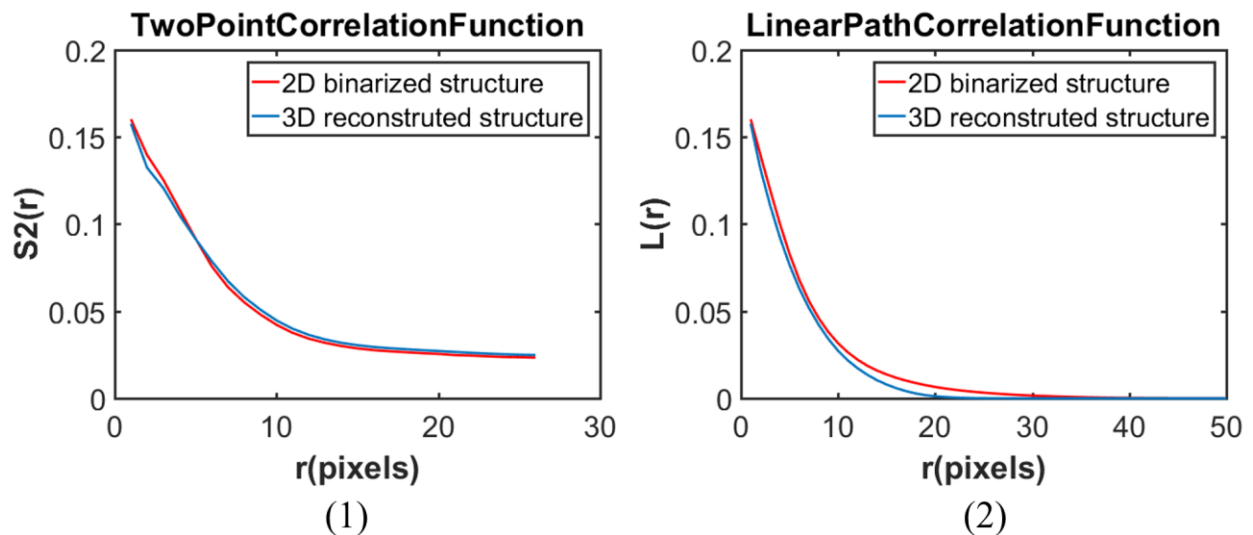


Figure S3 Comparison of (1) the two-point correlation functions for 2D and 3D structures, (2) the linear-path correlation functions for 2D and 3D structures.

A simple explanation of the two correlation functions are ⁴: (1) two point correlation function($S_2(r)$) gives the probability that two randomly chosen points, separated by distance r , fall in the same phase, (2) lineal path correlation($L(r)$) means the probability that a randomly selected line segment of length r falls entirely in the same phase.

The good agreement between the two correlation functions in Figure S3 shows that the 2D microstructure and the 3D reconstruction share a set of statistical information that ensures the generalization of argument that we achieved from 2D FEA simulations to 3D cases.

3. Reference

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3. Yeong, C. L. Y.; Torquato, S., Reconstructing random media. *Physical Review E* **1998**, *57* (1), 495-506.
4. Jiao, Y.; Chawla, N., Three dimensional modeling of complex heterogeneous materials via statistical microstructural descriptors. *Integrating Materials and Manufacturing Innovation* **2014**, *3* (1), 3.