Supplementary Information: Elastically driven phase separation in liquid crystals

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Abstract

This document contains supplementary simulation data regarding response to linear elastic perturbations and the binary phase diagram.

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I. RESPONSE TO LINEAR DEFORMATIONS

In addition to the nonlinear fields described in the text, we have examined the possibility of fractionation due to a linear ramp profile, $\theta(x) = \pi x/L$. We first examine a linear ramp profile, depicted in Figure 1. At this applied field, no demixing is observed within the system in contrast to the nonlinear fields within the main text.

II. COEXISTENCE DATA

Tables I–VI present further coexistence data determined in our simulations, expanding on results plotted in Fig. 2 of the main text. Chemical potentials reported were computing using reweighting as described in the main text. Values corresponding to pure A or B species are labeled with N/A as the values were not explicitly computed.
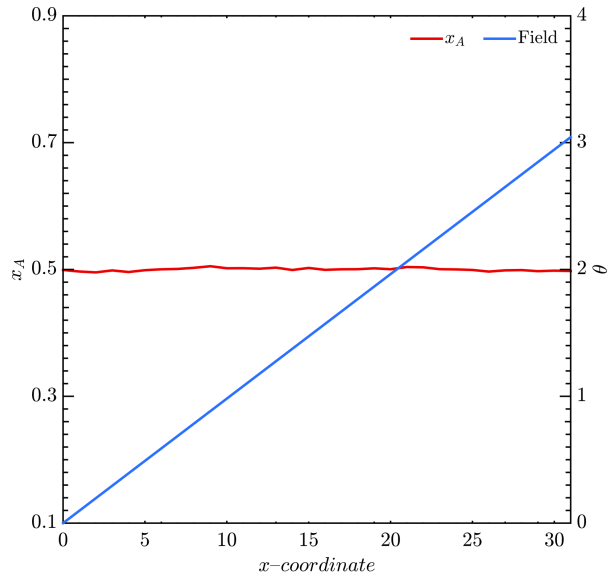
Figure 1. The application of a linear field to the binary mixture $\varepsilon_{AA}/\varepsilon_{BB} = T^* = 0.40$, with $x_B = 0.5$. No segregation is observed in the system, highlighting the role of nonlinear stress in inducing elastically-driven demixing.

Table I. Coexistence data for $\varepsilon_{AA}/\varepsilon_{BB} = 0.20$

T^*	T^*/T_{NI}^B	x_B^α	x_B^β	$\Delta\mu_{eq}$
0.0500	0.0445	0.00006	1.00000	2.32081
0.1000	0.0889	0.00006	0.99994	2.22953
0.1600	0.1423	0.00198	0.99744	2.12331
0.1700	0.1512	0.00275	0.99642	2.10198
0.1800	0.1601	0.00358	0.99501	2.08339
0.1900	0.1690	0.00448	0.99341	2.06117
0.2000	0.1779	0.00525	0.99149	2.04144
0.2100	0.1868	0.00582	0.98944	2.01933
0.2200	0.1957	0.00576	0.98688	1.99836
0.2300	0.2046	0.00314	0.98451	1.97101
0.2400	0.2135	0.00352	0.98227	1.94254
0.2500	0.2224	0.00410	0.97933	1.91719
0.2700	0.2401	0.00608	0.97325	1.86453
0.3000	0.2668	0.01101	0.96346	1.78181
0.4000	0.3558	0.05261	0.91859	1.52354
0.5000	0.4447	0.15015	0.85886	1.26555
0.6000	0.5337	0.31932	0.81281	0.96053
0.7000	0.6226	0.46672	0.73153	0.65992
0.8000	0.7116	0.61622	0.72553	0.25419
0.9000	0.8005	0.74459	0.77813	-0.29331
1.0000	0.8894	0.86541	0.86925	-1.14114
1.1243	1.0000	1.00000	1.00000	N/A

Table II. Coexistence data for $\varepsilon_{AA}/\varepsilon_{BB} = 0.25$

T^*	T^*/T_{NI}^B	x_B^α	x_B^β	$\Delta\mu_{eq}$
0.0500	0.044	0.00006	1.00000	2.178190
0.1000	0.089	0.00038	0.99955	2.106259
0.1600	0.142	0.00768	0.99110	2.016015
0.2000	0.178	0.02112	0.97376	1.950065
0.2500	0.222	0.04570	0.93382	1.863135
0.2700	0.240	0.05222	0.91104	1.826176
0.3000	0.267	0.02381	0.87597	1.765221
0.4000	0.356	0.06507	0.79780	1.526591
0.5000	0.445	0.16116	0.73373	1.281408
0.6000	0.534	0.30130	0.68068	1.010631
0.7000	0.623	0.45616	0.65736	0.690000
0.8000	0.712	0.59950	0.68569	0.286363
0.9000	0.800	0.73123	0.76246	-0.262816
1.0000	0.889	0.85664	0.86086	-1.111535
1.1243	1.000	1.00000	1.00000	N/A

Table III. Coexistence data for $\varepsilon_{AA}/\varepsilon_{BB} = 0.30$

T^*	T^*/T_{NI}^B	x_B^α	x_B^β	$\Delta\mu_{eq}$
0.0500	0.0445	0.00006	0.99402	2.03916
0.1000	0.0889	0.00192	0.99802	1.97639
0.1500	0.1334	0.01802	0.98098	1.91145
0.1900	0.1690	0.05205	0.94194	1.85693
0.2000	0.1779	0.06507	0.92593	1.84329
0.2100	0.1868	0.08108	0.90691	1.82953
0.2200	0.1957	0.10010	0.88488	1.81565
0.2300	0.2046	0.12312	0.85786	1.80166
0.2400	0.2135	0.15115	0.82282	1.78761
0.2500	0.2224	0.19219	0.77678	1.77349
0.2600	0.2313	0.25125	0.70370	1.75932
0.2700	0.2401	0.47210	0.49280	1.73064
0.3000	0.2668	0.00000	0.00000	N/A
0.3500	0.3113	0.01981	0.02401	1.98993
0.4000	0.3558	0.07447	0.17337	1.59496
0.4500	0.4002	0.11522	0.40070	1.45364
0.5500	0.4892	0.22568	0.52072	1.19598
0.6000	0.5337	0.29240	0.54010	1.05610
0.6500	0.5781	0.36430	0.55880	0.90309
0.7000	0.6226	0.43520	0.57880	0.73452
0.7500	0.6671	0.50660	0.60480	0.54449
0.8000	0.7116	0.57800	0.64360	0.32957
0.8500	0.7560	0.64620	0.68930	0.07791
0.9000	0.8005	0.71800	0.74770	-0.22859
0.9500	0.8450	0.78350	0.79850	-0.59720
1.0500	0.9339	0.90850	0.91460	-1.79403
1.1243	1.000	1.00000	1.00000	N/A

Table IV. Coexistence data for $\varepsilon_{AA}/\varepsilon_{BB} = 0.35$

T^*	T^*/T_{NI}^B	x_B^α	x_B^β	$\Delta\mu_{eq}$
0.0500	0.044	0.00006	0.99921	1.89762
0.0700	0.062	0.00100	0.99900	1.87355
0.1000	0.089	0.00701	0.99299	1.84200
0.1300	0.116	0.02603	0.97297	1.80864
0.1500	0.133	0.05205	0.94494	1.78603
0.1600	0.142	0.07007	0.92593	1.77458
0.1700	0.151	0.09409	0.89990	1.76319
0.1800	0.160	0.12713	0.86386	1.75170
0.1900	0.169	0.17317	0.81381	1.74017
0.2000	0.178	0.25626	0.72973	1.72862
0.2100	0.187	0.51123	0.54074	1.71687
0.5000	0.445	0.14094	0.21742	1.45123
0.6000	0.534	0.26727	0.39159	1.13502
0.7000	0.623	0.40721	0.49790	0.79867
0.8000	0.712	0.55135	0.59980	0.38419
0.9000	0.800	0.69459	0.71652	-0.17461
1.0000	0.889	0.83430	0.83890	-1.03139
1.1243	1.000	1.00000	1.00000	N/A

Table V. Coexistence data for $\varepsilon_{AA}/\varepsilon_{BB} = 0.40$

T^*	T^*/T_{NI}^B	x_B^α	x_B^β	$\Delta\mu_{eq}$
0.4500	0.4002	0.0000	0.0000	N/A
0.5000	0.4447	0.0781	0.0911	1.7555
0.5500	0.4892	0.1521	0.1813	1.4707
0.6000	0.5337	0.2227	0.2774	1.2634
0.6500	0.5781	0.2963	0.3596	1.0779
0.7000	0.6226	0.3702	0.4277	0.8872
0.7500	0.6671	0.4498	0.4810	0.6843
0.8000	0.7116	0.5164	0.5466	0.4597
0.8500	0.7560	0.5980	0.6259	0.1906
0.9000	0.8005	0.6724	0.6931	-0.1151
0.9500	0.8450	0.7450	0.7566	-0.4850
1.0000	0.8894	0.8204	0.8320	-0.9869
1.0500	0.9339	0.8899	0.8917	-1.6555
1.1243	1.0000	1.0000	1.0000	N/A
0.1635	0.1454	0.5000	0.5000	N/A
0.1630	0.1450	0.4702	0.5482	1.6449
0.1620	0.1441	0.3900	0.6000	1.6357
0.1610	0.1432	0.3466	0.6426	1.6469
0.1600	0.1423	0.3066	0.6870	1.6479
0.1500	0.1334	0.1737	0.8207	1.6576
0.1400	0.1245	0.1151	0.8809	1.6674
0.1300	0.1156	0.0781	0.9189	1.6771
0.1200	0.1067	0.0531	0.9449	1.6869
0.1100	0.0978	0.0348	0.9644	1.6964
0.1000	0.0889	0.0217	0.9777	1.7060
0.0900	0.0800	0.0127	0.9870	1.7163
0.0800	0.0712	0.0067	0.9932	1.7247
0.0700	0.0623	0.0029	0.9969	1.7354
0.0600	0.0534	0.0011	0.9988	1.7441
0.0500	0.0445	0.0003	0.9997	1.7529

Table VI. Coexistence data for $\varepsilon_{AA}/\varepsilon_{BB} = 0.50$

T^*	T^*/T_{NI}^B	x_B^α	x_B^β	$\Delta\mu_{eq}$
0.0500	0.044	0.00601	0.99399	1.46487
0.0600	0.053	0.01702	0.98198	1.45824
0.0700	0.062	0.03804	0.96196	1.45080
0.0800	0.071	0.07407	0.92492	1.44366
0.0900	0.080	0.14214	0.85586	1.43650
0.1000	0.089	0.42202	0.56800	1.42934
0.6000	0.534	0.07347	0.07514	1.98063
0.6500	0.578	0.16486	0.17357	1.51000
0.7000	0.623	0.25335	0.26754	1.20574
0.7500	0.667	0.34024	0.35345	0.93928
0.8000	0.712	0.42938	0.44640	0.67120
0.8500	0.756	0.51772	0.53483	0.38151
0.9000	0.800	0.60768	0.61357	0.05443
0.9500	0.845	0.69638	0.70387	-0.33849
1.0000	0.889	0.78350	0.78580	-0.83520
1.0100	0.898	0.80608	0.80608	-0.96320
1.0200	0.907	0.82112	0.82112	-1.08870
1.0300	0.916	0.83981	0.83981	-1.23234
1.0400	0.925	0.85792	0.85792	-1.39000
1.0500	0.934	0.86995	0.86995	-1.54500
1.1243	1.000	1.00000	1.00000	N/A