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In silico assessment of dielectric constants of magnetic composite sorbents for capillary electrochromatography

Alexey Yu. Shmykov, Anton L. Bulyanitsa and Andrei R. Timerbaev

Method

Briefly, BaTiO3 particles doped with Fe (500 ± 20 nm; US Research Nanomaterials, Inc. Houston, TX, USA) were dispersed in the oligomeric diisocyanate Crosslinker CX-100 (Cytec, Woodland Park, NJ, USA; M_n ~ 1500), and the mixture was applied to polydimethylsiloxane substrates (Sylgard-184, Dow Corning, Midland, MI, USA) using a die, followed by drying at 50 °C for 60 min. The capacitance and tangent of the dielectric losses for the obtained composites were measured using an E7-20 impedance meter (MNINI, Minsk, Belarus) at a frequency of 1 kHz, and the dielectric constant was calculated according to the method by Mjakin *et al.*[S1]

Table S1 Comparison of experimental and calculated dielectric constants ε^* at $\varepsilon_1 = 0.10$.[a]

φ_1 (%)	Experimental ε^*	Calculated ε^*				
		Model 1	Model 2	Model 3	Model 4	Model 5
20	1.75	1.98	1.98	1.82	1.73	1.76
25	1.74	1.86	1.74	1.68	1.57	1.56
35	1.38	1.63	1.35	1.41	1.27	1.26
45	1.35	1.39	1.04	1.17	1.01	0.94
50	1.16	1.28	0.91	1.05	0.89	0.79
Average RSD (%)		10.3	10.8	6.1	12.3	14.8

[a] Models are sequentially numbered as expressions (1)–(5) in the main article, respectively.

Table S2 Comparison of experimental and calculated dielectric constants ε^* at $\varepsilon_1 = 0.15$.[a]

φ_1 (%)	Experimental ε^*	Calculated ε^*				
		Model 1	Model 2	Model 3	Model 4	Model 5
20	1.75	1.97	1.93	1.80	1.68	1.74
25	1.74	1.85	1.69	1.66	1.51	1.56
35	1.38	1.61	1.29	1.38	1.20	1.22
45	1.35	1.37	0.99	1.13	0.92	0.88
50	1.16	1.25	0.86	1.11	0.80	0.71
Average RSD (%)		8.8	13.3	5.4	17.2	17.2

[a] Models are sequentially numbered as expressions (1)–(5) in the main article, respectively.

Reference

S1 S. V. Mjakin, N. A. Bubis, L. M. Kuznetsov, M. V. Zhukov and A. Yu. Shmykov, *Phys. Solid State*, 2022, **64**, 747; https://doi.org/10.21883/PSS.2022.06.53842.291.