

Electronic Supplementary Material

Multivariate Analysis of Nanoparticle Translocation through a Nanopore to Improve the Accuracy of Resistive Pulse Sensing

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Description of the finite element simulation model

The simulated 3-dimensional geometry is shown in Fig. S1†. Studying the off-axis via an axisymmetric model is impractical. Furthermore, the nanopore has a finite depth. Therefore, 2-dimensional axisymmetric and 2-dimensional models are inapplicable in the present study. Boundary conditions are available in Table S1†. For the mesh independence study, we have assumed two coefficients, including α and β , to refine the mesh in the nanopore domain and vicinity of the particle, respectively. α indicates the coefficient multiplied by the maximum and minimum size of the elements in the nanopore domain.

Furthermore, β is the number of the points considered on the nanoparticle's surface as the distribution. First, we have considered a constant β value and reduced α values. The error is computed concerning the most-refined mesh, and the optimized value is adopted. The same procedure has been repeated for the β coefficient for increasing β values. The selected values for α and β are available in Tables S2† and S3†. The generated mesh for the geometry is available in Fig. S2†, consisting of nearly 170k free tetrahedral elements. The legends in Figure S2 represent the size range of elements within the meshed domain, indicating both upper and lower limits. According to the figure, the nanopore and particle vicinity domains have finer elements. The maximum and minimum element sizes are $0.11 \mu\text{m}$ and 0.37 nm , respectively. The validation of the present model has been conducted with the analytical model.¹ Constant values and the parameters used in the simulation are available in Table S4†.

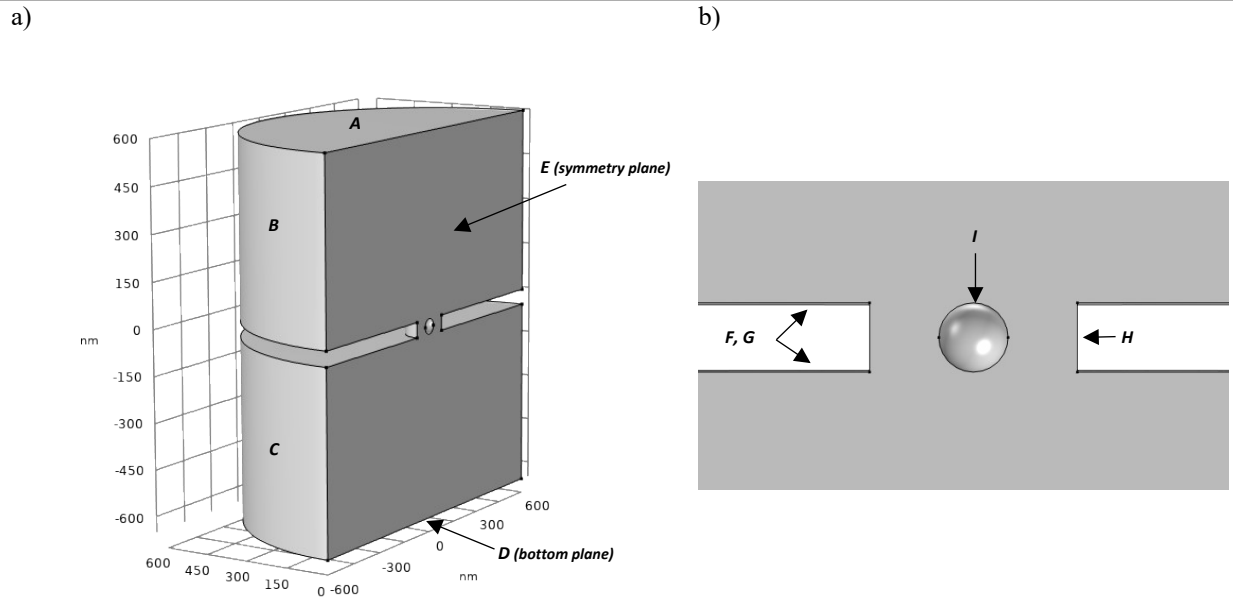


FIG. S1. (a) The simulated geometry and (b) the detailed view of the nanopore and the characterized boundaries. The electrolyte solution is KCl with a salt concentration of 10 mM.² The cylindrical nanopore's diameter and thickness and the nanoparticle's diameter are 150 nm, 50 nm, and 30 nm, respectively.³

TABLE SI. Boundary conditions for the Poisson, Nernst-Planck and Stokes equations.

Boundary	Poisson	Nernst-Planck	Stokes
A, D	A: $V=0$ V, D: $V=0.2$ V	$c_i=10$ mM	$P=0$
B, C	$n \cdot (\epsilon \vec{E})=0$	$n \cdot N_i=0$	$\vec{U}=0$
E	symmetry	symmetry	symmetry
F, G, H	$n \cdot (\epsilon \vec{E})=\sigma_w$	$n \cdot N_i=0$	$\vec{U}=0$
I	$n \cdot (\epsilon \vec{E})=\sigma_p$	$n \cdot N_i=n \cdot (c_i \vec{U})$	$\vec{U}=\vec{u}_p \mathbf{e}_z$

TABLE SII. Mesh refinement study for α , considering $\beta = 100$.

α	I (nA)	%Deviation
0.5	3.076575	%-0.23
0.15	3.084445	%0.0251
0.14	3.0840845	%0.0134
0.13	3.084293	%0.0202
0.12	3.08381	%0.004509
0.1	3.08367	0

Table SIII. Mesh refinement study for β , considering $\alpha = 0.5$.

β	I (nA)	%Deviation
50	3.075098	%-0.0699
100	3.076574	%-0.01893
150	3.074887	%-0.0737
200	3.076547	%-0.01981
250	3.077619	%-0.01502
300	3.076648	%-0.0165
350	3.077157	0

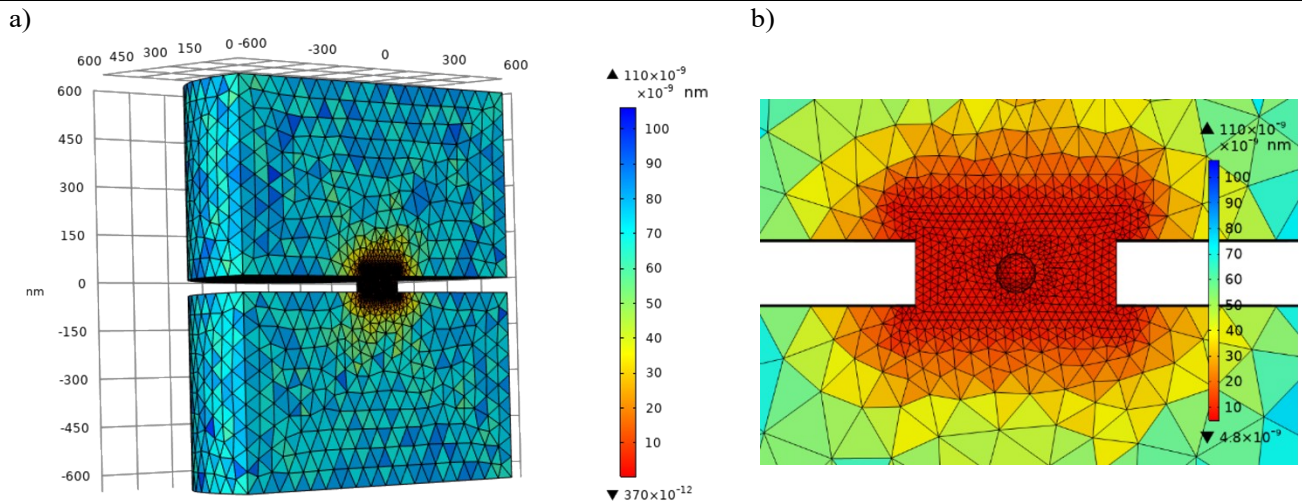


FIG. S2 The generated mesh for (a) the whole domain and (b) the nanopore and particle vicinity. We have considered α and β to edit the meshes in the nanopore and around the nanoparticle.

TABLE SIV. Constants and the parameters used in the simulation.

parameter	value	unit	details
N_A	6.022×10^{23}	1/mol	Avogadro constant
e	1.602×10^{-19}	C	electron charge
μ_{K^+}	7.62×10^{-8}	$m^2/(s.V)$	mobility of K^+
μ_{Cl^-}	7.91×10^{-8}	$m^2/(s.V)$	mobility of Cl^-
F	96485.3321	C/mol	Faraday constant
T	298	K	temperature
R	8.3145	J/(mol.K)	Gas constant
k_B	1.380649×10^{-23}	$m^2/(kg.s^{-2}.K^{-1})$	Boltzmann constant
ϵ_0	$8.8541878 \times 10^{-12}$	F.m ⁻²	Vacuum permittivity
ϵ_r	80	-	Relative permittivity of water
η	1.0016×10^{-3}	Pa.s	Dynamic viscosity of water
z_{K^+}	+1	-	the charge of K^+
z_{Cl^-}	-1	-	the charge of Cl^-
c_0	10	mM	Electrolyte solution concentration

Particle velocity calculation

In the case of the particles with surface charge density, the velocity (eq. S1†) has been achieved via electrophoretic mobility (μ_{EP}) of the particle. The electrophoretic mobility of a charged particle is calculated via eq. S2†.^{4,5,6} Where κ , a , and $f(\kappa a)$ are Debye-Hückel parameter, particle radius, and Henry's function respectively. The Debye-Hückel parameter (κ) is inversely equal to the Debye length (λ_D).⁷ Henry's function is obtained based on κa values for the particles with constant surface charge density.⁶ In this case, the oblate- and prolate-shaped particles translocate parallel to the minor and major semi-axis, respectively. Consequently, the applied coefficients for the particles are available in Table S5. Fig. S3† illustrates the velocity of the particles translocating through the nanopore concerning case I and case II.

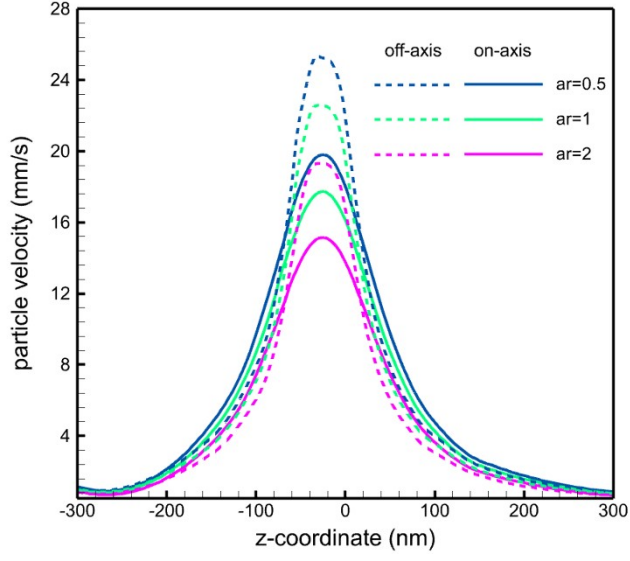
$$U_{EP} = \mu E \quad (S1)$$

$$\mu = \frac{\varepsilon_0 \varepsilon_r \zeta_p}{\mu} f(\kappa a) \quad (S2)$$

TABLE S5. The coefficients used in nanoparticle velocity calculations.

	oblate	sphere	prolate
$f(\kappa a)$	0.65	0.76	0.85

a)



b)

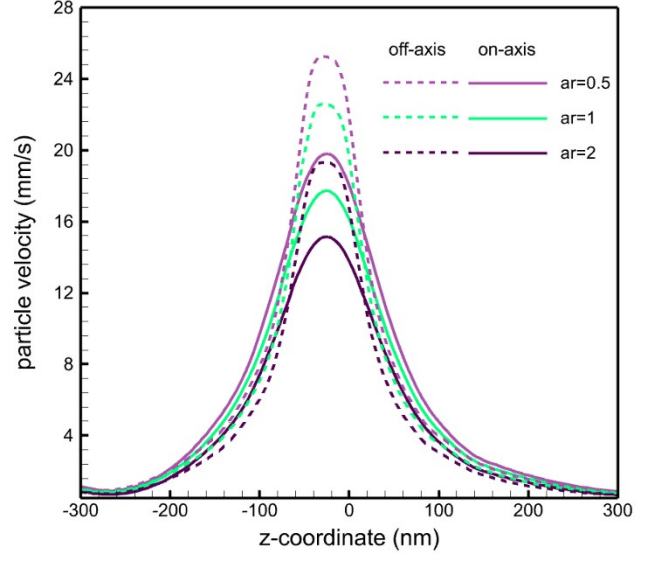


FIG. S3 Velocity variation for (a) case I and (b) case II concerning oblate, sphere, and prolate as the translocating particles.

The zeta potential of the particle is related to the surface charge density of the nanoparticle via eq. S7†.⁷ For the case of the particle with a surface charge density of -8.7 mC/m^2 , the absolute value of the zeta potential equals 34.95 mV according to the constants and parameters used in the present numerical simulation.

$$\sigma_p = \frac{2k_B T \epsilon_0 \epsilon_r \kappa}{e} \sinh\left(\frac{e\zeta_p}{2k_B T}\right) \quad (\text{S7})$$

Pulse waveshapes

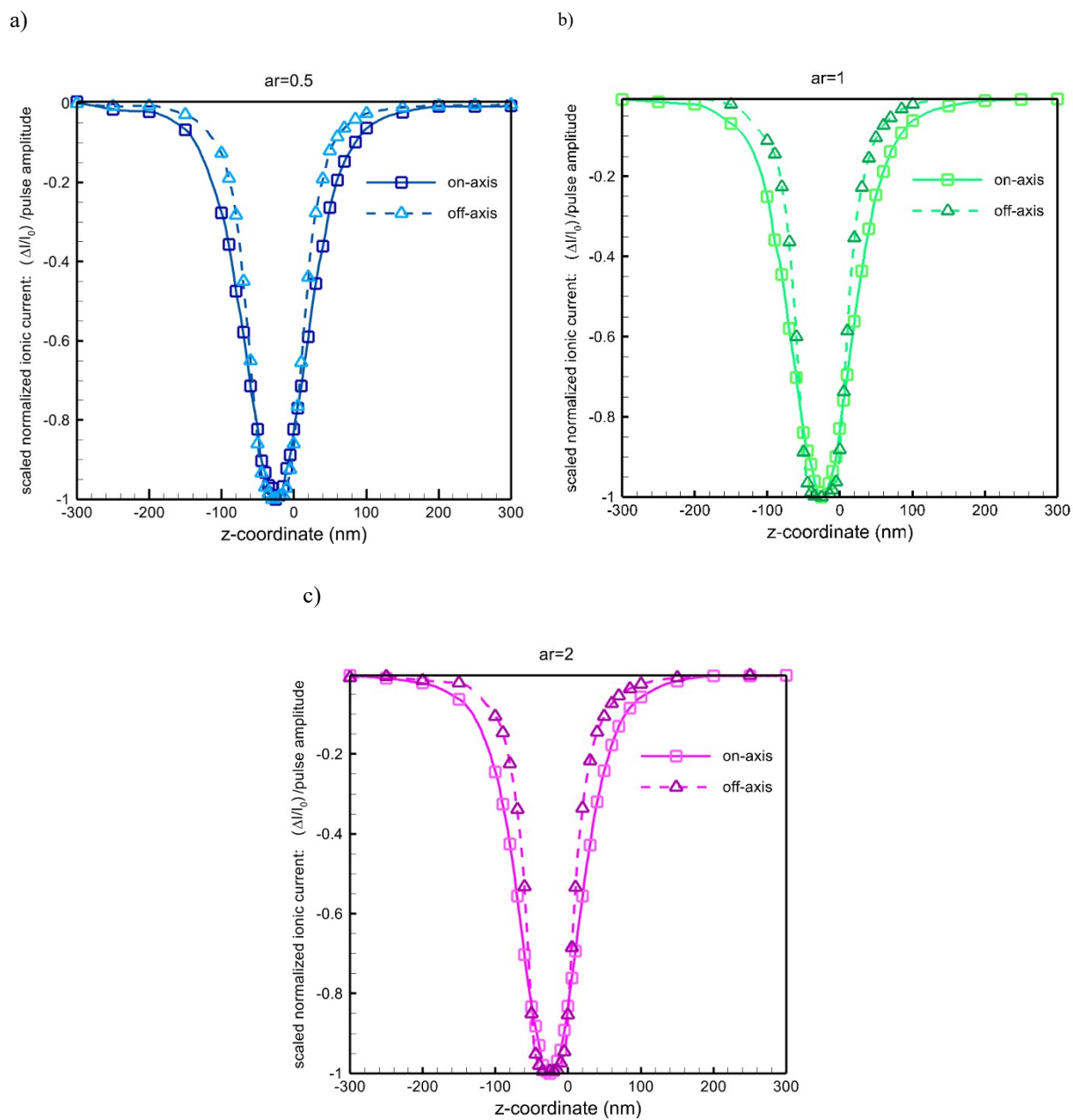


Fig. S4 Pulse waveshapes for the nanoparticles (without surface charge density) featured in Table 2, with aspect ratios of (a) 0.5, (b) 1, and (c) 2.

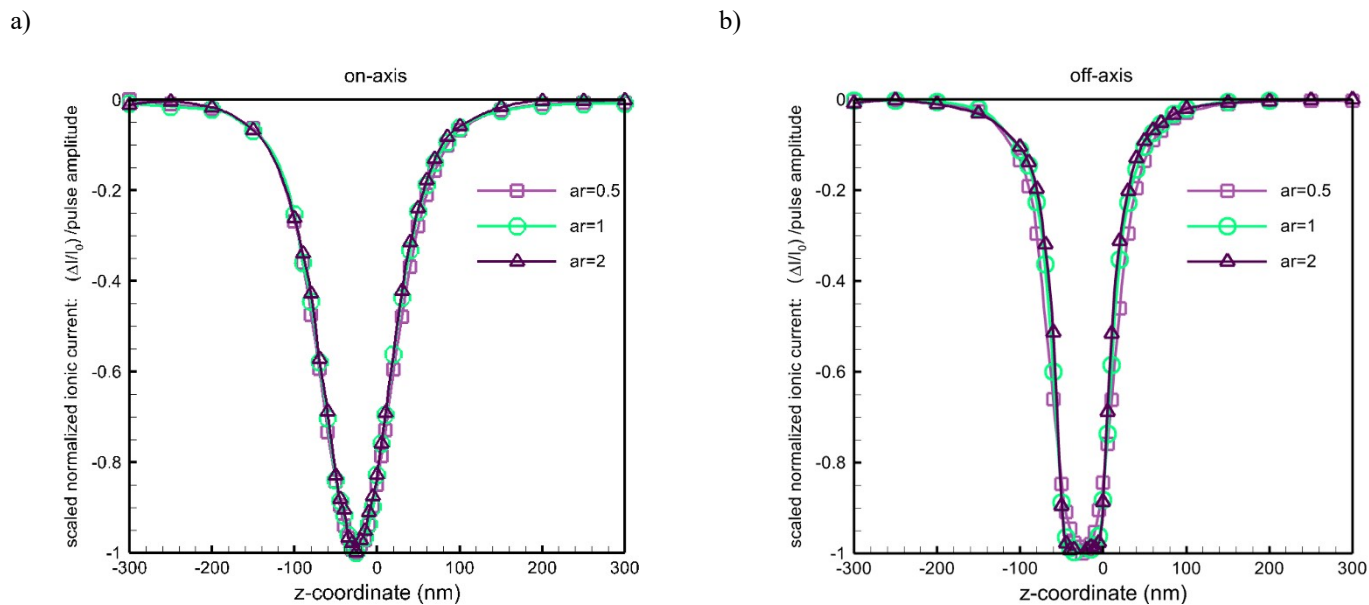


Fig. S5 Resistive pulse waveshapes in the (a) on-axis and (b) off-axis mode for the nanoparticles (without surface charge density) featured in Table 2b. The coincidence of the resistive pulse waveshapes of particles with different aspect ratios shows the pulse profiles' dependency on the particle's location.

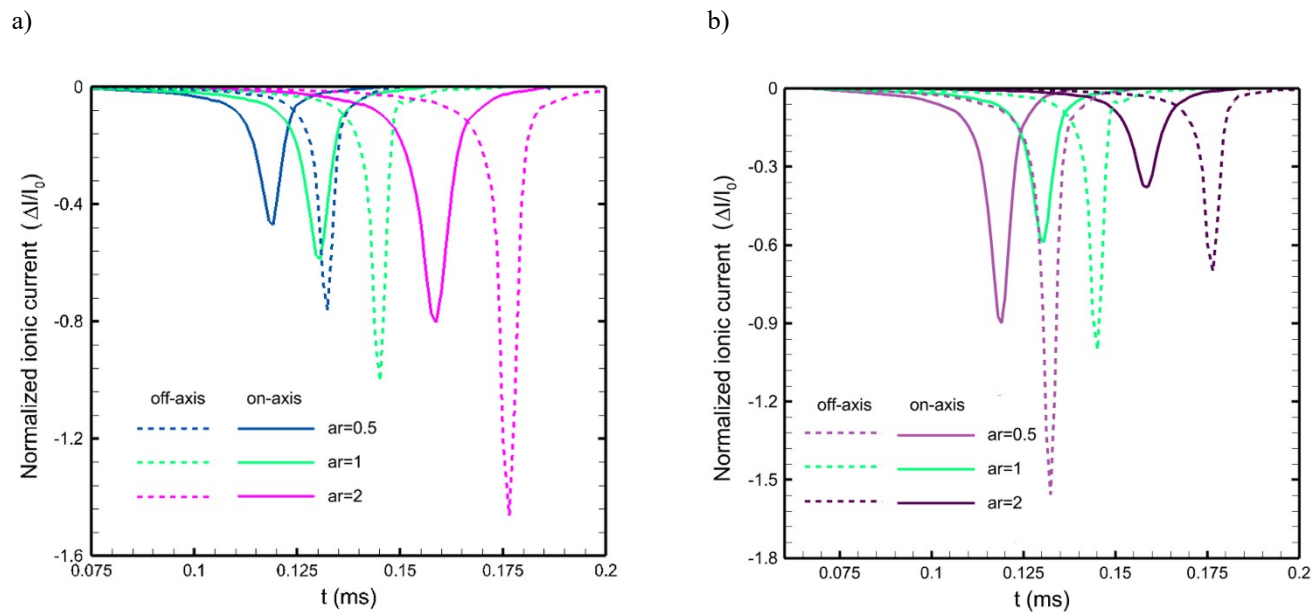


Fig. S6 (a) Resistive pulses of the particles with surface charge density equal to -8.7 mC/m^2 , featured in Table (a) 2a (case I: constant volume), and (b) 2b (case II: constant area). The on-axis and off-axis modes represent $x=0 \text{ nm}$ and $x=55 \text{ nm}$, respectively.

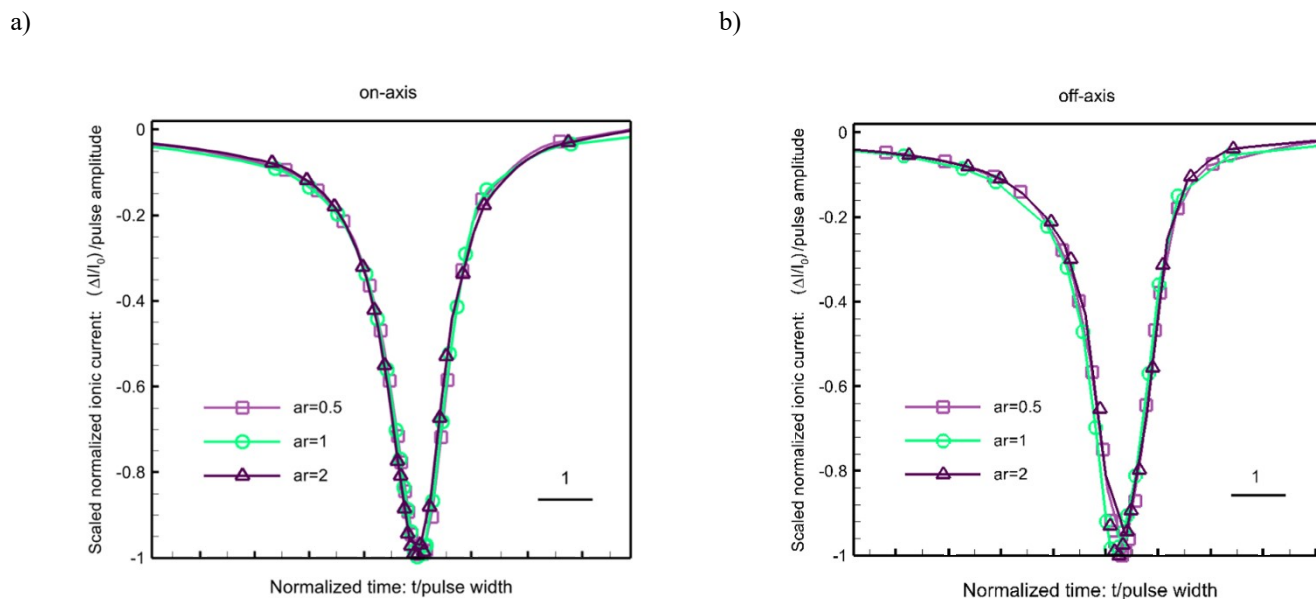


Fig. S7 Resistive pulse waveshapes in the (a) on-axis and (b) off-axis mode for the nanoparticles (with surface charge density) featured in Table 2b. The coincidence of the resistive pulse waveshapes of particles with different aspect ratios shows the pulse profiles' dependency on the particle's location. The incorporation of a scale bar serves the purpose of representing time, which is scaled relative to pulse width.

References

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