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Electrostatic interaction between two interpenetrating soft particles

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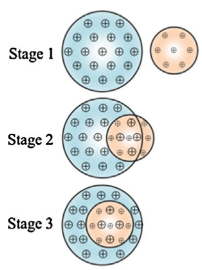
HIGHLIGHTS

- A three-stage model for interaction of two interpenetrating spheres is presented.
- The interaction energy and force of two interpenetrating spheres are calculated.
- The interaction force reaches a maximum in magnitude during interpenetration.
- The zero separation between likely charged spheres corresponds to unstable equilibrium.

GRAPHICAL ABSTRACT

Three-stage model for interaction of two spheres.



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ABSTRACT

A three-stage model of the electrostatic interaction between two interpenetrating charged spherical soft particles with no particle core (space-charged porous spheres) in an electrolyte solution is presented. That is, (i) interaction before contact of the two spheres, (ii) partial interpenetration, and (iii) full interpenetration, i.e., engulfing of one sphere by the other. This is an extension of the work of Dähnert and Rödenbeck (J. Colloid Interface Sci., 163 (1994) 229), who considered the interaction between two interpenetrating vesicle-like surface-charged particles, to the case of the interaction of space-charge porous spheres. Analytic expressions for the interaction energy and force between two interpenetrating weakly charged porous spheres as a function of particle separation are derived for the respective stages on the basis of the linearized Poisson–Boltzmann equations for the electric potential distribution.

1. Introduction

Soft particles, which are hard particles covered with an ion-penetrable surface layer of polyelectrolytes, can be a model for biological cells. Electrostatic interactions between soft particles are quite different from those for hard particles without surface structures in that the electrostatic interactions between soft particles are governed by their space-charges distributed within the particles or the Donnan potentials, while those for hard particles are determined by their surface charges or surface potentials. Theoretical studies on the interaction between soft particles have so far been confined mostly to the interactions before contact of the surface layers of interacting soft particles [1–11]. Concerning the interaction between soft particles after contact, the author discussed the electrostatic interaction between two parallel planar polyelectrolyte brushes before and after their contact [12,13].

In the present article we consider the electrostatic interaction between two interpenetrating charged soft particles with no particle core, i.e., space-charged porous spheres in an electrolyte solution. We consider three interaction stages, that is, (i) interaction before contact of the spheres, (ii) partial interpenetration, and (iii) full interpenetration, or engulfing of one sphere by the other (Fig. 1). This is an extension of the work of Dähnert and Rödenbeck [14], who considered the interaction between two interpenetrating vesicle-like surface-charged particles. The present three-stage interaction model can be a model for interactions between biological cells, which in some cases exhibit interpenetration or engulfing [15]. We derive analytic expressions for the electrostatic interaction

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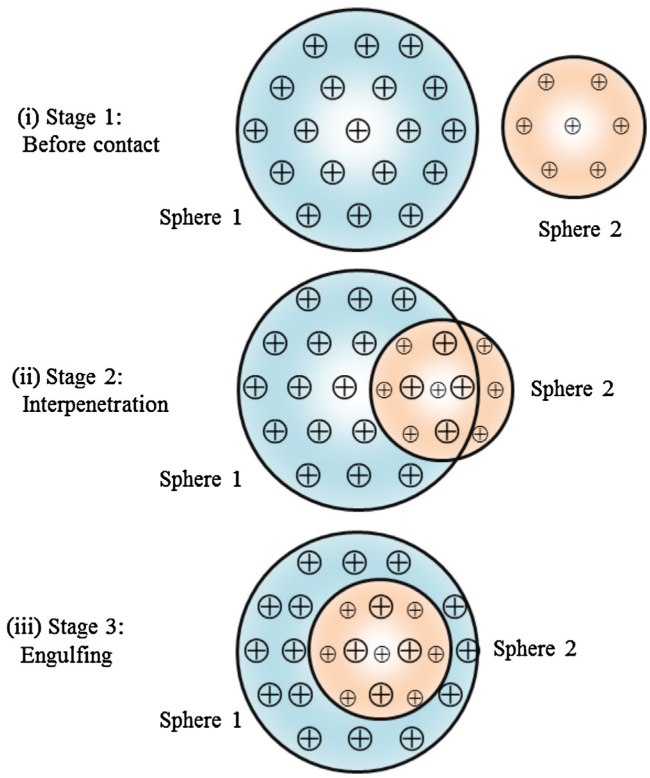

Fig. 1. Three-stage model for the electrostatic interaction between two charged soft particles (porous spheres) 1 and 2: (i) before contact, (ii) interpenetration, and (iii) engulfing.

between two interpenetrating weakly charged spherical soft particles (space-charged porous spheres) in an electrolyte solution on the basis of the linearized Poisson–Boltzmann equation for the electric potential distribution.

2. Linearized Poisson–Boltzmann equations for two interacting charged porous spheres

Consider two charged porous spheres of radii a_1 and a_2 carrying fixed charges of constant volume densities ρ_1 and ρ_2, respectively, at separation R between their centers O_1 and O_2 in an electrolyte solution containing N ionic species with valence z_i and bulk concentration (number density) n_i ($i = 1, 2, \ldots, N$) (in units of m^{-3}) in three stages, that is, (i) interaction before contact, (ii) interpenetration, and (iii) engulfing (Figs. 2–4). If dissociated groups of valence Z_j are distributed at a uniform density N_j in sphere j ($j = 1, 2$), then the fixed-charge density ρ_j in sphere j is related to the density N_j by $\rho_j = Z_j e N_j$ ($j = 1, 2$) (where e is the elementary electric charge). Without loss of generality, we may treat the case in which the radius a_1 of sphere 1 is larger than or equal to the radius a_2 of sphere 2, viz.,

$$a_1 \geq a_2 \tag{1}$$

We assume that the relative permittivity in spheres 1 and 2 take the same value ε_r as that of the electrolyte solution and that the electrical potential ψ is low enough to allow the linearization of the Poisson–Boltzmann equations for ψ.

The linearized Poisson–Boltzmann equation in the respective regions can generally be given by

$$\Delta\psi = \kappa^2\psi - \frac{\rho}{\varepsilon_r\varepsilon_o} \tag{2}$$

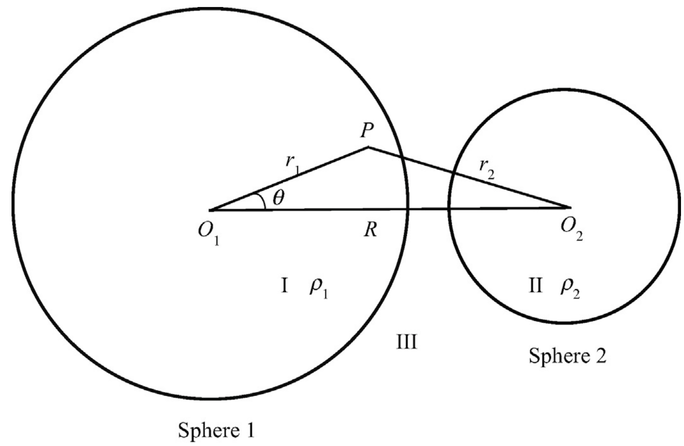

Fig. 2. Stage 1: interaction between spheres 1 and 2 before contact with each other at separation R between their centers. $R \geq a_1 + a_2$. Region I: inside sphere 1 and outside sphere 2. Region II: inside sphere 2 and outside sphere 1. Region III: outside both spheres 1 and 2. A reference point P lies in region I.

with

$$\kappa = \left(\frac{1}{\varepsilon_r \varepsilon_o kT} \sum_{i=1}^{N} z_i^2 e^2 n_i \right)^{1/2} \tag{3}$$

where κ is the Debye–Hückel parameter, ε_o is the permittivity of a vacuum, k is Boltzmann's constant, T is the absolute temperature, and ρ is the fixed-charge density in the respective regions in three stages, viz.,

(i) Stage 1: interaction before contact (Fig. 2)

$$\rho = \begin{cases} \rho_1 & \text{for region I} \\ \rho_2 & \text{for region II} \\ 0 & \text{for region III} \end{cases} \tag{4}$$

(ii) Stage 2: interpenetration (Fig. 3)

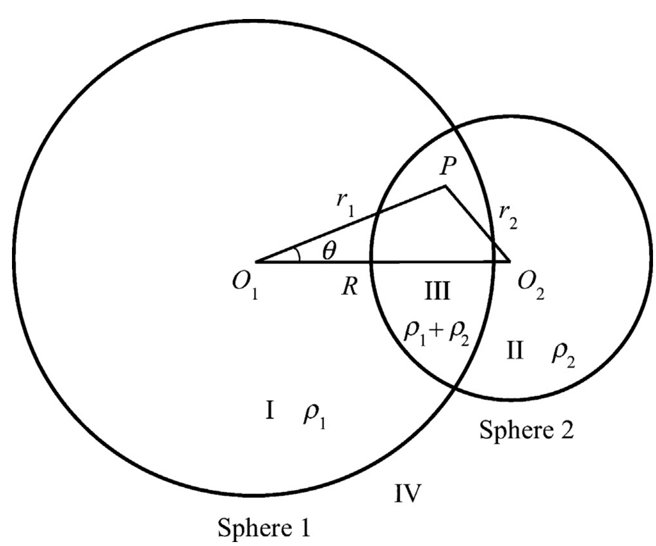

Fig. 3. Stage 2: interaction between two interpenetrating spheres 1 and 2 at separation R between their centers. $A_1 - a_2 < R < a_1 + a_2$. Region I: inside sphere 1 and outside sphere 2. Region II: inside sphere 2 and outside sphere 1. Region III: inside both spheres 1 and 2. Region IV: outside both spheres 1 and 2. A reference point P lies in region III.

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