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Modeling of the Electrical Current of the Polyaniline Microspheres

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To analyze the electrical conductivity of a polyaniline sphere, finite element analysis was conducted by COMSOL Multiphysics. A solid sphere between a probe and a planar electrode was modelled as 2D axisymmetric and the current density distribution was computed. The computed current was compared with the measured current, which yielded the conductivity of a polyaniline sphere.

Introduction

Polyaniline (PANI) is a conducting polymer whose conductivity depends on the oxidation state. The conductivity of PANI has been conventionally studied by measuring the *I-V* curves of compressed pellets of the micro- or nano structures using a standard four-probe method. To analyze the conductivity of a PANI microsphere, a 2D axisymmetric model using COMSOL Multiphysics program was constructed.

Modeling

COMSOL Multiphysics program for a finite element analysis was used to study the electric current of a solid sphere. In the experiment to measure conductivity of the PANI microsphere placed on a micro-gold electrode, a probe tip of 4 μm in diameter was used to apply a voltage potential between the tip and bottom of the sphere. Since the tip and the gold surface had very high conductance, the measured conductance was due to the PANI microsphere. In our measurement using three different diameters of spheres, the contact resistance between the probe and microsphere was negligible in comparison to the resistance of the PANI microsphere which was in the range of mega ohms (**Fig. S1**). Thus the current from the numerical model could be directly compared with the measured current of the PANI sphere.

A solid sphere between a probe and a planar electrode was modeled as 2D axisymmetric (**Fig. S2**). The probe tip of 4 μm diameter was assumed to penetrate 1 μm inside the sphere in

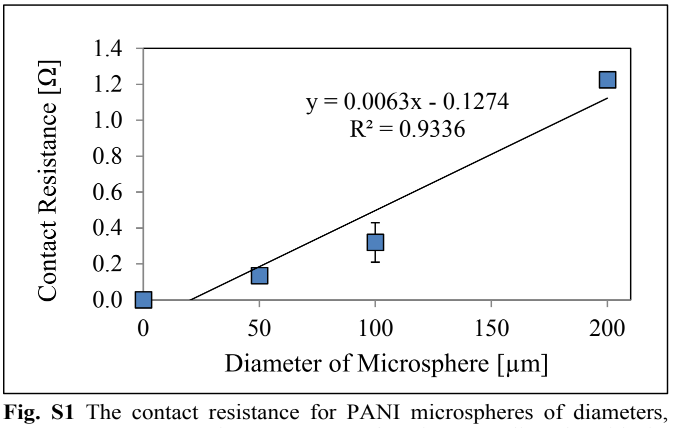

Fig. S1 The contact resistance for PANI microspheres of diameters, ~50 μm, ~100 μm and ~200 μm was found to vary linearly with the diameter of the microsphere. The contact resistance was negligible as compared to the bulk resistance of the microsphere which was in the mega ohm range.

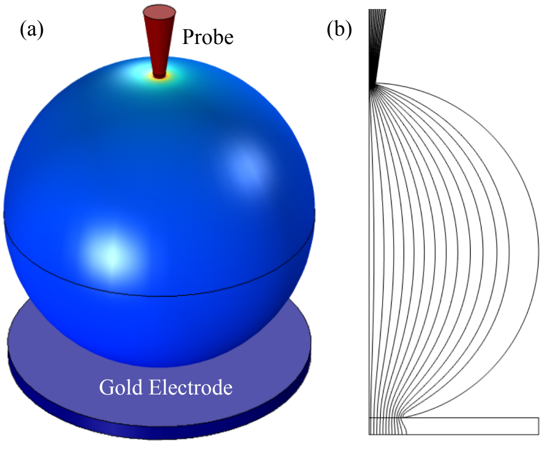

Fig. S2 (a) 2D axisymmetric model of a solid sphere (diameter: 50 μm) between a probe and a planar gold electrode. (b) Current density distribution in the sphere between the probe and the gold electrode.

the radial direction. The resulting current density distribution in the sphere due to an applied potential of 0.4 V between the probe and the gold electrode was solved by setting the potential of 0.4 V at the top of probe and the ground condition (V = 0) at the bottom of the sphere. The total current through the sphere was calculated by integrating the current density over the cross sectional area of the sphere center using trapezoidal numerical integration (Equation 1, **Fig. S3**).

$$I = \int_0^R f(r) r dr \int_0^{2\pi} d\theta \quad (1)$$

where *f(r)* is the current density extracted from the model above.
Pouillet's law (Equation 2) was used to compute the conductivity from the current.

$$\sigma = \frac{I}{V}\frac{l}{A} \quad (2)$$

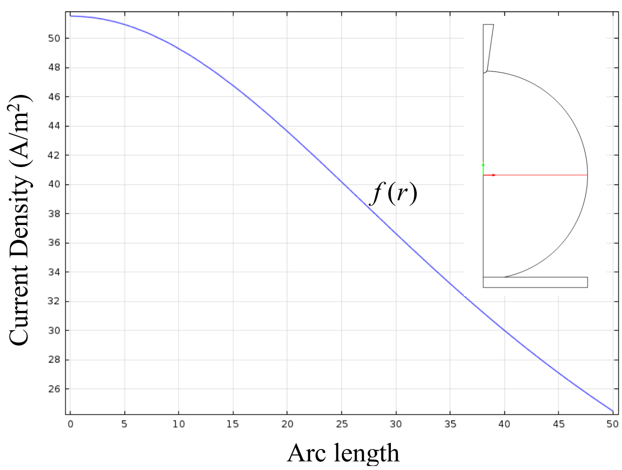

Fig. S3 Current density over the cross sectional area at the sphere center (the red line in the inset figure) was calculated.

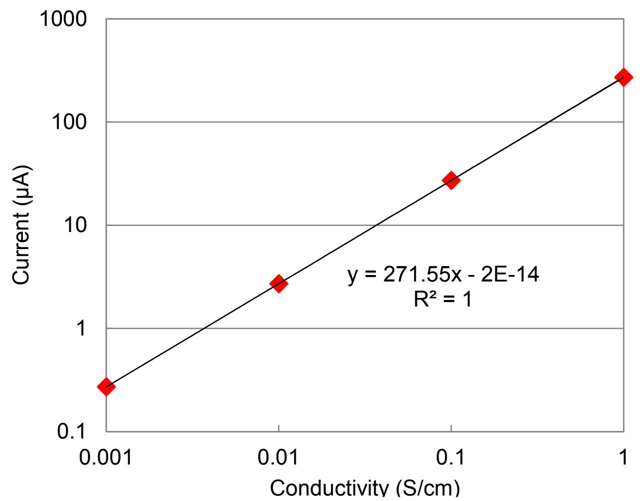

Fig.S4 There is a linear variation between the current and the conductivity values of a solid sphere.

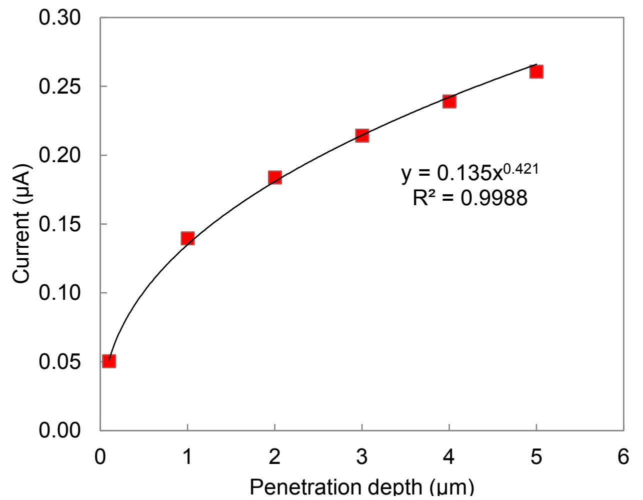

Fig.S5 The variation of current with the penetration depth of the probe inside the microsphere is shown.

Results and Discussion

The result shows the linear relation between the current through the sphere and the conductivity of sphere with the applied potential of 0.4 V (**Fig. S4**). The variation of the current with the penetration depth of the probe into the microsphere was also computed with the conductivity of 0.001 S cm^{-1} (**Fig. S5**). The current change between 1 μm and 5 μm was less than 0.2 μA, which could be neglected for the estimation of the conductivity.

Using the linear relation, the conductivity values of the PANI microspheres were predicted from the current measured at 0.4 V experimentally using the two-point probe method.

Notes and references

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