

Kinetics and isotherm studies on electrosorption of NaCl by activated carbon fiber, carbon nanotube and carbon nanotube-carbon nanofiber composite films

Yankun Zhan, Chunyang Nie, Haibo Li, Taiqiang Chen, Likun Pan*, and Zhuo Sun

Engineering Research Center for Nanophotonics & Advanced Instrument,

Ministry of Education, Department of Physics, East China Normal University, Shanghai, China 200062

Water shortage has become one of the major problems worldwide with the continuing increase of the world population. Capacitive deionization, or electrosorption, is a low-voltage (1-2 V) non-membrane water desalination technology in which charged ions are forced to move towards oppositely charged electrodes by imposing an electric field and electrode regeneration is easily accomplished by electrically discharging the electrodes [1,2]. As a key component of electrosorption device, the development and optimization of electrode materials should be the focus. In this manuscript, we characterize the structures of commercial activated carbon fiber (ACF), carbon nanotube (CNT) and home-made carbon nanotube-carbon nanofiber (CNT-CNF) films and compare their electrochemical behaviors in NaCl solutions in order to better understand the electrosorption mechanism.

The field emission scanning electron microscope image of CNT-CNF shows that in the composite film, CNF with a diameter of around 600 nm consists of core palpus and a carbon layer sheath outside and serves as the frame for the CNT growth. The CNT and CNF are entangled and form a continuous electroconducting network microstructure. From Brunauer-Emmet-Teller analysis, ACF possesses enormous surface areas and 74% of pores belongs to micropores while there are only 40% and 35% micropores in CNT and CNT-CNF films, respectively. It is known that a large amount of mesopores and macropores is beneficial to electrosorption because the overlapping effect caused by micropores can prevent ions to move towards electrode surface via pore structures and lead to a lower electrosorption capacity [3,4]. Further experiments show that the contact angles of water onto ACF, CNT and CNT-CNF electrodes are 130°, 87° and 35°, respectively, indicating that the hydrophilicity of the three electrodes has the following order: ACF<CNT<CNT-CNF. The specific capacitances of these electrodes calculated by cyclic voltammetry testing at a scan rate of 5 mV/s are 5.2, 7.4 and 25.0 F/g, respectively, following a same order.

The electrosorption behaviors of ACF, CNT and CNT-CNF electrodes are displayed in Fig. 1(a). When 1.2 V voltage is imposed, ions are driven onto the electrodes and the conductivity decreases gradually till equilibrium. The equilibrium times for ACF, CNT and CNT-CNF are 120, 60 and 30 minutes and their removal percentages are 27%, 57% and 58%, respectively. The batch experiments with different initial conductivities at 290 K are carried out and Langmuir isotherm and Freundlich isotherm are used to fit the experimental data. It is found that Langmuir isotherm fits the experimental data of CNT and CNT-CNF electrodes better, suggesting that for modeling purpose, monolayer coverage and equal activation energy during electrosorption process can be assumed, while Freundlich isotherm works well for ACF electrode, indicating a

* Corresponding author. Tel:+86 21 62234132 Fax: +86 21 62234321. E-mail: lkpan@phy.ecnu.edu.cn

multilayer sorption of NaCl. The electrosorption rate constants of NaCl onto ACF, CNT and CNT-CNF electrodes are determined by the pseudo-first-order kinetics equation, as shown in Fig. 1(b). All the experimental data are found to be in agreement with the pseudo-first-order rate law very well with regression coefficient $r^2 > 0.95$. The rate constants of ACF, CNT and CNT-CNF electrodes are 0.0232, 0.0740 and 0.1517 min^{-1} , respectively.

In conclusion, CNT-CNF exhibits a better removal percentage and faster rate for electrosorption of NaCl than ACF and CNT due to its optimal pore structure and more hydrophilic surface.

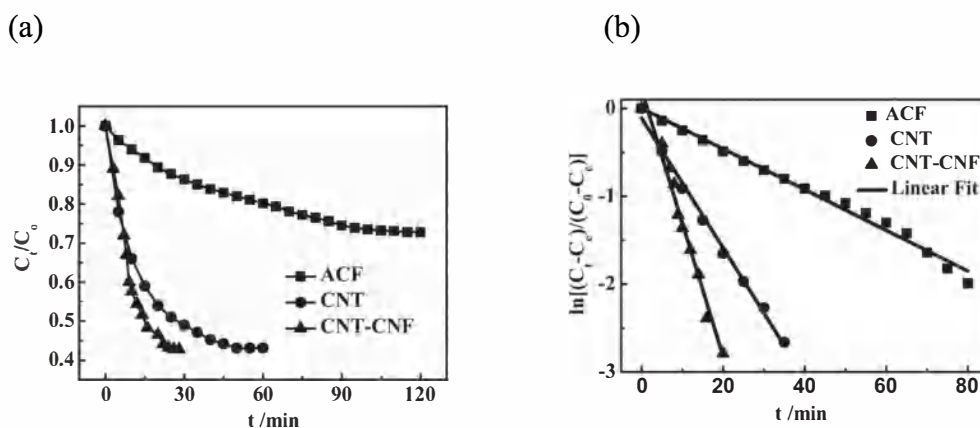


Fig.7 (a) The electrosorption of NaCl with reaction time by ACF, CNT and CNT-CNF electrodes; (b) the corresponding kinetic analysis using the pseudo first-order kinetics equation. C_0 , C_e and C_t (mg/l) are initial concentration, equilibrium concentration and the concentration at time t (min).

This work was supported by Special Project for Nanotechnology of Shanghai (No. 1052nm02700) and the Scientific Research Foundation for the Returned Overseas Chinese Scholars.

Reference

- [1] J. C. Farmer, D. V. Fix, G. V. Mack, R. W. Pekala, J. F. Poco, *J. Electrochem. Soc.* **143** 159 (1996).
- [2] K.L. Yang, T.Y. Ying, S. Yiacoumi, C. Tsouris, E. S. Vittoratos, *Langmuir* **17** 1961 (2001).
- [3] T.Y. Ying, K.L. Yang, S. Yiacoumi, C. Tsouris, *J. Colloid. Interf. Sci.* **250** 18 (2002).
- [4] M. W. Ryoo, J. H. Kim, G. Seo, *J. Colloid. Interf. Sci.* **264** 414 (2003).