Extended Abstracts of the 2004 International Conference on Solid State Devices and Materials, Tokyo, 2004, pp. 694-695

P13-12L

Model of Electrodiffusion of Metals in Fullerene Thin Films

B. P. Kafle, I. Rubinstein and E.A. Katz

Ben-Gurion University of the Negev, Dept. of Solar Energy and
Environmental Physics, Jacob Blaustein Institute for Desert Research
Sede Boker Campus, 84990, Israel
Phone: 972-8-6596793 E-mail: bpk@bgumail.bgu.ac.il

1. Introduction

Intercalation of fullerene C_{60}, by diffusion of non-alkali metals such as Au and Ag in the presence of electric field, have been experimentally demonstrated [1,2]. In this paper we propose an analytical model of metal diffusion into interstitial volume of C_{60} thin films under the action of electric bias and numerically analyze this model.

2. Theoretical model: The governing equation of our model based on mass conservation of mobile and bound charge carriers (electrons and metal ions) combined with the local electroneutrality approximation in the C_{60} thin film is

$$\frac{\partial \tilde{p}}{\partial \tilde{t}} = \frac{\partial}{\partial \tilde{x}}\left(\left(D_2 + \frac{\tilde{N} * A}{B}\right)\frac{\partial \tilde{p}}{\partial \tilde{x}} + \frac{\tilde{N} * \tilde{I}}{F \cdot \tilde{D}_m (B)}\right) \qquad (1)$$

Here,

$$D_2 = \frac{2\tilde{D}_m}{1 + \Gamma + \dfrac{\tilde{D}_m}{\tilde{D}_e}}, \quad \tilde{N}^* = \frac{\tilde{N} \cdot \tilde{D}_m}{(1+\Gamma_2)\left(1 + \Gamma + \dfrac{\tilde{D}_m}{\tilde{D}_e}\right)}$$

$$A = \left(1 - \frac{\tilde{D}_e}{\tilde{D}_m}(1+\Gamma)\right), \quad B = \tilde{p}\left(1 + \frac{\tilde{D}_e}{\tilde{D}_m}(1+\Gamma)\right) + \tilde{N}\frac{\tilde{D}_e}{\tilde{D}_m}$$

$$\tilde{p}(\tilde{x},0) = 0, \qquad \tilde{p}(0,t) = \tilde{p}(1,t) = \tilde{p}_o \qquad (2,3)$$

and $\tilde{p}$, $\tilde{N}$, Γ, $\tilde{D}_m$, $\tilde{D}_e$, $\tilde{I}$ are, respectively, concentration of mobile metal ions, concentration of intrinsic fixed positive charges (equal to the electrons in the conduction band), binding coefficient of metal ions, diffusivity of metal ions, diffusivity of electrons in C_{60} film and electric current, specified in the galvanostatic regime of operation.

3 Results:

The initial-boundary value problem (1)-(3) was solved numerically by an explicit finite difference method.
In Fig. 1-3 we present the numerically calculated concentration profiles of the metal ions in the 1 mm thick C_{60} film for different times at different electric current. We point out that the symmetry of these profiles (Fig. 1) typically for zero current is distorted as application of the electric current (Fig. 2). Moreover, from the Fig. 3, one notices monotonic increase in metal ions concentration, with time, at any position in the C_{60} film at constant electric current. On the other hand, in agreement with experimental observations [1-2] the numerical solution predicts a significant modification of the diffusion profiles and considerable speeding up of the metal ions penetration into C_{60} film by the electric current. Thus, the asymmetry of the dopant concentration profiles (Fig. 2-3) in C_{60} may be viewed as a measure of electrodiffusion in C_{60} films.
In conclusion, a considerable speeding up of the metal ions penetration into C_{60} film by the electric current is predicted.

Acknowledgement:
B. Kafle wishes to thank the Albert Katz Int. School for Desert Research and Bonna Terra foundation for financial support in this research.

References:

1. L. Firlej, A. Zahab, F. Brocard and N. Kirova, Phys. Rev. B **59** (1999) 16028.
2. E.A. Katz, D. Faiman, S.M. Tuladhar, S. Stutina, N. Froumin, M. Polak, Y. Strzhemenchny, *Sol. Energy mater.& Sol. Cells* ***75 (2003) 421.***

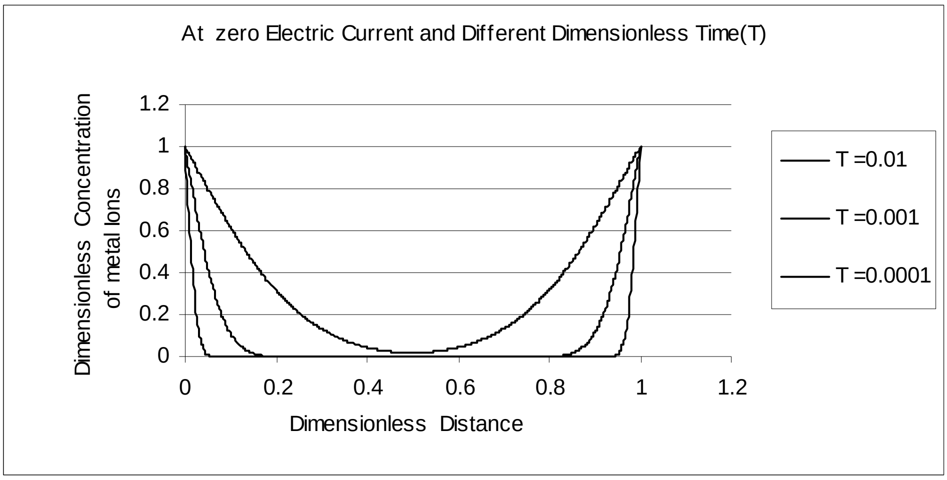

Fig. 1 Diffusion profiles of metal ions in C_{60} thin film at 150 °C without presence of the electric Current between the electrodes at dimensionless time 0.0001, 0.001, and 0.01, corresponding to a, b, and c respectively.

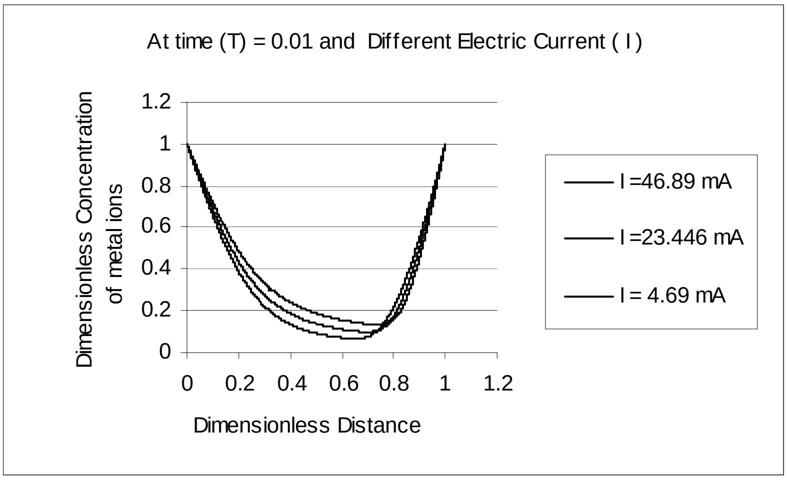

Fig. 2 Diffusion profiles of metal ions in C_{60} thin film at 150 °C at different electric current Values equal to 4.69, 23.46, and 46.89 mA, at constant dimensionless time equal to 0.01, as represented by a, b, and c respectively.

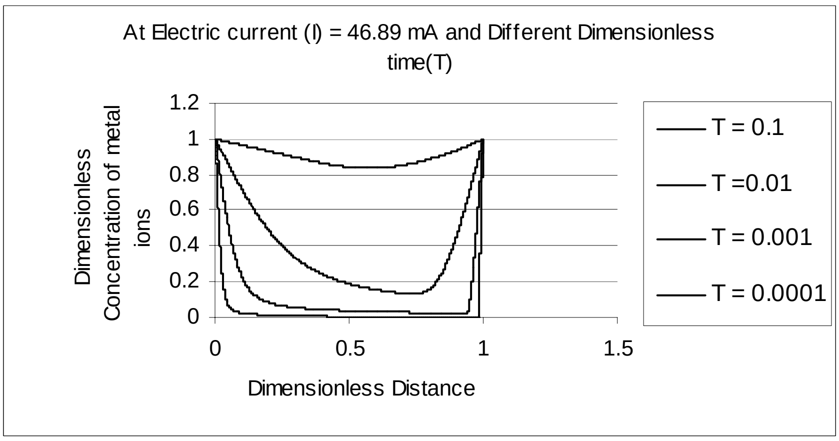

Fig. .3. Diffusion profiles of metal ions in C_{60} thin film at 150 °C at constant applied electric current between the electrodes (I = 46.89 mA) at different dimensionless time 0.0001, 0.001, 0.01, and 0.1 (a, b, and c and d respectively).