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Charge localization effects and transport in dendritic nanostructures for photovoltaic applications

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ABSTRACT

Charge localization effects and transport properties in dendritic interfaces are investigated in the framework of a coherent scattering formalism. Due to the large surface area, tree shaped interfaces enhance the overall efficiency of bulk heterojunction photovoltaic applications. The charge localization effects are analyzed for different tree shapes, band offset potentials and in the context of varying the thickness of the tree branches. Two types of localization are pointed out – on the tree branches or inbetween. The transfer characteristics are influenced by the band offsets and the energy of the charged particles. A detailed statistical analysis shows the correlation between the average transmission function and the surface area of the dendritic interface. The current study provides a framework for the characterization and optimization of dendritic interfaces.

1. Introduction

Dendritic nanostructures are promising candidates for a variety of applications, such as the next-generation electrocatalysts [1], photovoltaic cells [2–4], supercapacitors [5] or sensing devices [6,7]. Metallic nanostructures of this kind are also used as surface enhancement Raman scattering (SERS) active surfaces, for which new techniques based on thermal annealing have been recently developed [8]. Other examples include hierarchical dendritic gold nanostructures [9] prepared by electrochemical techniques, silver nanofractals [10] which exhibit thermally induced morphological transitions or mixed Au/Ag bimetallic dendrites produced by AC electrodeposition method [11]. In addition, during the past few years controllable growth of dendritic nanowire arrays has been achieved [12–14].

Bulk heterojunction (BHJ) solar cells are promising options for low cost and highly scalable renewable energy [15]. The morphology of the active layer is essential to attain a high power conversion efficiency and the investigation of these complex material systems requires specialized characterization techniques [16]. Recent theoretical investigations of BHJ organic solar cells employ the Monte Carlo approach [17] for identifying the optimal surface area and provide closed-form expression for exciton transport and carrier generation [18].

In BHJ photovoltaic applications a large surface area is necessary for efficient carrier generation and nanostructured interfaces also provide an enhanced light-harvesting efficiency. Ideally, BHJs are made by creating interpenetrating, connected networks of the donor and the acceptor components, which ensure the carriers' free paths to the electrodes. However in practice it is quite challenging to produce perfectly aligned interdigitating fingers made of the two materials. At the same time, the structures must ensure efficient charge collection and transfer to the electrodes, which may be impeded by enhanced scattering at the nanostructured interface. Therefore, from these two perspectives, the tree shaped interfaces are subject to optimizations.

In this paper we aim to characterize different types of dendritic interfaces (DIs), from the point of view of charge localization and coherent transport, focusing on the optimization of the interface for photovoltaic applications. We construct the tree structures using the diffusion limited aggregation (DLA) process, which was introduced by Witten and Sander [19]. This model is suitable for simulating electrodeposition processes and it is quite versatile in reproducing different growth conditions [8]. Next, we investigate the charge localization in different types of structures using a coherent scattering formalism, based on the R-matrix method [20–25]. This analysis provides the charge transfer characteristics through the DIs, emphasizing the correlation between scattering and the shape and the surface area of the DI.

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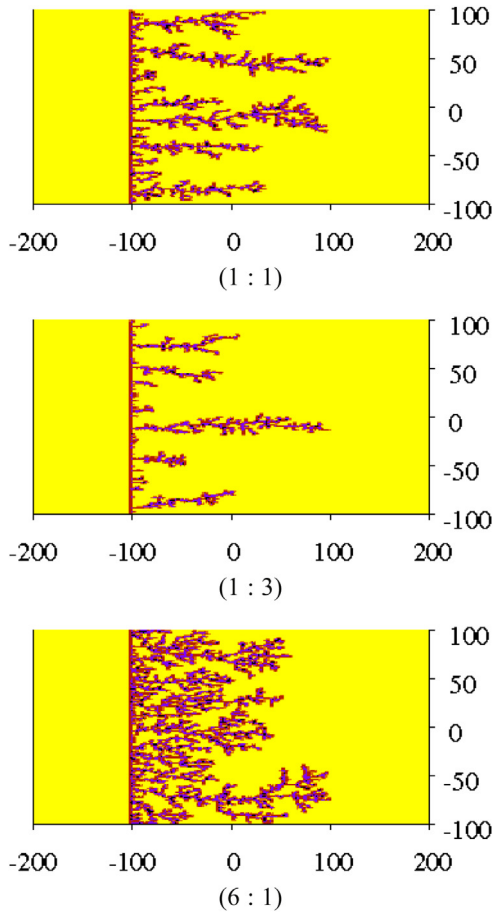

Fig. 1. Dendritic interfaces constructed by three different values of step probabilities ($p_x : p_y$) in the DLA process: normal (1:1), rarefied (1:3) and dense (6:1) trees. The half lengths of the scattering region are $L_x = 200$ nm and $L_y = 100$ nm.

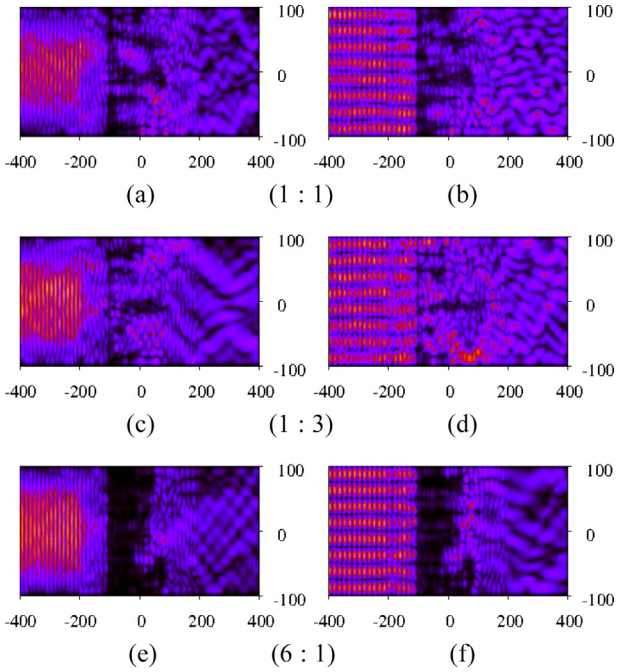

Fig. 2. Localization of the charge density for the three types of dendritic interfaces: normal (1:1), rarefied (1:3) and dense (6:1) trees, as indicated in Fig. 1, with the band offsets $V_{L/R} = V_{1,2} = 0$ and $V_t = -0.5$ eV. The 1st (a, c, and e) and 8th (b, d, and f) incident transversal modes correspond to particles incoming from the left hand side of the nanoribbon, with the total energy $E = 30$ meV.

The paper is organized as follows. In the next section we describe in detail the method used to construct the tree structures by DLA type processes and the R-matrix method employed to obtain the scattering wavefunctions. In the following section, we present the results obtained for the different tree structures, pointing out the differences in charge localization which occur by changing the band offset potentials and the width of the tree branches. Furthermore, a detailed statistical analysis shows the dependence of the transmission coefficient on the type and surface area of the interface, which allows the optimization of the DIs.

2. Methods

In the following we present the method employed to construct the dendritic interfaces and subsequently we describe the scattering formalism used for the analysis of charge localization effects and transport phenomena.

The dendritic interface is modeled by the (DLA) process, which is a diffusion based model, where the particles are moving in random directions until they reach a pre-formed cluster of particles. At this point they stick to the existent cluster. We consider a two-dimensional model, where the seed cluster is a straight line and the source of the particles is distributed on a parallel line. The resulting structures are Brownian trees, depicted in Fig. 1. The movement of the particles is restricted to the four directions $-x$, x, $-y$, y. The investigated structure is a nanoribbon type system, with the dendritic interface contained in a rectangular region, which has hardwall boundary conditions perpendicular to the seed cluster line. By employing an anisotropic random walk, different shapes of trees are produced. This is achieved by adjusting the relative step probabilities in the x and y directions, i.e. the ratio p_x/p_y. We consider equal probabilities in the $-x$ and x directions and similarly for the y direction. The tree shaped structures are labeled in the following as ($p_x : p_y$). A similar approach can be used to obtain three dimensional (3D) structures.

The charge localization effects and transport through the dendritic interface are characterized within a coherent scattering formalism, based on the R-matrix method, which is described in detail in Refs. [20–24]. This quantum transport model allows an efficient computation of the transmission functions for a wide range of energies and arbitrary scattering potentials. We consider a uniform confinement potential along the nanoribbon structure with vanishing wavefunction conditions at the edges. The system is partitioned into leads, which are invariant along the transport direction and active region which contains the DI. In our calculations we use material parameters as in GaAs/Al_xGa_{1-x}As heterostructures, like typical band offsets and effective mass $m^* = 0.0655 m_0$. We denote the band offsets in each region by $V_{L/R}$ for the left and right lead, respectively, V_t for the tree region and $V_{1,2}$ for the regions to the left and to the right of the DI, inside the scattering region, defined by the half lengths L_x and L_y. Using this approach based on the scattering formalism we are able to characterize the DIs in open quantum system calculations.

3. Results

We start by investigating the localization effects for three DIs, namely for the normal (1:1), rarefied (1:3) and dense (6:1) tree structures. The charge density maps obtained from the scattering wavefunctions are depicted in Fig. 2, for the 1st and the 8th incident transversal modes. The particles are incoming from the left hand side of the nanoribbon. The DIs partly reflect the incoming wavefunctions, producing quasi-stationary waves at the left end of the nanoribbon, while at the right end the wavefunctions are a

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