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Multiscale design and optimization of polymer-based photonic crystals for solar shielding

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ABSTRACT

Protecting from solar radiation remains a very stimulating field of research and development. Improvement of performances of UV/IR radiation shielding devices is thus constantly pursued. With increase of computer strength and code efficiency, simulation becomes a real asset in this investigation. In this study, we report an efficient multiscale simulation protocol to design and optimize such photonic devices based on polymers. The simulation approach combines atomistic-level techniques, i.e. classical molecular mechanics, and linear scaling-DFT in order to get full description of the optical properties of polymers over a large wavelength range. At each step of the procedure, validation with experimental data is carried out, confirming the accuracy of the approach. The resulting optical constants enable designing of a multilayer photonic heterostructure purposely optimized for UV/NIR-radiations protection. The ensuing simulated device reveals very promising optical performance. It exhibits a transparency higher than 90% in the visible range and shows high UV absorptance. Moreover, a strong NIR-shielding ability of 96% is achieved.

1. Introduction

Solar shielding materials and devices are highly attractive for different applications such as contact lenses, heat mirrors and thermal insulators in automobiles and buildings. The shielding of solar radiation prevents the increase of temperature inside automotive cabins, improves the comfort of passengers and reduces the use of air conditioning [1,2]. For this purpose, significant efforts have been made to investigate different thin film materials with excellent transparency and a strong IR-shielding ability, such as rare-earth hexaborides, titanium nitride (TiN), tin-doped indium oxides (ITOs), antimony-doped tin oxides (ATOs), metal-doped tungsten oxides (M_xWO_3) and vanadium dioxide (VO_2) [3–8]. In most cases, doped transparent-conductive oxides (TCOs) were used as thin film coatings owing to their interesting optical properties. However, their fabrication involves expensive deposition techniques such as chemical vapor deposition and magnetron sputtering, and also requires high-temperature/vacuum post-treatment which is energy-consuming. In addition, TCO coatings can shield radio waves and affect cellular phone reception within vehicles. To overcome these drawbacks, Liu et al. proposed to use polymer-ITO nanocomposites to allow radio wave permeability while maintaining strong IR-shielding ability [9]. Thanks to their high physical performances such as lightweight, flexibility, good mechanical strength, durability, low processing temperature and low production cost, polymeric materials are interesting candidates to address these issues [10]. Moreover, their high processability in different shapes such as thin films, or fibers is definitively an additional asset. Their ability to combine with other polymers (polymer blend), to be mixed with specific fillers, and to be functionalized are also stimulating properties [11]. Among the huge number of existing polymers, transparent ones are natural candidates to be used in developing optical devices. However, additional constraints must be put forward such as refractive indices between 1.70 and 1.30 [12], low thermal stability and stress birefringence [13]. A specific strategy to design and optimize polymer-based optical devices with high transparency and high NIR reflectivity is thus required. In this study, we propose a very efficient multiscale simulation approach to address this important issue.

The simulation approach combines two atomistic-level techniques [14], i.e. classical molecular mechanics (MM) and quantum mechanics (QM) in order to get optimal description of the optical properties of

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polymers over a large wavelength range (UV–visible-IR). The ensuing data are implemented in a photonic heterostructure device whose design has been optimized to tackle the aforementioned purpose. This photonic heterostructure consists of a combination of two chirped one-dimensional photonic crystals (1D PhCs), i.e. multilayer stacks made from alternating high and low refractive index polymers and possessing a linear thickness distribution. Such a device makes available the ultimate control of light propagation through the photonic structures according to the desired application [15]. The theoretical methods and computational aspects that intervene along the simulation process are first described. The ensuing results are then discussed and analyzed to optimize the optical device.

2. Methodology

The simplest case of a photonic crystal (PhC) is the Bragg mirror where alternating layers of high and low refractive index materials are organized in a one-dimensional periodic stack. In this study, those materials are amorphous transparent polymers, leading to polymeric 1D PhCs [16]. To get the optimal device, we took advantage of simulation. It first needs two suitable optical polymers with very different refractive index, that will constitute the layers of the 1D PhC. Eight candidates have been chosen to sample suitably polymers with refractive index between 1.70 and 1.30. From the higher (1.6037) to lower (1.3696), these are: Polystyrene (PS), Poly (acrylic acid) (PAA), Poly (2-hydroxyethyl methacrylate) (PHEMA), Poly (methyl methacrylate) (PMMA), Poly (methyl acrylate) (PMA), Poly (methacrylic acid) (PMAA), Poly[perfluoro (4-vinyloxy-1-butene)] (cyclic transparent optical polymer or Cytop) and Poly (4,5-difluoro-2,2-bis(trifluoromethyl)-1,3-dioxole-*co*-tetrafluoroethylene) (Teflon AF 2400) amorphous fluoropolymer. The chemical structures of their repeat unit are displayed in Fig. 1.

To better grasp the approach developed in this work, the whole protocol is summarized in the form of a workflow, and shown in Fig. 2: it starts with MM/QM atomistic-scale calculations, followed by simulation at device-scale of the PhC heterostructure. These steps are developed further in subsequent paragraphs.

2.1. Atomistic-scale description of polymer materials

At the atomistic scale, molecular mechanics approach makes available the depiction of the infrared region of molecular system thanks to a good description of the vibrational normal modes [17–19]. Besides, calculation methods based on quantum level first-principles, as the density functional theory (DFT) approach [20,21] are well documented as a versatile and powerful tool to disclose electronic absorption occurring in UV–visible region. However, the latter methods are computationally time demanding, especially for systems containing a great number of atoms, as for polymers. To circumvent this drawback, the methodology using the linear-scaling (LS) formulation of DFT is a very efficient alternative. It is thus employed in this study [22].

2.1.1. Simulation and optimization of the amorphous polymers structures

Amorphous polymer structures are first to be prepared. A crucial point in simulation is the appropriate depiction of the configurational space to properly represent the systems under study [23]. For this purpose, we used a procedure that has shown its efficiency in computing the glass transition temperature of polymers [23–25]. It is herein outlined. Interactions are described by a class II force field. The choice of this category of force field is important since it uses anharmonic and cross-coupling terms to better represent the potential energy surface (PES) obtained from *ab initio* calculations [26], hence leading to efficient description of the vibrational normal modes [27]. Moreover, based on previous validation studies, we chose the PCFF force field (Polymer Consistent Force Field) derived from the CFF [18,19,28,29]. This force field is described in the literature [18,26,30]. The Amorphous_Cell© module from Accelrys Materials Studio [31] was then considered to generate 100 amorphous polymer systems consisting of cubic cells with imposed periodic boundary conditions. The chain generation procedure is based on the self–avoiding walk algorithm adapted by Theodorou and Suter [32], and combined with the Meirovitch's scanning method [33]. Each configuration contains a single chain of 100 repeat units. From the whole set of configurations, ten configurations are then selected according to two criteria. The first criterion is related to the occupancy of the cell: the computed radius of gyration of the selected configurations must be around the maximum value [24]. The second criterion is purely energetic: configurations with the highest energy are discarded.

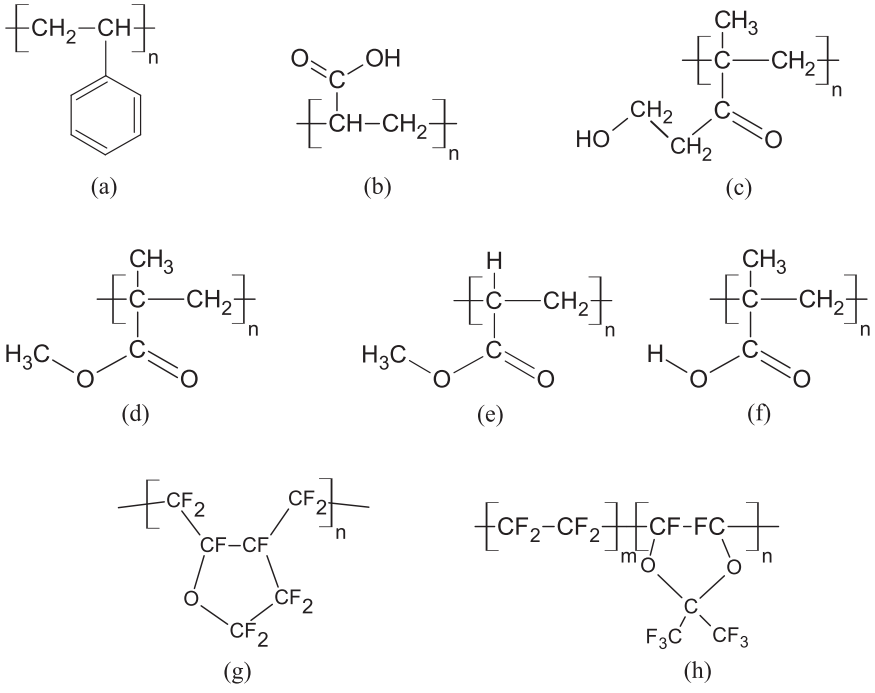

Fig. 1. Chemical structure of monomer repeat units of the chosen amorphous polymers, (a) PS, (b) PAA, (c) PHEMA, (d) PMMA, (e) PMA, (f) PMAA, (g) Cytop, (h) Teflon-AF 2400.