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Theoretical study of electronic transport through quasicrystalline nanotubes using mesh inflation approach

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ABSTRACT

This work introduces the mesh inflation method to construct (dodecagonal) quasicrystalline shell structures, and investigates the properties and functions of quantum transport through quasiperiodic components, e.g. the nanotube device. We model the quantum dynamics of a system described by a nearest neighbor tight-binding formulism, and apply the non-equilibrium Green's function technique to calculate the electronic transport properties, in which the non-equilibrium (transmitted) electronic density is self-consistently determined by solving Poisson's equation in capacitive network modeling. Numerical results find that the transmission spectrum of the quasicrystalline nanotube illustrates crossover characteristics from local order (like in periodic lattices) to global disorder (like in amorphous solids) with varying energy. Moreover, the electronic transport properties of nanoprobes through multiple atomic channels follow the rule of Landauer's formula.

1. Introduction

Considerable efforts have recently been dedicated to the fabrication of quasicrystals, including metallic alloys [1], mesoporous silica [2], dendritic liquid crystals [3], ABC-star polymers [4], colloids [5] and inorganic nanoparticles [6], in which the lack of translational symmetry is compensated by rotational symmetries not achievable by conventional periodic crystals, hence generating exciting questions and applications. The literature shows that the formation of quasicrystals should obey either energy-driven [7,8] or entropy-driven [9,10] "special" growth rules and have direct influences on their physical properties and thermodynamic stability [11]. In particular, quasicrystalline surfaces from metallic alloys (a few angstroms in scale) exhibit unusual surface properties, e.g. low friction, low adhesion, good oxidation resistance, and promising catalytic attributes [12], rendering them good candidates for coating (or composite) applications and for the study of interface mechanisms. As a result, the properties and functions of the quasicrystalline surface (or shell [13,14]) morphology through a quantum size effect can be further investigated. In this work we mainly study the tubular configuration [15] which presents unique electronic properties due to the surface curvature, quasiperiodicity, and the quasi-one-dimensional formation (large length-to-diameter ratio).

To realize quasiperiodic configurations, most previous works construct quasicrystals using the formal multi-grid method [16]. Other works obtain the quasicrystalline structure by an irrational cut of hyper-lattices (periodic lattices in a higher dimension than that of the physical space) [16–18] or by the iterative inflation approach [19,20] in rigid Cartesian dimensions. Caspar and Klug [13,14] proposed a geometrical scheme to generate the construction of icosahedral shells for spherical virus capsids. Our work introduces the mesh inflation method to establish the quasicrystalline shell structures, and investigates the properties and functions of quantum transport through quasiperiodic components, i.e. nanotube and nanoprobe devices. This method proceeds with the mesh generation and geometry processing for objects and continues with the inflation rule [19,20] on the mesh tiles to obtain the quasicrystal structures.

To study quantum dynamics, we adopt a nearest-neighbor tight-binding model for describing the system Hamiltonian, which allows the treatment of systems comprising a large number of atoms. The implementation of the non-equilibrium Green's function technique within the tight-binding framework [21,22] enables us to perform computations of the electronic transport properties. The transmitted electronic density (obtained by the non-equilibrium Green's function) and the Hartree potential (needed for the tight-binding Hamiltonian) are self-consistently determined by solving Poisson's equation with open-boundary

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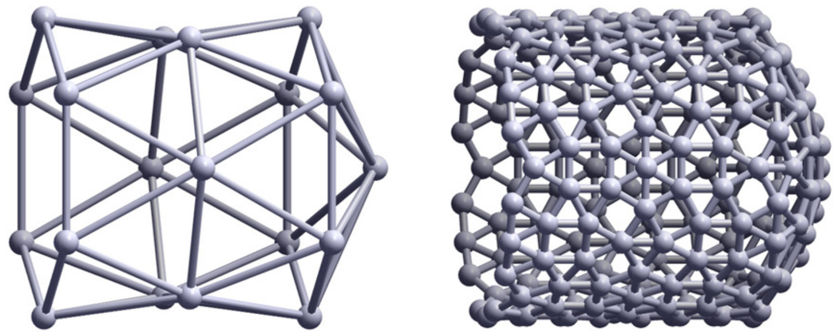

Fig. 1. (Left plot) Equilateral triangle mesh for the nanoprobe and (right plot) the schematic quasicrystalline nanoprobe by the inflation rule.

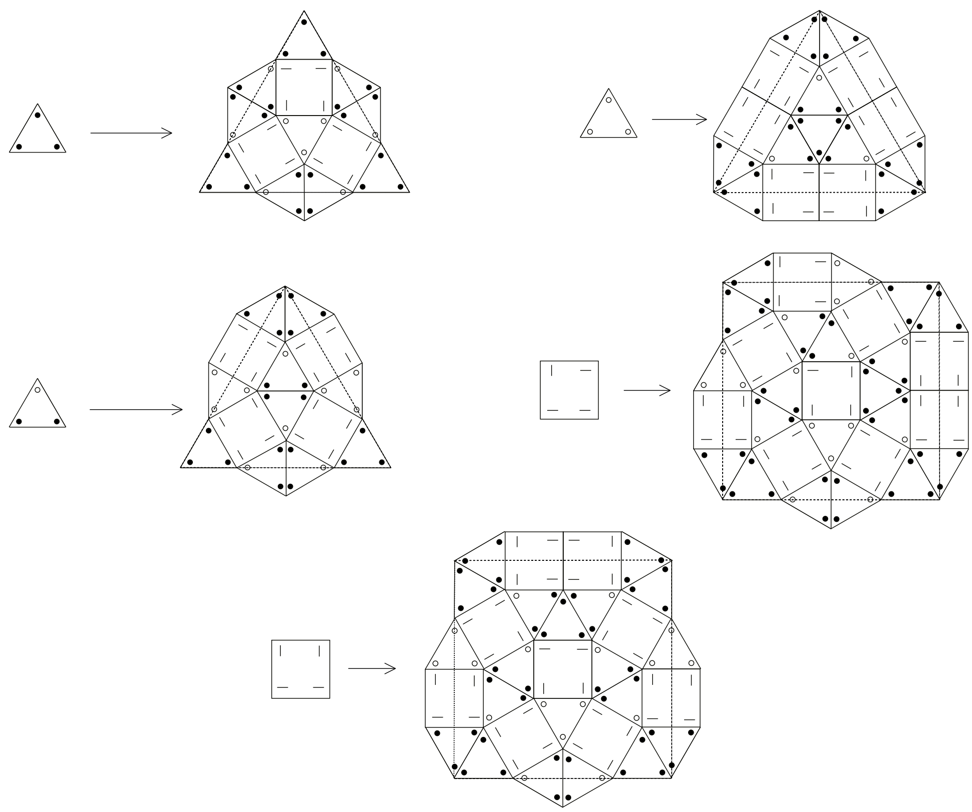

Fig. 2. Inflation rule by Schlottmann for dodecagonal tilings.

conditions naturally encountered in transport problems. In this work, Poisson's equation is solved efficiently in terms of the capacitive network model [23,24] to take into account the multiscale considerations.

This present article is organized as follows. Section 2 describes the mesh inflation method, and illustrates the quasicrystalline geometry of the nanoprobe for the following study. Section 3 formulates Green's function technique for non-equilibrium transport. This section also reports the self-consistent solution with the capacitive circuit model. Section 4 is devoted to numerical analyses. Section 5 contains the main conclusions.

2. The mesh inflation method

This section introduces the mesh inflation method to construct the arrangement of atoms conforming with quasicrystalline criterions on curved surfaces or closed shells. We first apply the Delaunay triangulation technique, e.g. by SurfRemesh [25], to mesh surfaces with the (approximate) equilateral triangle that has a bounded aspect ratio. The operation is based on the principle of finding points on a given surface until the topology and geometry of a desired surface pattern are nearly recovered and then meshing them with Delaunay triangles restricted to the surface. It hence maintains the topology and approximates the geometry of the original surface. The assumption about the input surface is that it actually approximates a smooth surface both point-wise and normal(vector)-wise. This means that if the given surface has a very sharp edge (dihedral angle less than 90 °), then the algorithm may not work. One example for a segment of a nanoprobe with an equilateral triangle mesh is shown in Fig. 1 (left plot).

A dodecagonal tiling composed of squares and triangles now can be produced by the inflation rule proposed by Schlottmann [19,26] (see Fig. 2), which includes a set of prototiles T_i, an inflation factor λ, and a rule regarding how to replace the enlarged prototiles λT_i with congruent copies of the prototiles. We start with the triangle tilings obtained by the above mesh generation and geometry processing, and decorate them by squares and triangles (Fig. 2), which are smaller by a factor $\lambda = (2+\sqrt{3})$, to make a new tiling of the smaller squares and triangles. We then rescale these to the original size, and continue the process iteratively. Thus, the