PO3072

3D kinetic Monte-Carlo modeling of random metallic network: optical and electrical characterizations

Jérôme Müller, Stéphane Lucas

University of Namur, Namur, Belgium

jerome.muller@unamur.be

Conductive transparent devices have numerous applications today, such as transparent electrodes (like front-side electrodes of solar cells), thin-film heaters… Many recent technologies related to this research field can provide those characteristics: transparent conducting oxides, metallic nanowires or carbon nano-tubes for example.
Our work focuses on the numerical modeling of random metallic networks obtained by atomistic deposition of silver or aluminum on a substrate (glass, TCO…). An optical and electrical characterization of such structures is done to optimize its transparency in the direction normal to the substrate and its electrical conductivity in the lateral and/or the normal direction. The modeling of the network is done thanks to the Nascam software, which is based on a 3D kinetic Monte-Carlo method. Then the reflectance and the transmittance are computed by using the effective medium theory based on the Maxwell-Garnett and Bruggeman models. The effective electrical conductivity of the network is also estimated by solving the Maxwell-Faraday equation by finite-element analysis. The investigated parameters are the average thickness of the metallic network, the substrate coverage, the energy of deposited atoms and the influence of the roughness/nanostructuration of the substrate surface.
We show that the deposition of high-energy metallic atoms on a flat substrate is needed to obtain a significant electrical conductivity of the network without increasing too much the average thickness, and then the reflectance. Indeed, a low-energy atomic deposition can induce the formation of islands not connected electrically. However, the structuration of the substrate allows to decrease the energy of deposited atoms while avoiding the apparition of such islands.

Keywords
kinetic Monte-Carlo modeling
metallic network
transparent conductive thin-film