Impact of Geometric and Material Variability on Electromagnetic Wave Guidance Characteristics of Arrays of Nanoparticles

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Arrays of nanoparticles are employed in the design of metamaterial structures, nanocircuits, nanoantennas, among others. Most commonly, the modeling of such devices is usually done assuming a perfect periodicity of the array. In reality, however, the manufacturing process yields a disordered pattern of particles due to variability in particle size, placement, and electrical properties. In view of this, we are interested in quantifying the impact of such disorder on the electromagnetic behavior of structures composed by such arrays of nanospheres. The investigation of the impact of disorder has been presented in the literature for the case of a periodic chain of nanoparticles using a simple dipole model approximation (F. Rüting. Physical Review B, vol. 83, no. 11, 2011). In addition, Alù and Engheta have presented an analytical approach to account for cases of small disorder for such nanoparticle chains; however, the presence of a supporting substrate is not considered in their physical model (A. Alù and N. Engheta, New Journal of Physics, vol. 12, no. 1, 2010).

In the present work, we adopt a rigorous full-wave approach to characterize the impact of such disorder. As such, no small-disorder approximation needs to be made. Furthermore, in contrast to previous modeling approaches, no independence is assumed of the random variables that quantify the disorder in the periodic chain. Instead, a more realistic model is considered by taking into account the correlation of the random variables of the disordered spheres. Such correlation depends on a variety of factors, among which the proximity between spheres stands out as an important one.

Our statistical modeling makes use of a sampling methodology based on the Smolyak algorithm and ideas from the high-dimensional model representation (HDMR) (X. Ma and N. Zabaras. J. Comp. Physics, vol. 229, no. 10, pp. 3884-3915, 2010). First, a principal component analysis is performed to reduce the random space that quantifies the disorder in the finite-length array of particles; thus, the statistical simulation is done more efficiently. Next, HDMR is employed to extract the statistics of the wave propagation attributes of the structure, while the number of iterations is minimized. A series of numerical studies are used to both contrast the proposed methodology to previous ones for the case of infinite periodic chains, and also examine the range(s) of validity of the assumption of small disorder and the modeling simplifications resulting from it for accurate prediction of the electromagnetic behavior of the disordered nanoparticle chain.