Augmented coupling interface method for computing frequency band of nanostructure

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Abstract

Due to the advance of processing technology, it is now possible to produce many new composite materials at nanoscale. Understanding their mechanical and optical properties is very important in applications. This in turn can be studied through the help of the frequency band structure of these composite material. By assuming the nanostructure of these materials is periodic and using the Bloch theory, the problem is reduced to just one period with two materials separated by an interface. For metal-dielectric composite material, the corresponding problem is a nonlinear eigenvalue problem because the dielectric coefficient of the metal depends on the eigenvalue (i.e. the frequency). The governing partial differential equation (the Maxwell equation) changes type. In fact, the dielectric coefficients change sign with several order of difference in magnitude across the metal-dielectric interface, sometimes the dielectric coefficient may even become complex-valued. Further, the electromagnetic field changes rapidly near the interface. These physical complexity creates computational difficult. In this talk, I will present an augmented coupling interface method to compute metal-dielectric composite material with periodic nano structure. The main ingredients of this method contains (i) an introduction of an additional quantity to reduce this nonlinear eigenvalue problem to a quadratic eigenvalue problem where a standard technique can be applied, (ii) an augmented coupling interface method, where the above new variable is discretized uniformly on the interface, the rest of variables are discretized on an underlying rectangular grid. A proper interpolation between these two grids are designed to reduce the number of stencil point. The method is second order. Frequency band structure for metal-dielectric material will be demonstrated.

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