Accurate Homogenization of Layered Structures and a Breakdown of Effective Medium Theory

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In recent years, a curious "breakdown of effective-medium theory" has been theoretically predicted and experimentally observed in layered media (Sheinfux *et al.*, Phys. Rev. Lett. 113, 243901, 2014; Zhukovsky *et al.*, Phys. Rev. Lett. 115, 177402, 2015; Lei *et al.*, Phys. Rev. B 96, 035439, 2017). This effect is particularly pronounced in the vicinity of the critical angle of incidence, where the standard quasi-static effective tensors may produce inaccurate and inconsistent results for the reflection (R) and transmission (T) coefficients, even though the thickness of the layers and even the thickness of the whole structure (Zhukovsky *et al.*) may be much smaller than the vacuum wavelength.

Also in recent years, we have developed a local and nonlocal homogenization theory applicable to any reasonable size and composition of a periodic lattice cell (Tsukerman & Markel, Proc Royal Soc A 470, 2014.0245 & Phys. Rev. B 93, 024418, 2016; Tsukerman, Phys Lett A 381, 1635–1640, 2017). Central in the procedure are the fine-scale and coarse-scale basis sets approximating the fields; these are Bloch waves and the corresponding generalized plane waves. Depending on the choice of these bases, the homogenization procedure can produce effective parameters valid for a broad range of illumination conditions or, alternatively, tailored to a subset of these conditions; there is usually a trade-off between the accuracy of homogenization and its range of applicability. An automatic general outcome of the procedure is an effective tensor containing, in addition to the permittivity and permeability entries, magnetoelectric coupling terms.

It is from the perspective of our general homogenization theory that we revisit the "effective-medium breakdown". We use the examples by Sheinfux *et al.* and Zhukovsky *et al.* as our case studies and pay particular attention to the role of magnetoelectric coupling and to the dependence of the effective material tensor on the range of illumination conditions chosen – that is, either a broad range of the angles of incidence or, alternatively, a narrow range around the critical angle. We also show that nonlocal homogenization improves the accuracy of homogenization (as measured by the RT errors) by at least an order of magnitude in typical cases.