Comment on "Existence of a Photonic Gap in Periodic Dielectric Structures"

Indisputably, one of the hallmarks in the study of photonic band gap structures is an article by Ho, Chan, and Soukoulis [1]. It opened a way for the fabrication of the first photonic structure with a complete photonic band gap (CPBG) [2] and advanced the field considerably. One of its main conclusions is that, regarding a CPBG, the diamond structure fares much better than a simple face-centered-cubic (fcc) one: (i) the threshold value of the dielectric contrast ε to open a CPBG is 4 (8.2 for an fcc structure [3]), (ii) a CPBG opens between the 2nd and 3rd bands (the 8th-9th bands for an fcc structure), and, consequently, is much more stable against disorder, and (iii) a CPBG is significantly larger (15% and 5%, for the respective diamond and fcc closed packed lattice of spheres with a dielectric contrast $\varepsilon = 12.96$).

Recently, motivated by advances in the fabrication of colloidal crystal structures of spheres with a complex unit cell, I have recalculated the photonic bandstructure of a diamond lattice for a sphere filling fraction f varying from 0 till the close-packed case $f_{cp} = 0.34$ and for $\varepsilon \in (1, 25]$. In agreement with Ref. [1], in this range of f, there is no CPBG for the case of air spheres in a dielectric. (The case of overlapping air spheres with high f is not considered here.) Surprisingly, in the reciprocal case of dielectric spheres in air, quantitatively different results from earlier calculations were found (although, qualitatively, regarding band degeneracies and splitting differences are minute) (see Figs. 1, 2), with potentially important consequences for photonic structures made from colloids. The results are compared against an fcc lattice of air spheres in a dielectric [3]. A diamond lattice can have simultaneously two CPBG, that between the 2nd-3rd bands, and, as in an fcc case, between the 8th-9th bands. Regarding a CPBG, a diamond lattice fares still better than an fcc lattice. However, the lower CPBG is, in the range of parameters considered, not the dominant one (see Fig. 2). For its optimal $f = f_{cp}$ it does not exceed 2.3% (for $\varepsilon = 9$), only persists for $\varepsilon \in [5.2, 16.3]$, and closes already for $f = 32\%$. The dominant CPBG is the upper one (cf. Fig. 2). For

$f = 17\%$ and $\varepsilon = 12.96$ it can reach 12%, however, the threshold value of ε for its opening is 7.9, comparable to that for an fcc lattice. I have several reasons to believe that my results are correct. I have performed band structure calculations using the photonic KKR method [3], which is optimized for lattices of spheres, whereas results computed in early days of the plane-wave expansion method have often turned out imprecise, an example being Ref. [4]. Indeed, 6 years later, for the test case in Fig. 1, the plane-wave method (see Fig. 4 of Ref. [5]) yielded a lower CPBG width of only half that presented in Ref. [1]. The two lowest bands in Fig. 1 (but not the higher ones) agree well with those calculated in Ref. [5]. The effective refractive index n_{eff}, as calculated from the band structure in the L direction, is 1.604, only 10% larger than $n_{eff}^{MG} = 1.456$, calculated by the Garnett formula [6], which usually provides a very good fit to n_{eff}. For comparison, the upper edge of the bands at the L point in Ref. [1] seems to be almost 20% lower than in my case, resulting in more than 30% deviation from n_{eff}^{MG}.

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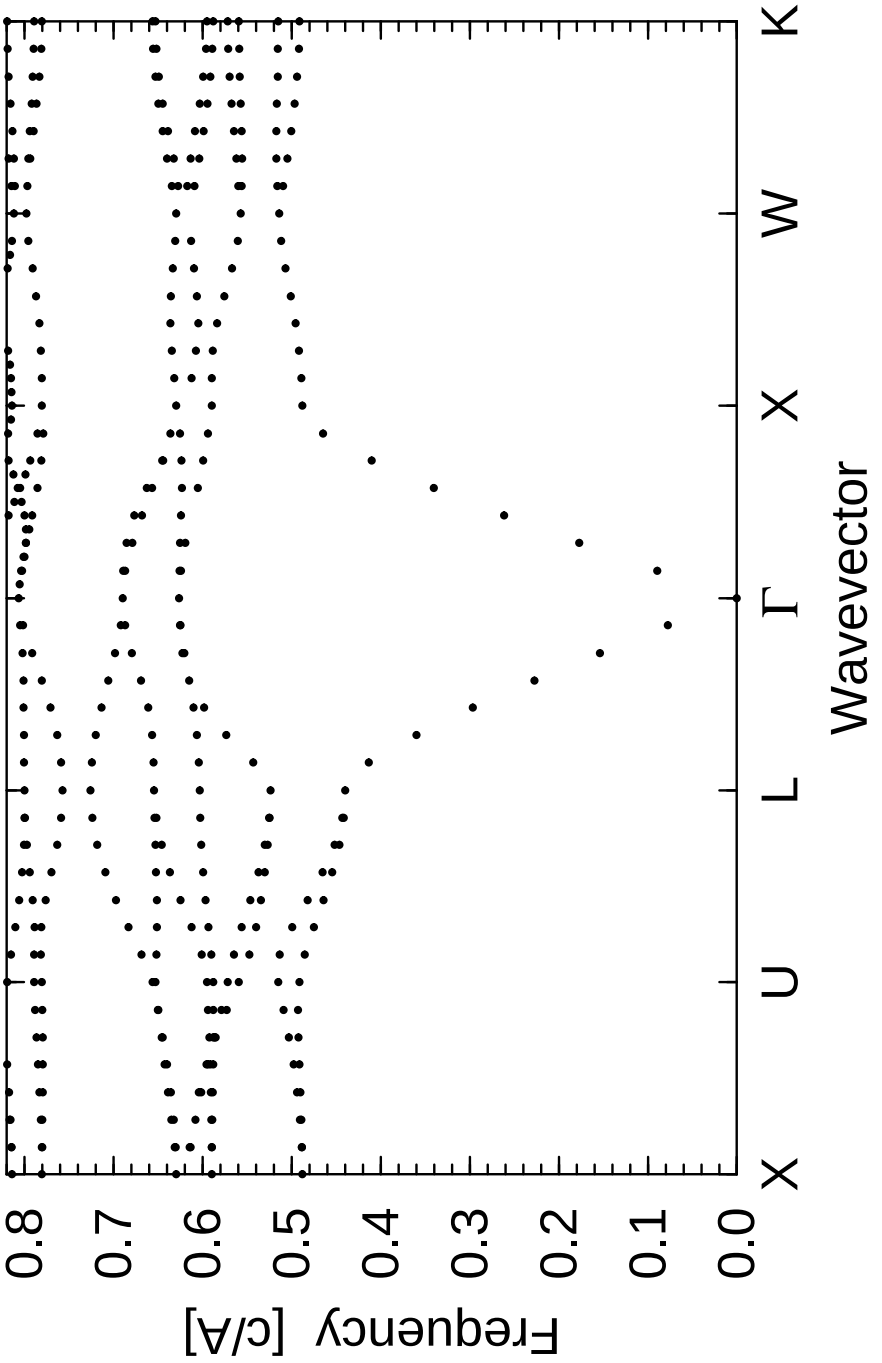

FIG. 1. Photonic band structure for a close-packed diamond lattice of spheres of dielectric constant $\varepsilon = 12.96$ in air (the same set of parameters as in Ref. [1]). Frequency in units [c/A], where c is the speed of light in vacuum and A is the lattice constant of a conventional cubic unit cell of the diamond lattice. Two CPBG open in the spectrum with the respective gap to midgap frequency ratios 1.3% and 4.2%.

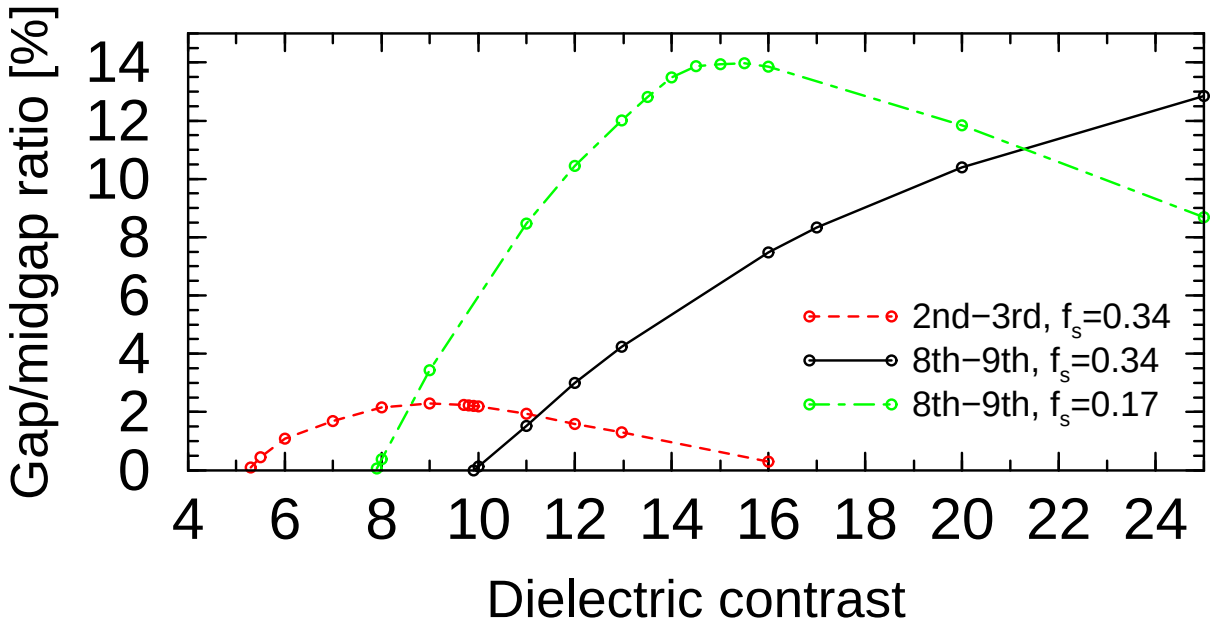

FIG. 2. Gap to midgap frequency ratio for a diamond lattice of dielectric spheres in air as a function of the dielectric contrast ε.