

Comparative studies on photonic band structures of diamond and hexagonal diamond using the multiple scattering method

This article has been downloaded from IOPscience. Please scroll down to see the full text article.

2004 J. Phys.: Condens. Matter 16 741

(<http://iopscience.iop.org/0953-8984/16/6/005>)

View [the table of contents for this issue](#), or go to the [journal homepage](#) for more

Download details:

IP Address: 129.252.86.83

The article was downloaded on 27/05/2010 at 12:40

Please note that [terms and conditions apply](#).

Comparative studies on photonic band structures of diamond and hexagonal diamond using the multiple scattering method

Hui Chen^{1,2}, Weiyi Zhang^{1,2} and Zhenlin Wang²

¹ Jiangsu Provincial Laboratory for NanoTechnology and Department of Physics, Nanjing University, Nanjing 210093, People's Republic of China

² National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing 210093, People's Republic of China

Received 27 October 2003, in final form 5 December 2003

Published 30 January 2004

Online at stacks.iop.org/JPhysCM/16/741 (DOI: 10.1088/0953-8984/16/6/005)

Abstract

Photonic band structures are investigated for both diamond and hexagonal diamond crystals composed of dielectric spheres, and absolute photonic band gaps (PBGs) are found in both cases. In agreement with both Karathanos and Moroz's calculations, a large PBG occurs between the eighth and ninth bands in diamond crystal, but a PBG in hexagonal diamond crystal is found to occur between the sixteenth and seventeenth bands because of the doubling of dielectric spheres in the primitive cell. To explore the physical mechanism of how the photonic band gap might be broadened, we have compared the electric field distributions ($|E|^2$) of the 'valence' and 'conduction' band edges. Results show that the field intensity for the 'conduction' band locates in the inner core of the sphere while that of the 'valence' band concentrates in the outer shell. With this motivation, double-layer spheres are designed to enhance the corresponding photonic band gaps; the PBG is increased by 35% for the diamond structure, and 14% for the hexagonal diamond structure.

Periodically space modulated dielectric structures, termed photonic crystals (PCs), have been investigated extensively in recently years, and the aim was to search for PCs with a photonic band gap which forbids the propagation of electromagnetic waves within that frequency range [1–3]. This novel feature of PCs leads to considerable efforts both in experimental and theoretical research works, and results in various practical applications in modern optical devices, such as selective reflectors, optical polarizers, band filters and low-threshold microcavity lasers [4, 5]. Although it is more difficult to fabricate three-dimensional (3D) PCs than two-dimensional (2D) ones, in order to control the light propagation at optical wavelengths in all directions, many groups have devoted themselves to developing

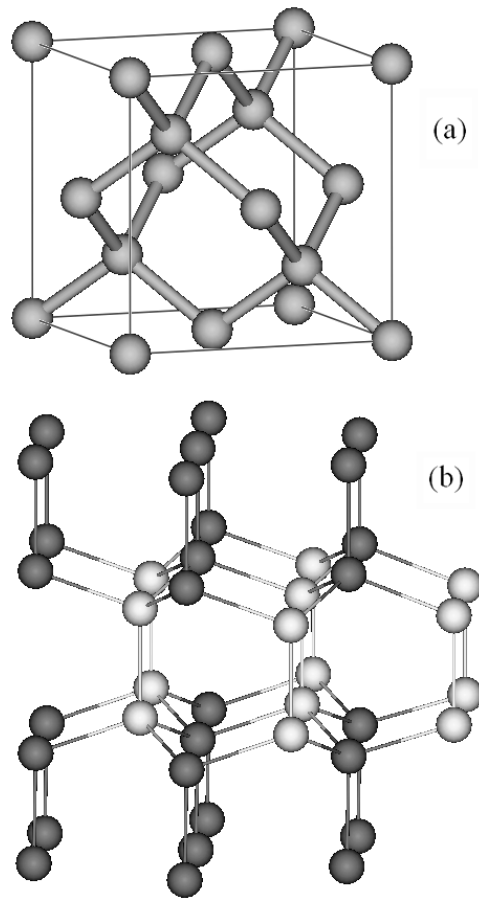


Figure 1. Schematic diagrams for the crystal structures of (a) diamond; (b) hexagonal diamond.

various methods to synthesize 3D PCs. Among those, the most promising methods are self-assembly [6–8] and microfabrication [9, 10], which can acquire stop bands in infrared and near-infrared regions.

The theoretical study of photonic crystals concentrates on the search for structures possessing photonic band gaps. Among the numerical methods used for calculating the photonic band structures, the most frequently adopted technique is the plane-wave expansion method [11–19], since it is straightforward and easy to implement. In most circumstances the plane wave expansion method gives reliable results. However, it may cause slow convergence of the solution or even inaccuracy in the case where very rapid change of electromagnetic waves takes place in space. It is, therefore, not surprising that a great discrepancy exists among different groups concerning the calculated photonic band structures for diamond crystals composed of dielectric spheres in air, though all used the plane-wave expansion method [17–19]. To overcome this difficulty, the transfer-matrix method and finite difference time domain method have also been in wide use recently to calculate the transmission spectra [20, 21] and pseudo-local density of states [22–25], respectively. These methods have the advantage of treating the general type of dielectric modulation and they can be used for all kinds of material components such as dielectric, ionic, as well as metallic elements. However, to achieve high numerical accuracy, a fine mesh size is needed which makes the calculation very CPU intensive.

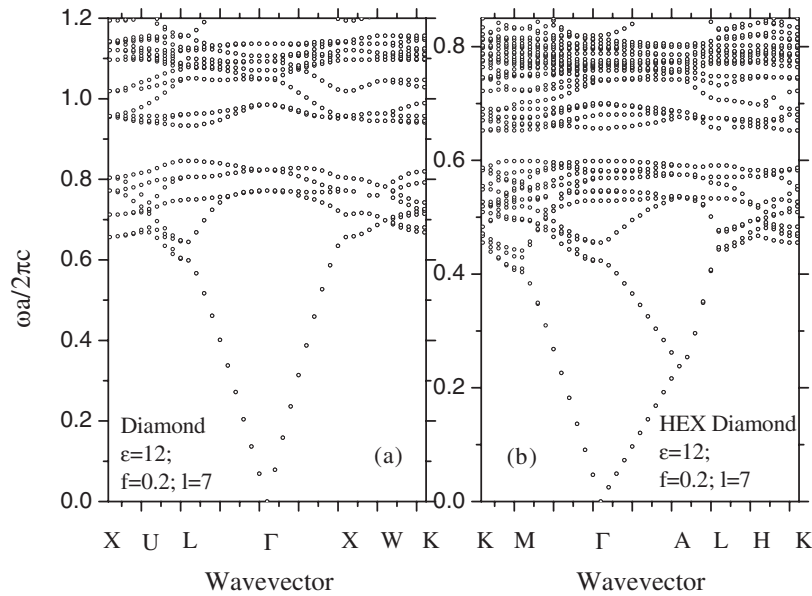


Figure 2. The photonic band structures of diamond and hexagonal diamond crystals made of dielectric spheres in air, with dielectric constant $\epsilon = 12$ and filling ratio $f = 0.2$. (a) Diamond crystal; (b) hexagonal diamond crystal. Note that the lattice constant a of FCC diamond is larger by a factor of $\sqrt{2}$ than that of hexagonal diamond.

In dealing with the situation of rapid variation of the dielectric constant in space, another advantageous method is the multiple scattering method, which formulates the problem in real space compared with the expansion in reciprocal space for the plane-wave method. It treats the variation of the dielectric constant with the background as scattering potentials. In particular, for a simple spherical scattering potential, the scattering T -matrix can be calculated exactly since the effect of the scattering centre can be included in the boundary condition. Therefore, it generally offers much higher numerical accuracy and less computer time. Thus, it has been widely used in the calculation of electronic structures in solids, as well as photonic band structures in PCs [26–37]. Recently, the multiple scattering method has been successful in calculating photonic band structures with a variety of material components such as dielectric, ionic, as well as metallic and even coated elements [32–37], and it is worth pointing out that the comparison of experiment and theory using the multiple scattering method has so far been more than satisfactory [34, 38]. We have written a general computer code to implement the multiple scattering method for the photonic band structures in 3D photonic crystals. The program code is very efficient and less CUP expensive.

In this paper, we make a comparative study of the photonic band structures of two types of diamond-like crystals, *diamond* and *hexagonal diamond*. The schematic diagrams of their crystal structures are presented in figure 1. The former is the common diamond with face-centred-cubic (FCC) lattice type: the primary cell is composed of two spheres separated by one fourth of the cubic diagonal. The latter, known as *Lonsdaleite* and rare in nature, belongs to the hexagonal-close-packed (HCP) crystal type, but each ‘atom’ is also composed of two spheres separated by $\sqrt{6}/4$ of the lattice constant in the basal plane.

In figure 2, the photonic band structures for single-layer spheres of high dielectric constant $\epsilon = 12$ in air are shown; the left-hand and right-hand panels display the bands for the diamond and hexagonal diamond crystals. The x -axis is the wavevector in the first Brillouin zone along

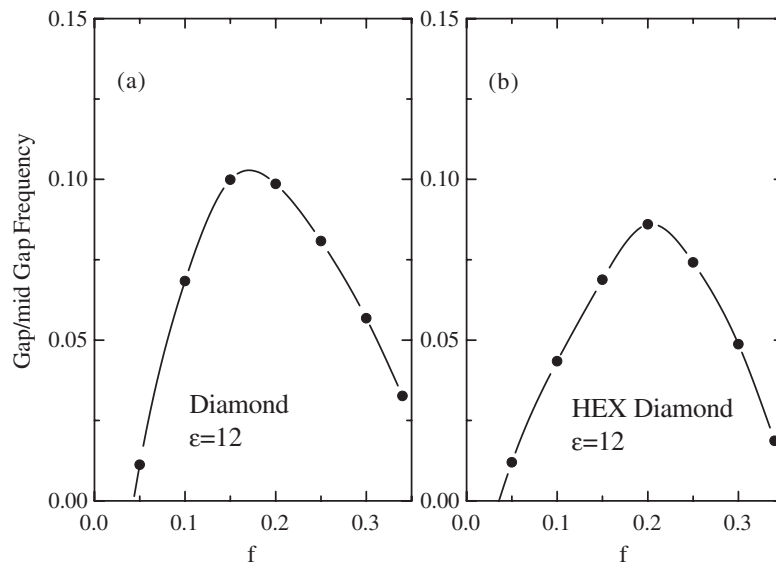


Figure 3. The gap/mid-gap frequency as a function of filling ratio f ; the dielectric constant of the spheres is $\epsilon = 12$. (a) FCC diamond crystal; (b) HCP diamond crystal.

the high symmetry points and the y -axis is the reduced frequency $\omega a/2\pi c$ with respect to the lattice constant a . The filling ratio of the spheres is $f = 0.2$, and the results are obtained with angular momentum $l = 7$. Comparing with that calculated with $l = 5$, exactly the same results are obtained for the low frequency range displayed here, which indicates that the code possesses fast convergence. Figure 2 shows that there is a large photonic band gap in both crystal types: the band gap for diamond is between the eighth and ninth bands, while it is between the sixteenth and seventeenth bands for hexagonal diamond. This is so since the primitive cell of hexagonal diamond contains twice the number of spheres as that of diamond. Because the lattice constant for FCC is larger than that of HCP by a factor of $\sqrt{2}$, the scales of frequency in figure 2 are almost the same for these two crystal types. In fact, the band gap in the diamond structure between the eighth and ninth bands was first pointed out by Karathanos *et al* in 1994 [29]. Although it may also occur between the second and third bands in some cases [37], the gap size divided by the mid-gap frequency barely exceeds 3%; thus the high band gap is always dominant in the diamond structure. This result also reminds us that the plane wave expansion method must be treated with care in dealing with the situation of rapid variation of electromagnetic field in space.

The dependence of the gap size/mid-gap frequency as a function of the filling ratio of the spheres f is presented in figure 3. These curves resemble inverted parabolas. The band gap starts to appear around $f = 0.05$, increases rapidly with f for small filling ratio, reaches its maximum value at $f = 0.17$ for diamond and $f = 0.21$ for hexagonal diamond, then shrinks slowly as the spheres approach close to touching each other. Note that the photonic band gap changes from an indirect gap at small f to a direct gap at larger filling ratio. For diamond, this change takes place around $f = 0.2$ from an indirect gap between the 'valence' band L-point and the 'conduction' band X-point to a direct gap between L-points, while for hexagonal diamond, the indirect gap is between the 'valence' band M-point and the 'conduction' band X-point, the direct gap is between the M-points, and the crossover filling ratio also takes the value $f = 0.2$. The reason why the dependence of gap size/mid-gap frequency

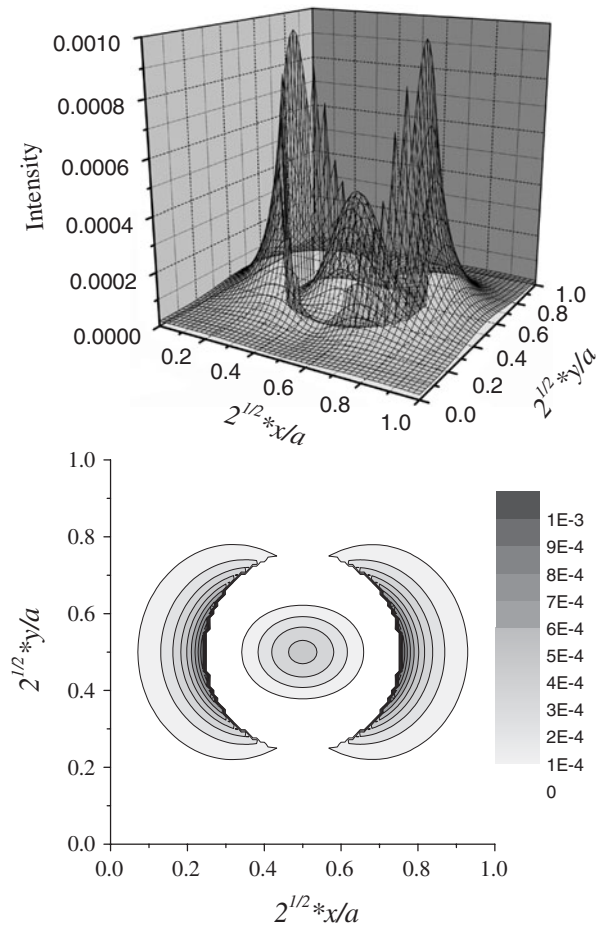


Figure 4. The electric field intensity of the ‘conduction’ band at the L-point of the Brillouin zone for the diamond crystal. The figure is plotted along the (001) direction; the x and y axes are both in the interval $(0, a/\sqrt{2})$. The upper panel is the 3D plot while the lower panel is the contour plot.

resembles inverted parabolas will become clear when we discuss the field distribution of the eigenmodes near the gap edges.

As was proposed by Zhang *et al* [35] for 2D photonic crystals, the double layer structure of the cylinders can often be used to enhance the photonic band gap. To broaden the photonic band gap in three dimensions using the specially designed layer structure of dielectric spheres, it is of interest to know the spatial distribution of electric fields for the modes near band gap edges. Such information offers a valuable insight concerning the characteristics of the modes, and their patterns can be explored to maximize the energy difference of the modes by properly choosing suitable double layer spheres. To illustrate, the electric field intensities ($|E|^2$) of the modes located at the L-point of the ‘conduction’ and ‘valence’ bands are calculated for a diamond crystal of high dielectric spheres embedded in air, with filling ratio $f = 0.2$ and dielectric constant $\epsilon = 12$, and the results are presented in figures 4 and 5. We find that the field distributions for both modes are primarily concentrated inside the high dielectric spheres, but there are also significant differences. The field intensity of the ‘conduction’ band has a shell-like structure—the intensities in the core and outer-shell region of the sphere are rather

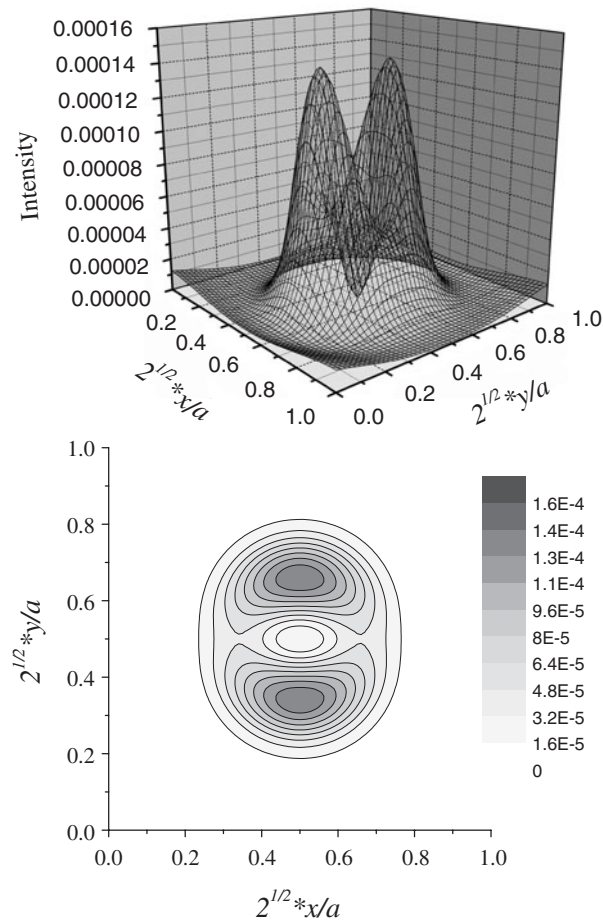


Figure 5. The electric field intensity of the ‘valence’ band at the L-point of the Brillouin zone for the diamond crystal. The figure is plotted along the (001) direction; the x and y axes are both in the interval $(0, a/\sqrt{2})$. The upper panel is the 3D plot while the lower panel is the contour plot.

high, while the intensity of the ‘valence’ band is practically zero in the core region. Thus if we lower the dielectric constant in the core region to increase the potential energy, the energy of the ‘conduction’ band will increase due to its higher intensity, but it has negligible effect on the ‘valence’ band.

From the field distributions of ‘conduction’ and ‘valence’ band states, it is also easy to understand the inverted parabola shapes of the gap size/mid-gap frequency. When the filling ratio is rather low, the spheres are very small and only the core regions are effective. Since the ‘conduction’ band state at the L-point has higher field intensity at the high dielectric core region than that of ‘valence’ band state at the L-point, the ‘conduction’ band state is actually lower in energy than the corresponding ‘valence’ band state; this means band crossing and no photonic band gap. As the filling ratio increases so that the spheres enter the intermediate region of the field distribution of the ‘conduction’ band, the energy of the ‘conduction’ band remains almost unchanged due to the low field intensity in this region, while that of the ‘valence’ band decreases continuously because of the high field intensity in the same region. Thus this opens up the photonic band gap and causes a continued enhancement. With further increasing the

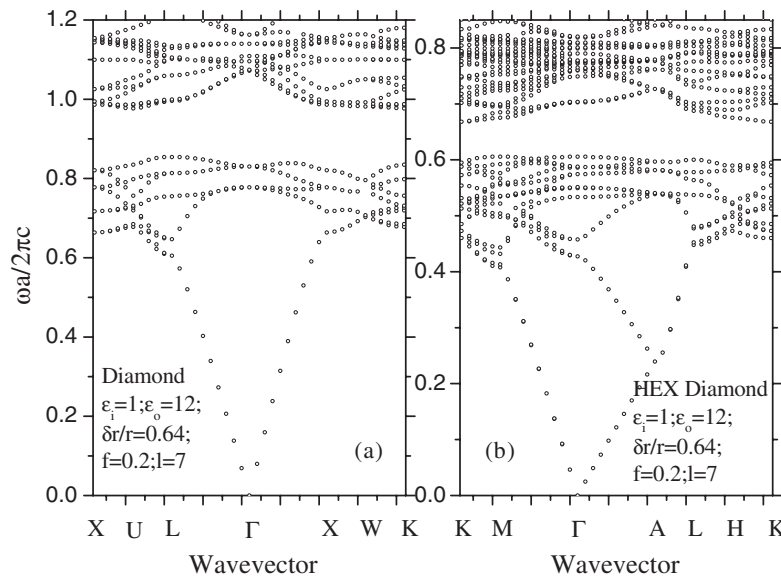


Figure 6. The photonic band structures of diamond and hexagonal diamond crystals made of double layer dielectric spheres in air. The inner and outer dielectric constants are $\epsilon_i = 1$ and $\epsilon_o = 12$, respectively. The filling ratio of spheres is $f = 0.2$, and the outer layer thickness is 64% of the sphere radius. (a) Diamond crystal; (b) hexagonal diamond crystal.

filling ratio, the outer-shell region of the ‘conduction’ band also starts to play a role; this lowers the energy of the ‘conduction’ band and reduces the overall photonic band.

The above physical mechanism paves the way to use double-layer spheres to widen photonic band gaps. In figure 6 the photonic band structures of the double-layer spheres are presented for both diamond and hexagonal diamond crystals. The outer layer dielectric constant takes the same value as before $\epsilon = 12$, the inner core is taken as air, the filling ratio of the spheres is $f = 0.2$, and the outer layer thickness is 64% of the sphere radius for both crystals. The other parameters are the same as in figure 2. The left-hand and right-hand panels display the band structures for diamond and hexagonal diamond crystals, respectively. With the double layer structure specified above, the photonic band gap is enhanced by 35% for diamond crystal and 14% for hexagonal diamond crystal, respectively. Our study suggests that the gap formation is mainly contributed by the high dielectric outer layer while the inner core can be used to adjust the detailed field distribution so as to maximize the difference of the field distribution between the two modes.

In summary, we have studied in this paper the photonic band structures of diamond-like crystals made of single layer spheres and double-layer spheres. It is shown that large band gaps exist in hexagonal diamond crystal as well as in diamond crystal composed of single layer high dielectric spheres in air, and double-layer spheres can efficiently broaden the band gap size by fully exploring the difference of the electric field distribution between the ‘conduction’ band and the ‘valence’ band.

Acknowledgments

The present work is supported in part by the National Natural Science Foundation of China under Grant No. 19934003, 90103022 and ‘Excellent Youth Foundation’ [10025419] as well as the ‘Climbing Program’ of NSTC [G19980614].

References

- [1] Yablonovitch E 1987 *Phys. Rev. Lett.* **58** 2059
- [2] Yablonovitch E, Gmitter T J and Bhat R 1988 *Phys. Rev. Lett.* **61** 2546
- [3] Yablonovitch E and Gmitter T J 1989 *Phys. Rev. Lett.* **63** 1950
- [4] Tarhan I I and Watson G H 1996 *Phys. Rev. Lett.* **76** 315
- [5] Vos W L *et al* 1996 *Phys. Rev. B* **53** 16231
- [6] Ozin G A and Yang S M 2001 *Adv. Funct. Mater.* **11** 95
- [7] Velev O D, Lenhoff A M and Kaler E W 2000 *Science* **287** 2240
- [8] Jiang P, Bertone J F, Hwang K S and Colvin V L 1999 *Chem. Mater.* **11** 2132
- [9] Lin S Y *et al* 1998 *Nature* **394** 251
- [10] Fleming J G and Lin S Y 1999 *Opt. Lett.* **24** 49
- [11] Leung K M and Liu Y F 1990 *Phys. Rev. Lett.* **65** 2646
- [12] Zhang Z and Satpathy S 1990 *Phys. Rev. Lett.* **65** 2650
- [13] Meade R D, Rappe A M, Brommer K D, Joannopoulos J D and Alerhand O L 1993 *Phys. Rev. B* **48** 8434
- [14] Chan C T, Datta S, Ho K M and Soukoulis C M 1994 *Phys. Rev. B* **50** 1988
- [15] McGurn A R and Maradudin A A 1993 *Phys. Rev. B* **48** 17576
- [16] Sigalas M M, Chan C T, Ho K M and Soukoulis C M 1995 *Phys. Rev. B* **52** 11744
- [17] Ho K M, Chan C T and Soukoulis C M 1990 *Phys. Rev. Lett.* **65** 3152
- [18] Sözüer H S, Haus J W and Inguva R 1992 *Phys. Rev. B* **45** 13962
- [19] Simeonov S, Bass U and McGurn A R 1996 *Physica B* **228** 245
- [20] Pendry J B 1994 *J. Mod. Opt.* **41** 209
- [21] Li Z Y and Lin L L 2003 *Phys. Rev. E* **67** 046607
- [22] Chan Y S, Chan C T and Liu Z Y 1998 *Phys. Rev. Lett.* **80** 956
- [23] Fan S, Villeneuve P R and Joannopoulos J D 1996 *Phys. Rev. B* **54** 11245
- [24] Ward A J and Pendry J B 1998 *Phys. Rev. B* **58** 7252
- [25] He S L, Xiao S S, Shen L F, He J P and Fu J 2001 *J. Phys. A: Math. Gen.* **34** 9713
- [26] Ohtaka K 1980 *J. Phys. C: Solid State Phys.* **13** 667
- [27] Stefanou N, Karathanos V and Modinos A 1992 *J. Phys.: Condens. Matter* **4** 7389
- [28] Wang X D, Zhang X-G, Yu Q L and Harmon B N 1993 *Phys. Rev. B* **47** 4161
- [29] Karathanos V, Modinos A and Stefanou N 1994 *J. Phys.: Condens. Matter* **6** 6257
- [30] Tayeb G and Maystre D 1997 *J. Opt. Soc. Am. A* **14** 3323
- [31] Stefanou N, Yannopapas V and Modinos A 1998 *Comput. Phys. Commun.* **113** 49
- [32] Moroz A and Sommers C 1999 *J. Phys.: Condens. Matter* **11** 997
- [33] Zhang W, Wang Z L, Hu A and Ming N 2000 *J. Phys.: Condens. Matter* **12** 9361
- [34] Zhang W, Lei X Y, Wang Z L, Zheng D G, Tam W Y, Chan C T and Sheng P 2000 *Phys. Rev. Lett.* **84** 2853
- [35] Zhang X D, Zhang Z Q and Li L M 2000 *Phys. Rev. B* **61** 1892
- [36] Fang A, Zhang W, Wang Z, Hu A and Ming N 2001 *J. Phys.: Condens. Matter* **13** 8489
- [37] Moroz A 2002 *Phys. Rev. B* **66** 115109
- [38] Velikov K P, Moroz A and Van Blaaderen A 2002 *Appl. Phys. Lett.* **80** 49