Special points for superlattices and strained bulk semiconductors

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Special **k** points for performing integrals over the Brillouin zone of [001] and [111] superlattices are obtained and discussed. If the superlattice period is taken properly, the number of special points required in order to reach suitable convergence can be greatly reduced. Twelve and ten special points will give the same accuracy for $N\times M$ [001] and [111] superlattices, respectively, as Chadi's and Cohen's ten special points for bulk semiconductors, provided we have $N+M=4n$, with n an integer. These special points can also be used to calculate the corresponding integrals for strained bulk semiconductors.

I. INTRODUCTION

In many theoretical investigations involving the electronic structures of solids, one often needs to calculate integrals over the first Brillouin zone. Baldereschi[1] and Chadi and Cohen[2] suggested that such integrations can be accurately approximated by summing over a rather small number of special **k** points in the Brillouin zone, with different weights for each point. (Elaborations of the special point method have been given by Monkhorst, Pack, Chadi, and Cunningham.[3,4]) For example, ten special points give very satisfactory results for the Green's functions of bulk cubic semiconductors.[5]

In this paper we extend the special points method to [001] and [111] lattice-matched $N\times M$ superlattice such as $(GaAs)_N(AlAs)_M$, determining the special points for cases such that $N+M=4n$, where N and M are the numbers of two-atom-thick layers of each slab of a superlattice (e.g., $Na_L/2$ and $Ma_L/2$ are the thicknesses of the GaAs and AlAs slabs in a [001] GaAs-AlAs superlattice period, where a_L is the lattice constant of either bulk material), and n is an integer. The number of special points needed to obtain reasonable accuracy of such integrals can be greatly reduced if such a requirement is satisfied. In this paper we assume that the two components of the superlattice are perfectly lattice matched. For [001] super- lattices the three-dimensional lattice translation vectors can be taken to be the following: $(a_L/2)(1,1,0)$, $(a_L/2)(1,-1,0)$, and $(a_L/2)(0,0,N+M)$ for $N+M$ even, or $(a_L/2)(1,1,0)$, $(a_L/2)(1,-1,0)$, and $(a_L/2)(0,1,N+M)$ for $N+M$ odd. For [111] superlattices the corresponding translation vectors are taken to be $(a_L/2)(1,-1,0)$, $(a_L/2)(0,1,-1)$, and $(a_L/2)(N+M, N+M,0)$. We choose the unit of wave vector **k** and the reciprocal lattice vectors **G** as $2\pi/a_L$, and k_1, k_2, and k_3 are the three components of the reduced wave vector **k** in the x, y, and z directions

$$\mathbf{k}=(k_1,k_2,k_3)(2\pi/a_L)\ .$$

Since the theoretical formalism is the same for any superlattice consisting of cubic semiconductors, for simplicity of presentation, we discuss only zinc-blende GaAs/AlAs superlattices.

II. GENERAL APPROACH

We follow the general approach of Chadi and Cohen for generating special points. They begin with one or more wave vectors and, by subjecting these wave vectors to symmetry operations, generate the special points. For zinc-blende crystals with a face-centered-cubic Bravais lattice, they generated ten special points **k**, based on the starting points $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$, and $(\frac{1}{8},\frac{1}{8},\frac{1}{8})$. We see the equivalent special points for superlattices composed of zinc-blende layers.

In generating the special points for zinc-blende materials, Chadi and Cohen actually used three types of symmetry: (i) time-reversal invariance (**k** and $-\mathbf{k}$ are equivalent); (ii) point-group symmetry (**k** and $T\mathbf{k}$ are equivalent, where T is an element of the point group T_d for zinc-blende structures[6]); and (iii) translational symmetry (**k** and $\mathbf{k}+\mathbf{G}$ are equivalent, where **G** is a reciprocal-lattice vector).

For a superlattice, time-reversal invariance still applies, but the point-group symmetry is lower (C_{2v} for a [001] superlattice and C_{3v} for a [111] superlattice, instead of T_d for the bulk), and the translational symmetry is different: Certainly the reciprocal-lattice vectors in the direction of growth are different and some reciprocal-lattice vectors in perpendicular directions might be changed also for some superlattices.

At first glance, the reduced symmetry appears to greatly increase the number of special points needed to obtain the same accuracy as obtained by the ten special points of Chadi and Cohen. For example, because of the lower symmetry of a [001] superlattice, its starting points corresponding to the three bulk generators $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, $(\frac{1}{4},\frac{1}{4},\frac{1}{4})$,

and $(\frac{1}{8},\frac{1}{8},\frac{1}{8})$ are $(\pm\frac{1}{2},\pm\frac{1}{2},\pm\frac{1}{2})$, $(\pm\frac{1}{4},\pm\frac{1}{4},\pm\frac{1}{4})$, and $(\pm\frac{1}{8},\pm\frac{1}{8},\pm\frac{1}{8})$, and produce, in principle, $8^3=512$ special points instead of the ten points of Chadi and Cohen. Here we show how the number of special points can be reduced from 512 to 12 for the [001] superlattice and to 10 for the [111] superlattice—provided one restricts one's attention to superlattices of special periods, namely $N\times M$ superlattices, such that $N+M=4n$, with n an integer.

III. [001] SUPERLATTICES AND STRAINS

A. Superlattices

For [001] superlattices, the C_{2v} symmetry dictates that the starting points corresponding to the bulk $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ generator be $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, $(\frac{1}{2},-\frac{1}{2},\frac{1}{2})$, and $(\frac{1}{2},\frac{1}{2},-\frac{1}{2})$, with weights $\frac{1}{4}$, $\frac{1}{2}$, and $\frac{1}{4}$, respectively. Combining either $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$, or $(\frac{1}{2},\frac{1}{2},-\frac{1}{2})$ with $(\pm\frac{1}{4},\pm\frac{1}{4},\pm\frac{1}{4})$ for an arbitrary [001] superlattice, using the method of Chadi and Cohen, we find six special points: Two have weights of $\frac{1}{16}$ and four have weights of $\frac{1}{32}$. Recombining these six points with $(\pm\frac{1}{8},\pm\frac{1}{8},\pm\frac{1}{8})$ will give 40 points: 24 with weight $\frac{1}{128}$ and 16 with weight $\frac{1}{256}$. Repeating this procedure, but starting with $(\frac{1}{2},-\frac{1}{2},\frac{1}{2})$, yields 64 points, each with weight $\frac{1}{128}$. This gives a total of $40+64+40=144$ superlattice special points corresponding to the 10 special points of bulk zinc blende. It is often impractical to use so many special points.

For [001] superlattices with special periods, the 144 special points can be reduced considerably by invoking translational symmetry. For example, consider a GaAs-AlAs $N_{\mathrm{GaAs}}\times M_{\mathrm{AlAs}}$ [001] superlattice such that $N_{\mathrm{GaAs}}+M_{\mathrm{AlAs}}=4n$, where n is an integer. (Here, for example, N_{GaAs} denotes the number of GaAs molecular layers per slab of GaAs. Hence a 1×1 superlattice consists of alternating layers of GaAs and AlAs, and a 2×3 superlattice alternates two GaAs layers and three AlAs layers.) In this case, the reciprocal-lattice vectors of the superlattice are $\mathbf{G}_1=(1,1,0)$, $\mathbf{G}_2=(1,-1,0)$, and $\mathbf{G}_3=(0,0,1/2n)$. Because of the symmetry of this special period, any two of the 144 special points (k_1, k_2, k_3) that have the same values of k_1 and k_2 coalesce into a single special point—reducing the number of distinct points to 20. Examination of the remaining symmetries reduces this set to 12 special points $\mathbf{k}$, each with weight α, denoted by $(\mathbf{k},\alpha)$:

$(\frac{7}{8},\frac{3}{8},\frac{1}{8};\frac{1}{8})$, $(\frac{5}{8},\frac{3}{8},\frac{1}{8};\frac{1}{16})$, $(\frac{7}{8},\frac{1}{8},\frac{1}{8};\frac{1}{16})$,

$(\frac{3}{8},\frac{1}{8},\frac{1}{8};\frac{1}{8})$, $(\frac{3}{8},\frac{3}{8},\frac{1}{8};\frac{1}{16})$, $(\frac{1}{8},\frac{1}{8},\frac{1}{8};\frac{1}{16})$,

$(-\frac{7}{8},\frac{3}{8},-\frac{1}{8};\frac{1}{8})$, $(-\frac{5}{8},\frac{3}{8},-\frac{1}{8};\frac{1}{16})$,

$(-\frac{7}{8},\frac{1}{8},-\frac{1}{8};\frac{1}{16})$, $(-\frac{3}{8},\frac{1}{8},-\frac{1}{8};\frac{1}{8})$,

$(-\frac{3}{8},\frac{3}{8},-\frac{1}{8};\frac{1}{16})$, and $(-\frac{1}{8},\frac{1}{8},-\frac{1}{8};\frac{1}{16})$.

These special points have been used to compute the Green's functions of superlattices, for energies in the fundamental band gaps.[7]

B. Strained bulk zinc blende

One can consider bulk GaAs to be a degenerate form of a GaAs-GaAs [001] superlattice. In this case, the superlattice has D_{2d} symmetry rather than C_{2v} symmetry (because the former AlAs of the GaAs-AlAs superlattice is now GaAs). Either the first six or the last six of the special points above (with their weights doubled) could be used for the D_{2d} symmetry, leading to results with the same accuracy as the ten special points of Chadi and Cohen. Of course, by viewing bulk GaAs as a 2×2 GaAs-GaAs superlattice, the Hamiltonian matrix is four times as large as for bulk GaAs, and so evaluating six special points for sums involving functions of the larger Hamiltonian will be more laborious than evaluating ten for bulk GaAs. Therefore it does not make sense to treat bulk GaAs as a GaAs-GaAs superlattice, but *bulk GaAs strained along the [001] direction has D_{2d} symmetry,* and so either the first six or the last six of the above 12 special points (with their weights doubled) can be used to evaluate integrals over the Brillouin zone for [001]-strained bulk GaAs.

IV. [111] SUPERLATTICES AND STRAINS

A. Superlattices

For [111] superlattices, the point group is C_{3v}, and the generators of special points are $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ and $(-\frac{1}{2},\frac{1}{2},\frac{1}{2})$, with weights of $\frac{1}{4}$ and $\frac{3}{4}$, respectively. Combining $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$ with $(\pm\frac{1}{4},\pm\frac{1}{4},\pm\frac{1}{4})$ and then $(\pm\frac{1}{8},\pm\frac{1}{8},\pm\frac{1}{8})$, we obtain ten distinct special points, with weights of $\frac{3}{64}$, $\frac{3}{128}$ or $\frac{1}{256}$. Starting with $(-\frac{1}{2},\frac{1}{2},\frac{1}{2})$, we obtain 40 special points with weights of $\frac{3}{128}$ or $\frac{3}{256}$, bringing the total number of special points to 50. This set can be reduced by considering $N_{\mathrm{GaAs}}+M_{\mathrm{AlAs}}=4n$, in which case $(1/4n,1/4n,1/4n)$ is a reciprocal-lattice vector. By adding this reciprocal-lattice vector, or its negative, to each of the 50 general special points, we reduce the number of distinct points to 20: eight lie in a plane on the superlattice Brillouin-zone boundary which is perpendicular to the [111] direction and passing through the point $(\frac{1}{8},\frac{1}{8},\frac{1}{8})$, and 12 lie on a parallel plane within the Brillouin zone. Using translational symmetry with reciprocal-lattice vectors $(1,-1,0)$, $(0,1,-1)$, and $(-1,0,1)$ together with C_{3v} point-group symmetry, these 20 points reduce to the following ten distinct special points $\mathbf{k}$ with weights α, $(\mathbf{k};\alpha)$:

$(\frac{3}{8},\frac{1}{8},-\frac{1}{8};\frac{3}{32})$, $(\frac{5}{8},-\frac{1}{8},-\frac{1}{8};\frac{3}{32})$, $(\frac{1}{8},\frac{1}{8},\frac{1}{8};\frac{1}{64})$,

$(\frac{7}{8},-\frac{3}{8},-\frac{1}{8};\frac{3}{16})$, $(\frac{9}{8},-\frac{3}{8},-\frac{3}{8};\frac{3}{32})$,

$(\frac{9}{8},-\frac{5}{8},-\frac{1}{8};\frac{3}{16})$, $(\frac{7}{8},-\frac{5}{8},\frac{1}{8};\frac{3}{32})$,

$(\frac{5}{8},-\frac{3}{8},\frac{1}{8};\frac{3}{32})$, $(\frac{1}{8},\frac{1}{8},-\frac{1}{8};\frac{3}{32})$, and $(-\frac{5}{8},\frac{3}{8},\frac{3}{8};\frac{3}{64})$.

B. Strain

The GaAs-GaAs [111] superlattice has C_{3v} symmetry, and so the above ten special points can be used for treating Brillouin-zone sums for [111]-strained bulk GaAs.

V. CONCLUSION

Special points for superlattices can be computed using the method of Chadi and Cohen. By limiting oneself to special-period superlattices, such as those for which $N_{GaAs}+M_{AlAs}=4n$, one finds that relatively few special points will provide accurate integrals over the superlattice Brillouin zone. We have presented 12 special points for $N\times M$ [001] superlattices and ten for $N\times M$ [111] superlattices, valid for $N+M=4n$, where n is an integer. However, our general approach can be used for generating special points that will produce more accuracy or for superlattices that do not satisfy the condition $N+M=4n$. These same special points obtained for $N+M=4n$ may be used for Brillouin-zone sums for strained bulk zinc-blende material.

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[3]An alternate approach for determining special points has been given by Monkhorst and Pack. See, for example, H. J. Monkhorst and J. D. Pack, Phys. Rev. B **13**, 5188 (1976); D. J. Chadi, *ibid.* **16**, 1746 (1977); J. D. Pack and H. J. Monkhorst, *ibid.* **16**, 1748 (1977).

[4]Special points for the two-dimensional Brillouin zone have been determined by S. L. Cunningham, Phys. Rev. B **10**, 4988 (1974).

[5]See, for example, S. Y. Ren, W. M. Hu, O. F. Sankey, and J. D. Dow, Phys. Rev. B **26**, 951 (1982).

[6]We use the notation of M. Tinkham, *Group Theory and Quantum Mechanics* (McGraw-Hill, New York, 1964).

[7]See, for example, S. Y. Ren, J. D. Dow, and J. Shen, Phys. Rev. B (to be published).