

AN EFFICIENT FULL-ZONE K-P METHOD FOR 'ON THE FLY' CALCULATION OF VALENCE BAND ENERGIES IN HOLE TRANSPORT STUDIES

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Abstract

A new computationally efficient full-zone k-p method for use in valence band transport and optical studies of Si and Ge has been developed. This method generalizes the traditional k-p method by avoiding, in part, the use of perturbation theory. New band parameters have also been computed.

I. INTRODUCTION

Full-zone carrier transport investigations are becoming increasingly popular. Band-structures used in these simulations are often calculated with the pseudopotential method, which uses plane waves as basis functions. However, due to the rapidly varying angular behavior exhibited by the true eigenfunctions, a large number of plane waves are needed (typically 50-100). Thus, band structure calculations usually require considerable CPU time, and full-zone transport calculations often resort to interpolation and to look-up tables, where the results of these pseudopotential calculations are stored. Under certain conditions, however, it may be preferable to calculate the band structure values while the transport simulation is taking place ('on the fly'). To allow for these circumstances, we have developed a full-zone k-p method, which very quickly calculates an eigenvalue anywhere in the zone for the relevant valence bands. Determining an eigenvalue requires approximately 5 milliseconds on a 486PC-33, and values agree well with results from pseudopotential calculations. The procedure is also invertible to give $k(\epsilon)$, making this method attractive for Monte Carlo calculations. The calculations have also lead to the development of new band parameters.

II. METHOD OF SOLUTION

The k-p method is based on second-order degenerate (Rayleigh-Schrödinger) perturbation theory applied to a one-electron crystal Schrödinger wave equation [1,2]; given a knowledge of a relatively small number of band energies at a particular point k_0 in k-space the method allows the band structure to be calculated very accurately for small deviations δk about k_0 . For sufficiently small δk analytic solutions are possible [1], while for somewhat larger δk , a numerical solution is required [2,3]. The k-p method has also been applied extensively to superlattice structures [4,5].

With our k-p calculations, we do not resort to perturbation theory, but solve exactly an 18 band k-p secular determinant with spin-orbit coupling included. Specifically, we have generalized the well-known 3×3 k-p valence band Hamiltonian of Dresselhaus *et al.* (DKK) [1] to include all momentum coupling arising from an underlying 18-band k-p Hamiltonian. This allows direct use of the Kane cubic [2], but now with energy-dependent coefficients. We have computed direct (momentum) coupling matrix elements using the five Luttinger parameters [6,7], and have computed new indirect coupling matrix elements using a fitting procedure.

Once the secular equation is established, we find the eigenvalues using a determinant decomposition method, which to our knowledge has never been applied to band calculations, and is

closely related to ‘‘Schur complement domain decomposition’’ [8]. With this method, the matrix is block-partitioned and then reduced to lower (block)-triangular form. This allows the associated determinant to be factored into a product of lower-order determinants. We then only have to solve the low-order determinant associated with the valence bands of interest. This 3rd order secular determinant is quickly solved with Newton’s method to obtain the eigenvalues. The mathematical basis of our method is as follows.

We wish to solve the eigenvalue problem

$$(H - \varepsilon)|\phi\rangle = (H_0 + H' - \varepsilon_n)|\phi\rangle = 0 \quad (1)$$

where the Hamiltonian has been split into two parts, one of which representing an independently soluble problem

$$(H_0 - \varepsilon_n)|\psi_n\rangle = 0; \quad H_0 = -\nabla^2 + V; \quad \{\psi_n\}_n \text{ complete on } \mathcal{H} \quad (2)$$

In the present context, H' represents the k·p terms, as well as (formally) spin-orbit coupling. Now, we partition \mathcal{H} as

$$\mathcal{H} = \mathcal{H}_A \oplus \mathcal{H}_B; \quad \mathcal{H}_A = \text{span}\{\psi_n\}_{n \in A}; \quad \mathcal{H}_B = \text{span}\{\psi_n\}_{n \in B} \quad (3)$$

and $|\phi\rangle$, accordingly, as

$$|\phi\rangle = P_A |\phi\rangle + (1 - P_A) |\phi\rangle; \quad P_A = \sum_{n \in A} |\psi_n\rangle \langle \psi_n| \quad (4)$$

Substitution of (4) into (1) then leads to the following eigenvalue problem, restricted to \mathcal{H}_A

$$\sum_{j \in A} \{ \langle \psi_i | P_A H' P_A | \psi_j \rangle + \delta_{ij} \varepsilon_i - \langle \psi_i | P_A H' (1 - P_A) [(1 - P_A)(H - \varepsilon)(1 - P_A)]^{-1} (1 - P_A) H' P_A | \psi_j \rangle - \delta_{ij} \varepsilon \} \langle \psi_j | \phi \rangle = 0 \quad (5)$$

This result follows in a more straightforward manner directly from (1), if we partition the matrix H in accordance with (3) and employ a determinant reduction formula involving the Schur complement

$$(H - \varepsilon)|\phi\rangle = 0 \rightarrow |H - \varepsilon| = \begin{vmatrix} A - \varepsilon & S \\ S^\dagger & B - \varepsilon \end{vmatrix} = |A - S(B - \varepsilon)^{-1} S^\dagger - \varepsilon| = 0, \quad (6)$$

the final reduced-order determinant being equivalent to (5) with the following identifications

$$\begin{aligned} (A)_{ij} &= \langle \psi_i | P_A H' P_A | \psi_j \rangle; \\ (S)_{ij} &= \langle \psi_i | P_A H' (1 - P_A) | \psi_j \rangle; \\ (B - \varepsilon)_{ij}^{-1} &= \langle \psi_i | [(1 - P_A)(H - \varepsilon)(1 - P_A)]^{-1} | \psi_j \rangle \end{aligned} \quad (7)$$

Standard k·p perturbation theory follows from (6) by treating $(B - \varepsilon)^{-1}$ as a perturbation. We do not do this, but instead analytically reduce (6) to an expression involving matrices of $O(A)$ only. We employ 18 (cubic harmonic) basis functions, partitioning this set in accordance with standard k·p perturbation theory applied to diamond-type semiconductors ($A_{(3 \times 3)} \sim \Gamma_{25}$ valence bands, $B_{(15 \times 15)} \sim$ all other bands). Our new reduced-order 3×3 k·p Hamiltonian replaces the DKK valence band Hamiltonian [1], and we then make use of the Kane solution [2], otherwise unmodified.

We have computed the required momentum matrix elements based on the measured Luttinger parameters of Hensel and Suzuki [6] for Ge and Lawaetz [7] for Si, and have generated new matrix elements associated with intra-conduction band coupling.

To compute valence band energies, we solve the reduced secular determinant using Newton-Raphson iteration, obtaining the three (heavy, light, and splitoff band) energies individually. Typically, fewer than 5 iterations are required to compute each energy to better than 6 decimal places for arbitrary (reduced) k . Running on a 486PC-33 computer this corresponds to about 20–25 milliseconds per energy determination for random k throughout the Brillouin zone, and to about 2–4 milliseconds per energy for closely spaced wavevectors.

III. COMPUTED VALENCE BANDS IN SI AND GE

Dispersion relations for the valence bands in Si computed using our extended k - p method are shown in Fig. 1, along with selected values given by the pseudopotential calculation of Chelikowsky and Cohen [9]. Agreement with the pseudopotential result is quite good throughout the Brillouin zone. It is also evident that for large k our bands tend to fit the local pseudopotential result somewhat better than the nonlocal result. The corresponding result for Ge is provided in Fig. 2. Agreement with the pseudopotential result is also good, though somewhat less dramatic than in Si. It is worth noting that each of these plots requires just over one second to compute on a 486PC-33 computer. Each dispersion curve consists of 100 energy evaluations (hence 300 per plot). Energy contours for the heavy and light hole bands in Si are illustrated in Figs. 3 and 4; these are surface projections in the $\langle 100 \rangle$ plane.

IV. SUMMARY

We have developed a computationally efficient method for computing valence band energies throughout the Brillouin zone in bulk diamond-type semiconductors. We have applied this method to Si and Ge, obtaining very good agreement with pseudopotential calculations. We have also computed new k - p valence band parameters. Our approach is to solve the underlying secular equation on a lower dimensional subspace exactly, rather than perturbatively as in traditional k - p perturbation theory. Our method is quite general, and in particular, application to both valence and conduction bands of zincblende materials is possible.

Acknowledgements

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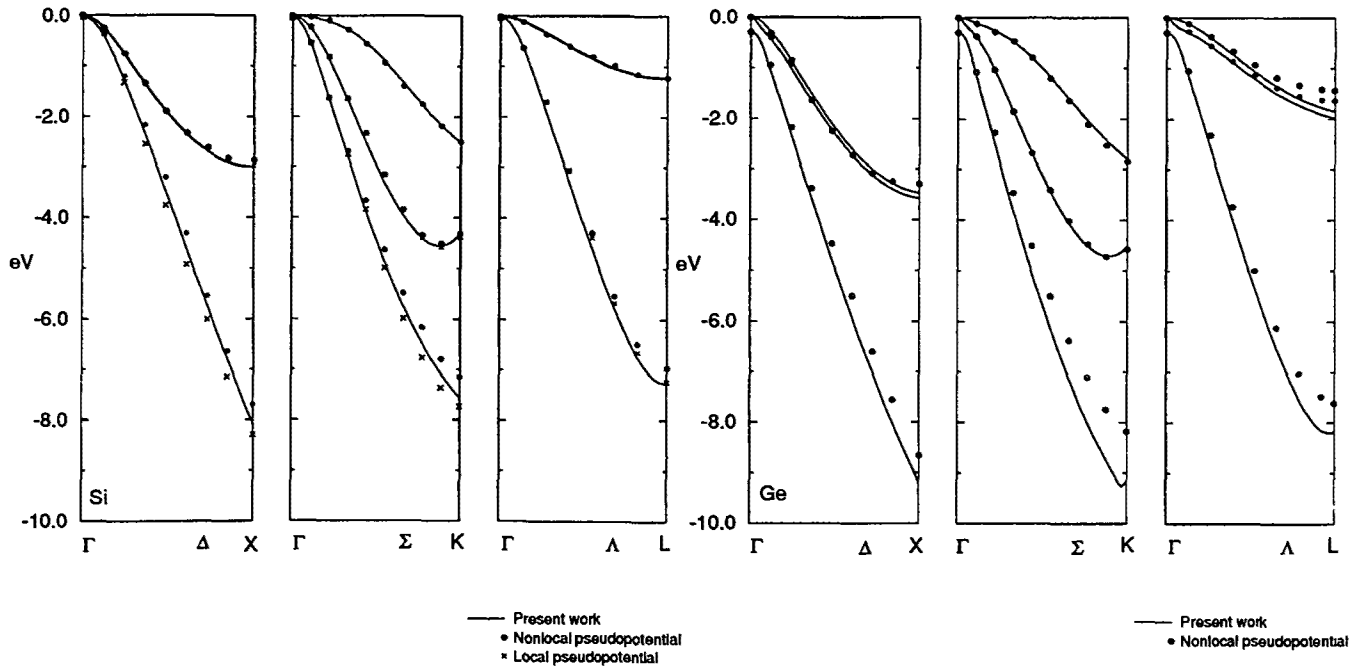
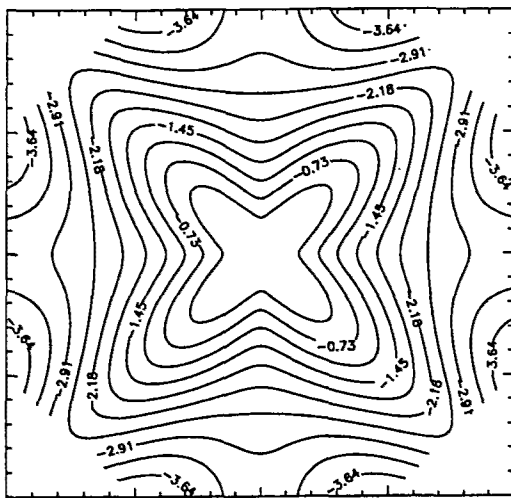
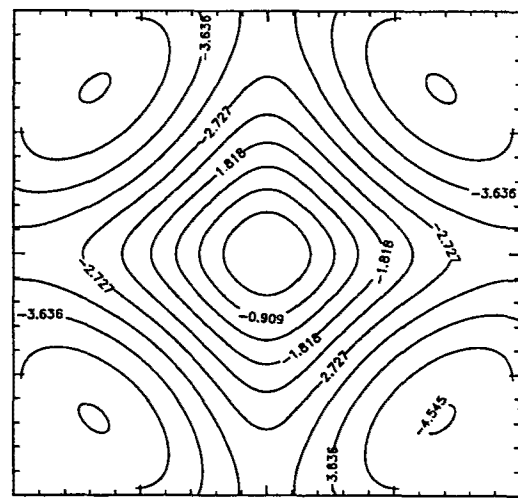


Figure 1: Comparison of present full-zone k-p valence band dispersion relations in Si with the pseudopotential result of Chelikowsky and Cohen [9].

Figure 2: Comparison of present full-zone k-p valence band dispersion relations in Ge with the pseudopotential result of Chelikowsky and Cohen [9].



[100] plane projection



[100] plane projection

Figure 3: Constant energy surfaces of the heavy hole band in Si.

Figure 4: Constant energy surfaces of the light hole band in Si.