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Pseudopotential-Based Full Zone k . p Technique for Indirect Bandgap Semiconductors: Si, Ge, Diamond and SiC

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Abstract: The k . p is a versatile technique that describes the semiconductor band structure in the vicinity of the bandgap. The technique can be extended to full Brillouin zone by including more coupled bands into consideration. For completeness, a detailed formulation is provided where the associated k . p parameters are extracted from the local empirical pseudopotential method in the form of band edge energies and generalized momentum matrix elements. We demonstrate the systematic improvement of the technique with the proper choice of the band edge states for the group-IV indirect bandgap semiconductors: Si, Ge, diamond and SiC of the 3C cubic phase. The full zone agreement is observed to span an energy window of more than 20 eV for Si, and 40 eV for the diamond with the 15-band pseudopotential-based k . p approach.

Key Words: Band structure, indirect bandgap semiconductors, pseudopotentials.

Keywords
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