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Optical properties of semiconductor alloys and superlattices HYEJUNG KIM, YIA-CHUNG CHANG, Department of Physics, University of Illinois at Urbana-Champaign, Urbana IL and Research center for Applied Sciences, Academia Sinica, Taipei, Taiwan, Y.D. KIM, Department of Physics, Kyung Hee University, Seoul, Korea — Optical properties of semiconductor alloys and superlattices are studied using a full-potential linear augmented-Slater-type orbital (LASTO) method. The LASTO method is highly efficient for dealing with large supercells to model alloys and superlattices in reasonable time frame. Bulk properties such as band structures, equilibrium lattice constants and bulk moduli are in good agreement with existing data. We calculate optical bowing parameters and dielectric functions of zincblende semiconductors and our calculations are compared with ellipsometric measurements for $InAs_xP_{1-x}$, $Zn_xCd_{1-x}Se$, $Al_xGa_{1-x}Sb$ alloys and $(GaSb)_m(AlSb)_n$ superlattices. To model alloys $A_xB_{1-x}C$, we consider 8-atom supercells of configurations B_4C_4, $A_1B_3C_4$, $A_2B_2C_4$, $A_3B_1C_4$, A_4C_4 (i.e., ratio of A to B atom equals 0, 0.25, 0.5, 0.75, 1). Atoms are allowed to relax to reach equilibrium positions. Complex dielectric functions are obtained after adding empirical GW corrections and semi-empirical excitonic effects.

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