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Effects of atomic randomness on the band structure calculation of $Si_{1-x}Ge_x$ via density functional theory MD HOSSAIN, Department of Mechanical Science and Engineering, University of Illinois at Urbana-Champaign, IL 61801, USA, JONATHAN FREUND, HARLEY JOHNSON, Department of Mechanical Science and Engineering,University of Illinois at Urbana-Champaign, IL 61801, USA — Electronic band structure calculations for compound semiconductors are usually performed by averaging fitting parameters using the virtual-crystal-approximation in either the pseudopotential method or the tight binding method. The effect of atomic randomness is completely ignored in such calculations. In this work, without using any fitting parameters, density functional theory is employed to calculate the band structure of the $Si_{1-x}Ge_x$ alloy system taking into account the effect of atomic randomness and, correspondingly, the local strain relaxation. The variation of band gap with 16 different Ge fractions in the alloy is computed to find bowing parameters for the two distinct composition ranges: $0 \leq x \leq 0.85$ and $0.85 \leq x \leq 1.0$. The calculation is carried out for a supercell of 64 atoms with P1 symmetry, and the randomly positioned atoms are relaxed up to a force tolerance of 0.0001eV/Å. Our results show much better agreement with experimental results for bandgaps, especially near $Si_{0.85}Ge_{0.15}$, than available empirical methods do. The results demonstrate the importance of accounting for the effect of randomness and local strain in band structure calculations.

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