

A microscopic supercell model for the dielectric function of germanium nanowires

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The observation of light, room temperature, visible photoluminescence from porous silicon has been the medium for much of the recent interest in luminescent group IV nanostructures. Though much of this initial interest was aimed at visible luminescent nanostructured Si more recently there has been increasing interest in Ge nanowires (GeNWs). In particular, porous germanium layers attract the considerable attention of numerous researchers [1] because they provide the formation of nanocrystals. Since the effective masses of the carriers in germanium are rather small, the quantum-dimensional effects in germanium nanocrystals should manifest themselves at considerably larger crystallite dimensions than in nanocrystals of other semiconductors. In this work the supercell model is applied to a semiempirical sp^3s^* tight-binding approach to calculate the electronic band gap and imaginary part of the dielectric function. Within the framework of the supercell model is possible to include the interconnection between nanowires present in real samples [2,3]. For modeling GeNWs, we start from a cell of eight Ge atoms with side $a=5.65 \text{ \AA}$ and take the periodic boundary condition only along z-direction, i.e., free boundary conditions are applied in x and y directions. For GeNWs with bigger cross sections, Ge atoms are added on (100) and (010) planes to obtain nanowires with larger width, conserving their square shapes. Each surface dangling bond is saturated with a hydrogen atom. The results of the variation band gap are compared with those obtained by TB- $sp^3d^5s^*$, the density functional theory, and experimental data in agreement with the quantum confinement scheme. The imaginary part of the dielectric function is calculated by including both the *intra-atomic* and *interatomic* dipole matrices by using the interconnected and free standing (without interconnection) models for the Ge skeleton. The calculation show that although the *intra-atomic* matrix elements are small in magnitude a quantitative treatment of the optical absorption spectrum of GeNWs may not be possible without the inclusion of *intra-atomic* matrix elements. Finally, this microscopic supercell model predicts the low frequency tail in the absorption spectrum, which appears even without the allowance for the indirect optical transitions.

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