AB-INITIO STUDY OF SILICON NANOWIRES

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SUMMARY

Four different size nanowires of Si have been studied by the density functional theory. We have shown that distinct from the bulk silicon with indirect band structure the one of the silicon nanowires is direct. Both valence band maximum and conduction band minimum are located at the Γ point. Optical properties of the nanowires have been studied.

1. INTRODUCTION

The use of nanostructures as wires, tubes or rods are found to exhibit good properties as an antireflection coating [1], passivation layer, and absorber layer [2,3], which present interest for solar cells. They might play a major role in enhancing the efficiency of photovoltaic devices [4] by increasing the light coupling into the active region of the solar cells. Recently it is reported [3] that Si nanowire arrays having less than 5% areal fraction of wires can achieve up to 96% peak absorption, and that they can absorb up to 85% of day-integrated, above-bandgap direct sunlight, with a peak external quantum efficiency of 0.89. The observed absorption enhancement and collection efficiency enable a cell geometry that not only uses 1/100th the material of traditional wafer-based devices, but also may offer increased photovoltaic efficiency owing to an effective optical concentration of up to 20 times. Here we study electronic structure and optical properties of Si nanowires.

2. METHODS

Bulk Si was used in the computations with the following optimized lattice parameters $a = b = c \approx 5.392$ Å in satisfactory agreement with experimentally determined parameters $a = b = c \approx 5.4307$ Å. For the study of the nanowires 1×1×2, 2×2×2, and 3×3×2 supercells have been prepared, which have been surrounded by vacuum along **x** and **y** directions [Fig. 1]. Along the **z** axis there is no vacuum and translational symmetry will be valid. So, the nanowires will mimic infinite wires. Dangling bonds of the outermost Si atoms located at the border of the wire with vacuum have been passivated by hydrogen. Optimization of the nanowires and studies of electronic structure has been performed for the Γ point.

The Vienna *ab initio* simulation package (VASP) [5,6] has been used for the computations within the generalized-gradient approximation (GGA) following the Perdew-Burke-Ernzerhof scheme (PBE) [7] for the exchange-correlation functional. Non-norm-conserving pseudopotentials generated in accordance to the projector-augmented-wave (PAW) method [8, 9] have been used. It allowed us to construct orthonormalized all-electron-like wave functions for the H-1*s* as well as Si-3*s* and -3*p* valence electrons. Full optimization of the lattice has been performed using the conjugate gradient method. Plane-wave cut-off 290 eV is employed to ensure the convergence. The convergence was achieved when the forces acting on the atoms were smaller than 20 meV $Å^{-1}$.

Imaginary part of the dielectric function was calculated. The real part of the dielectric function is then calculated using the Kramers-Kronig transformation. These two spectra were then used to calculate all the other optical spectra, such as the reflectivity, the absorption coefficient, the refractive index, the extinction coefficient, and the electron energy loss spectra for the energy range 0-12 eV.

3. RESULTS

Full geometrical optimization has been performed for the nanowires. The optimized structures are shown in Fig. 1. Band structures of bulk and nanowire Si have been studied [Fig. 2]. Analysis shows that distinct from bulk silicon with indirect band structure, the ones for silicon nanowires are direct [Fig. 2]. Both conduction band minimum and valence band maximum are located at the Γ point. The bottommost conduction band and topmost valence bands are dispersive. As the width of the wire increases the dispersion becomes more evident. Analysis of Fig. 2 shows that the band gap of the Si nanowires increases

with decreasing the width of the wires. As expected the band gaps are underestimated because of the well-known deficiency of the density functional theory (DFT).

The imaginary part of the optical dielectric function $\varepsilon_2(\omega)$, the reflectivity $R(\omega)$, the absorption coefficient $\alpha(\omega)$, the refractive index $n(\omega)$, the extinction coefficient $k(\omega)$ have been calculated from DFT for the nanowires along transversal and longitudinal polarizations. The results have been compared with experimentally established optical parameters for bulk Si [Fig. 3]. Because of the underestimation of the fundamental band gap in the DFT calculations, locations of all the peaks in the spectral distribution of $\varepsilon_2(\omega)$ are expected to be shifted toward lower energies compared to the expected ones. The absorption coefficient of the nanowires is larger, and the refractive index and the extinction coefficients are smaller than the experimentally determined ones. The absorption decreases with increasing the size of the nanowires.

4. CONCLUSION

Thus Si nanowires have been studied by the density functional theory. We found that distinct from the bulk silicon with indirect band structure the one for the nanowires is direct. Both valence band maximum and conduction band minimum are located at the Γ point. Optical properties of the nanowires are found to be anisotropic.

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Figure captions

FIG. 1. Schematic presentation of the n×n×2 (n=1,2,3) Si based nanowires.

FIG. 2. Band structure of the n×n×2 (n=(a) 1, (b) 2, and (c) 3) Si nanowires. Fermi level is set to zero.

Fig. 3. Optical spectra for the n×n×2 (n= (a)1, (b) 2, and (c) 3) Si nanowires.