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Influence of Porosity on the Structural and Electronic Properties of Porous Silicon

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INTRODUCTION

Porous silicon (PSi) is a promising material for several applications in significant and varied fields photoluminescence (PL), electroluminescence (EL) and gas and (bio) sensing, etc. In this work we have studied the influence of porosity on the structural and electronic properties of porous silicon and comparing them to those of the solid (c-Si) in order to understand changes in these properties when it is reduced to nanometric sizes.

THEORETICAL STUDY

In this work, structural and electronic properties investigations of PSi were performed using ab-initio pseudo potential plane wave (PP-PW) method founded on DFT. The exchange correlation energy is treated within the generalized gradient approximation of Perdew-Burke-Ernzerhof (GGA-PBE) included in the CASTEP program (Cambridge Serial Total Energy Package) [1]. The pseudopotential of Vanderbilt-type ultra-soft was utilized to compute the potential seen by the valence electrons. Supercell model was used to simulate porous silicon structures with four porosities (P = 3.12, 15.62, 28.12 and 40.62%) respecting the same space group P4 2 m (No.111). Hydrogen atoms were used to passivate all surfaces dangling bonds in silicon pores.

RESULTS AND DISCUSSION

Optimized structural parameters of all studied structures were obtained by geometry optimization step. For all porosities, the PS structures expand when compared to that of c-Si due to the hydrogen-hydrogen interaction. The electronic properties of PSi were studied by calculating the band structures, densities of states and electron density distributions. The electron band structures show for the different porosity, in contrary to the silicon crystal (c-Si) which possesses an indirect band gap, the feature of direct band gap. Otherwise, as shown in Fig. 1, The values of the gap of porosities 3.12, 15.62, 28.12, 40.62% are respectively 0.735, 1.196, 1.792, 2.090 eV unlike c-Si which has an indirect gap of 0.622 eV. There is a widening in the forbidden band which varies as a function of the porosity. This broadening is due to the increase in quantum confinement in the resulting structure and the increase in specific surface area as a function of porosity [2]. The densities of states and the electron

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charge maps of all PSi structures show that covalent bond Si-Si is conserved as in the case of c-Si.

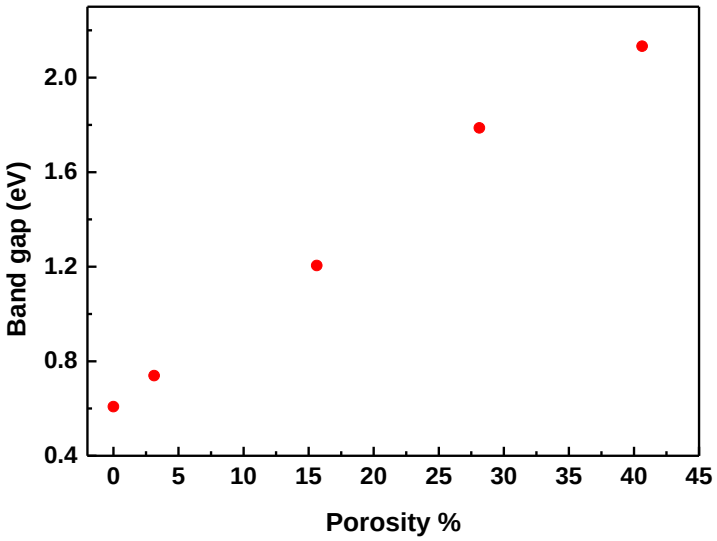

Fig 1: Evolution of band gap energy with porosity

CONCLUSION

Geometric optimization indicates expansion of the supercells, described by an increase in lattice parameters as a function of porosity. In addition, the electronic band structure of all PS structure shows direct band gap semiconductors for all studied porosities.

References

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