DFT study on the optical and vibrational properties of 3C porous Silicon Carbide

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In recent years there has been multiple investigations on the properties of silicon carbide nanostructures due to the attractive properties of SiC such as hardness and chemical inertness, and a wide band gap suitable for applications in harsh environments of high frequencies, and temperatures. Porous SiC (pSiC) is especially interesting due to its high core-surface ratio that makes it ideal for applications as sensors, additionally the binary nature of SiC allows for multiple chemical surface configurations that could be suitable for band gap and chemical properties engineering. There has been plenty of experimental studies on the hexagonal 6H-pSiC and only a few on the 3C-pSiC, however it has been observed that 3C-pSiC could be suitable for applications as a fast response H sensor, and there is no, at the best of our knowledge, theoretical investigations on the vibrational and optical properties of this material, which could be crucial for the development of future devices. In this work the vibrational and optical properties of 3C-pSiC were studied using the first principles density functional theory, the density functional perturbation theory and the supercell scheme [1,2]. The porous structures were modelled in the [001] direction by removing columns of atoms of an otherwise perfect SiC crystal, obtaining two surface configurations: one with only C atoms and one with Si atoms. Results indicate phonon optical modes of Si and C undergo a shift towards lower frequencies compared to their bulk counterparts due to phonon confinement effects. The dielectric function analysis shows a shift of the imaginary part of the dielectric function towards lower frequencies compared to the crystalline SiC, which could be due to the change of the band gap feature from an indirect band gap to a direct one, even though the 3C-pSiC band gap is higher than that of the crystalline bulk SiC. The highly porous case start their optical activity at higher frequencies compared to the lower porosity case which reflects the quantum confinement effects. These results could be important for the characterization and engineering of 3C-pSiC.

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