

Anisotropic electronic and optical properties of In nanowires on Si(111).

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Structural, electronic and optical properties of quasi-1D atomic wires of In on Si(111) have been intensively studied in the last years due to their potential applications as electronic nano-devices and outstanding physical properties as quasi-1D systems. However, the mechanism of the phase transitions between the 4×1 , 4×2 and 8×2 reconstructions is still under debate. It is well known that the electronic band structure is highly anisotropic. The consequences for the behavior of the electron gas in the In chains have to be understood. One possibility is to study its optical signatures related to intraband transitions. In this work we calculate the anisotropic plasma frequency considering the intraband contributions to the dielectric function. This calculation is performed using *ab-initio* density-functional theory, PAW pseudo-potentials and the supercell method. The atomic positions are taken from a previous calculation and are consistent with the experimental results[1]. We consider in detail each of the different reconstructions of this surface, specially 4×1 and 4×2 (keeping the metallic character) or 8×2 (with metallic or semiconducting behavior). The results of this study help to understand in more detail the optical spectra of these nanowires in the limit of low frequencies. The intraband contribution to the dielectric function indicates that HREELS measurements may also contribute to understand the properties of the electron gas on this surface. We acknowledge the partial financial support from CONACyT grants No. 36651-E and 36764-E. [1] Bechstedt *et al.*, Phys. Rev. B, **68**, 193406 (2003).