AB INITIO CALCULATIONS OF THE ANISOTROPIC DIELECTRIC TENSOR OF GaAs/AlAs HETEROSTRUCTURES.

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The dielectric and optical properties of periodic heterostructures have been widely investigated within the effective medium theory. This classical theory is expected to fail for very small hererostructures, where quantum confinement is important, but the size limit at which the classical approach breaks down is not known. On the theoretical side, calculations of the dielectric tensor of $(001)(\mathrm{GaAs})_p/(\mathrm{AlAs})_p$ superlattices have shown that the interplay between quantum confinement and local field effects is crucial [1]. For light polarized in the growth direction, it leads to the otherwise surprising justification of the use of a classical effective medium theory, even for the smallest periods.

In this work, the static dielectric properties of both $(001)(\mathrm{GaAs})_p/(\mathrm{AlAs})_{3p}$ superlattices, and periodic arrays of GaAs wires in an AlAs matrix, have been calculated as a function of the superlattice well width or the wire diameter (up to 13 Å) within Density Functional Perturbation Theory. The GaAs volume fraction has been fixed to 1/4 to fulfill the requirement that the wires are not interconnected. For the multilayer geometry, we found a generalization of the results obtained in Ref. [1]. In the direction perpendicular to the interfaces, $\varepsilon_\perp$ turns out to be constant and close to the classical limit, whereas in a direction parallel to the interfaces, quantum confinement is important even at large well width. Moreover, local field effects are found to be quantitatively identical and independent of the volume fraction of the well material in the multilayer geometry. Turning to the case of the interacting wires, the change in the geometrical form of the confinement and the resulting increase of the confinement have a drastic issue. Confinement effects are no longer equilibrated by the local fields effects, and consequently, the classical limit for $\varepsilon_\perp$ and $\varepsilon_\parallel$ is estimated to be reached at a well width by far larger than in the SL's.

[1] S. Botti, N. Vast, L. Reining, V. Olevano et L. C. Andreani, Phys. Rev. Lett. **89**, 216803 (2002).