Atomic and Electronic Structure of Si-Ge Superlattices

The $Si_4Ge_4(001)$ superlattice has received a lot of theoretical[1-4] and experimental attention.[5-7] In a recent Letter, Wong, Jaros, Morrison, and Hagon[1] (hereafter WJMH) suggested that this superlattice would adopt an atomic configuration that deviates from the commonly accepted structure. This would change the electronic band structure and bring the calculated optical transitions into better agreement with experiment. In this Comment, I point out that the suggested deviation is in conflict with first-principles calculations (the results of which were misinterpreted by WJMH), and with experiment. The changes in the electronic structure that follow from the atomic displacements in the WJMH model are therefore unphysical, and cannot be the correct explanation for the observed optical transitions.

The structure under discussion is lattice matched to a Si(001) substrate, and consists of four atomic monolayers of Si, alternated with four monolayers of Ge. (WJMH incorrectly refer to this configuration as "free standing." The term free standing applies to the case where the superlattice is free to adopt its own equilibrium in-plane lattice constant; i.e., it is no longer matched to Si.) The Si layers are cubic (lattice constant $a=5.43$ Å), while the Ge layers (equilibrium $a=5.65$ Å) are strained in order to match the Si in the plane of the interface ($a_{\parallel}=5.43$ Å). The strain in the perpendicular direction is then determined by minimizing the elastic energy[8]; this leads to a lattice constant in the perpendicular direction $a_{\perp}=5.83$ Å. Whe WJMH carry out their pseudopotential calculations for this system, they obtain a band structure which is in reasonable agreement with previous first-principles calculations.[2-4] The lowest-energy transition, at around 0.8 eV, is indirect. Various explanations[2,7] have already been advanced as to why this transition shows up strongly in electroreflectance,[5] a technique which in principle is only sensitive to direct transitions. In the meantime, photocurrent experiments have provided independent evidence for the indirect nature of this transition.[7]

Nonetheless, WJMH set out to construct a model in which the lowest calculated transition would be direct. They assume that the Ge layers would not be strained in accordance with elastic theory, but would remain "bulklike." One way in which this is implemented is by choosing the Ge form factors such as to represent bulk Ge, a procedure which conflicts with the atomic structure of the system. Another, physically quite distinct, way in which WJMH approach the bulklike Ge is by keeping $a_{\parallel}$ fixed, and increasing the Ge-Ge separation ($a_{\perp}$) along the superlattice axis in order to bring the Ge—Ge bond length closer to its bulk value. I note that a 1% change in the bond length requires roughly a 3% change in the perpendicular lattice constant, so that this procedure significantly enhances the magnitude of the uniaxial strain. This deviation in the atomic structure happens to lead to a similar narrowing of the (pseudo) direct gap as the modification of the form factors, although for physically quite different reasons: Deformation-potential theory[8] shows that changes in the strain components due to the expansion of the Ge layers push the valence band upwards and the conduction band downwards.

My major point here is that there is no physical basis for such a drastic change in the atomic structure of the superlattice. The atomic configuration obtained from minimizing the elastic energy indeed provides an excellent description of the system. This was confirmed by microscopic energy-minimization calculations in Ref. 8. These first-principles results showed that the strain in the perpendicular direction was within 1% of the elastic-theory prediction; i.e., in this case $a_{\perp}$ is predicted by elastic theory to better than 0.002 Å.[9] This theoretical approach was repeated and confirmed in Ref. 3.

Furthermore, channeling measurements[6] have provided a convincing experimental confirmation of the elastic-theory predictions, yielding data that are in very good agreement with $a_{\perp}=5.84$ Å.

In conclusion, WJMH's model of the atomic structure of the $Si_4Ge_4(001)$ superlattice is internally inconsistent and in conflict with other theory and experiment. Electronic structure results based on this model can therefore not be representative of the actual system.

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