Investigating local stoichiometry fluctuations in nm-thin semiconductor alloys: a case study on SiGe

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Semiconductor alloys allow tuning the electronic properties by changing the alloy composition. This adjustability makes them attractive materials for a wide range of applications. Thin layers of SiGe are of interest in semiconductor devices such as heterojunction bipolar transistors and field-effect transistors. When one or more dimensions are reduced to the nanoscale, local composition fluctuations in such alloys become crucial.

Using first-principles density functional theory[1] and the computationally faster extended Hückel theory[2], we simulate a large number of atomic structures to quantify the effect of local stoichiometry fluctuations on the band structure. We study unstrained alloys as well as alloys biaxially strained along the ⟨100⟩ directions. Our results show how introducing small fractions of carbon, which reduce the lattice mismatch with the Si substrate, lowers the band gap of the alloy. When carbon atoms occupy adjoining lattice sites, defect states are observed, which significantly reduce the band gap. However, by calculating the formation energy, we conclude that such atomic structures are energetically unfavorable.

By simulating few-nm thin SiGe layers sandwiched between Si, we show how the concept of an effective layer thickness can be used to describe the quantum confinement effect. Quantum confinement increases the band gap with decreasing layer thickness, counteracting the band gap reduction from increasing the Ge content. Applying results from the bulk alloy, we show how the numerical model of the finite quantum well can be used to describe the effect of local stoichiometry fluctuations on the band gap of thin layers. This model is in good agreement with results from calculations of multiple atomic structures of various alloy compositions and layer thicknesses.

References

1. F. Fuchs, W. Roscher, D. Dick, C. F. Irmscher, J. Schuster, S. Gemming, J. Phys. Chem. C 2025, 129, 2, 1546
2. D. Dick, F. Fuchs, J. Schuster, S. Gemming, PSS RRL, 2500087, in press

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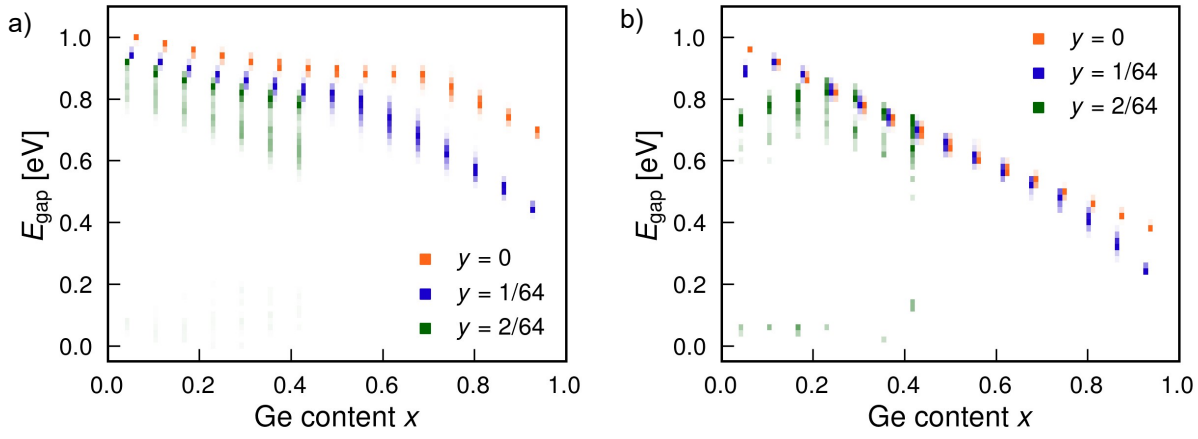

Figure 1: Band gap of unstrained (a) and ⟨100⟩ biaxially strained (b) $Si_{1-x-y}Ge_xC_y$ alloys as a function of the alloy composition. The shaded region depicts the variation in band gap observed from the simulation of 200 atomic structures.

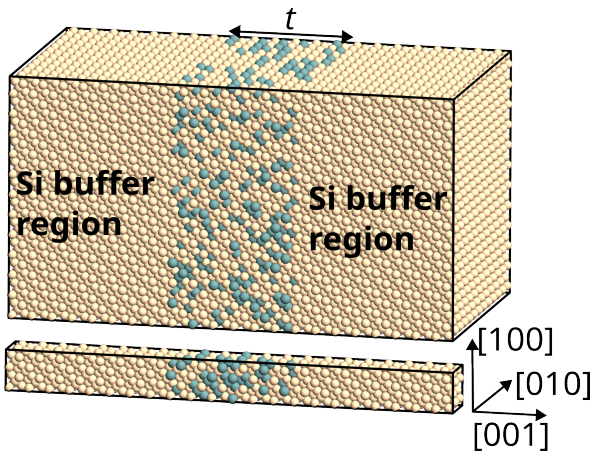

Figure 2: Example of the simulated atomic structure of a 3 nm thin SiGe layer between Si. Beige atoms are Si, green atoms are Ge.

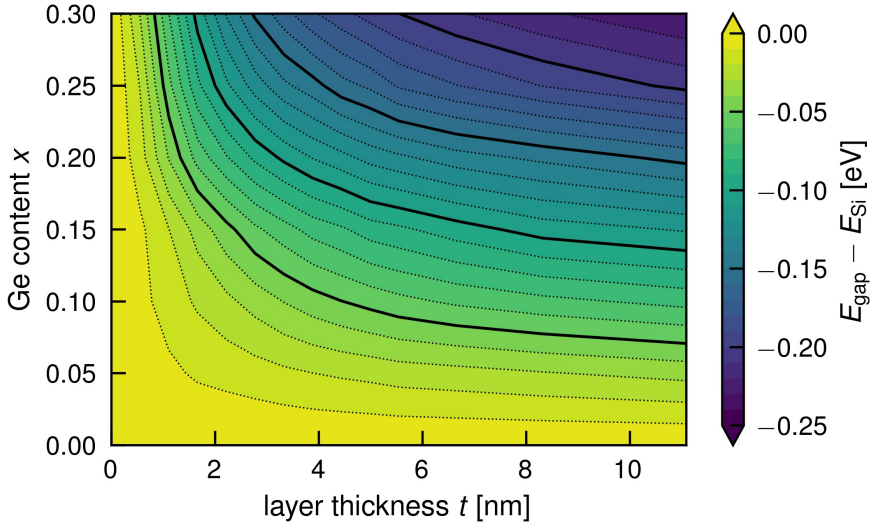

Figure 3: Effect of alloy composition and layer thickness on the band gap of biaxially strained SiGe layers. It is calculated as the mean value of 36 atomic structures.