First-principal calculations for giant valley splitting in stressed silicon thin films

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Since the discovery of giant valley splitting (~ 20 meV) [1] at the interface between buried-oxide (BOX) and silicon-on-insulator (SOI), we have experimentally found some related characteristics in the field-effect current [2] and the Stark effect [3]. Although some theoretical models for traditional valley splitting (< 1meV) at the interface between Si and thermal oxide had been already well-established [4,5], the main mechanism of giant valley splitting remains unclear yet. The uniqueness of our device is that, after the implantation of oxygen atoms, the BOX and SOI layers were annealed at very high temperature (1350 ºC) which is near the melting point of Si (1414 ºC) to obtain an atomically flat interface. Considering this fact, we build a hypothesis [6], that is, an extraordinary strong strain exists in the $[110]$ direction at the interface after cooling and that induces the giant valley splitting. Up to date, some papers have discussed the stress effect on the electric states in Si thin films mainly with perturbative-type calculations [5,7], starting from one-electron Hamiltonian. On the other hand, in this work, we extensively performed first-principal calculations on stressed Si slabs to prove the hypothesis discussed above.

The super cell of Si slabs is constructed so that the unit vectors are taken in the $[\bar{1}10]$, $[110]$, and $[001]$ directions. Each Si layer parallel to the x-y plane contains one atom, and they form a spiral staircase in the super cell. Both upmost and downmost Si atoms are terminated by two hydrogen atoms to passivate the surfaces. Then, the Si slabs are sandwiched with thick vacuum layers to prevent possible interaction between consecutive Si slabs. In the calculations we used local density approximation (LDA) as the approximation to the exchange-correlation energy and norm-conservative pseudopotentials for both Si and H. The cutoff energies for wavefunction and electric density are 60 and 540 Rydberg, respectively. The mesh of k-point sampling is set to be 6x6x1.

The quantized energy levels are clearly seen at Γ point in the energy diagrams. The valley splitting is defined as the energy separation of the lowest sublevel in the conduction band. In Fig. 1, the valley splittings are plotted as a function of electric field applied perpendicular to the Si slab (30 ML) with various strengths of stress in the $[110]$ direction. Even without stress (0.0 GPa), the valley splitting increases with increasing the electric field due to the confinement effect, as predicted by the theoretical models [4,5]. Clearly the stress magnifies this field effect to the level of the giant valley splitting.

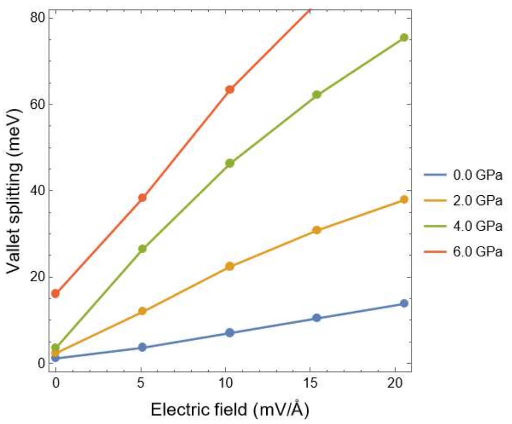

Fig.1. Valley splitting as a function of electric field with various strengths of stress.

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