Capping and core layer-dependent carrier dynamics on Ge/Si NC memory

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Nonvolatile memory devices based on Ge/Si core-shell nanocrystals (NCs) [1], have attracted attention due to their ability to handle the trade-off between the programming speed and the retention time by minimizing tunnel oxide thickness. Recently, several experimental groups have highlighted the effect of Si-cap (Ge-core) thickness and overall size distribution of Ge/Si dome shaped structure on various device parameters, including retention lifetime of the charge (hole) [2]. Theoretical groups tried to analyze the effect of confinement on these structures using effective mass and pseudopotential methods by assuming bulk band alignment and valence band offset between the Ge and Si region. To understand the effect of capping and core layer thickness on the electronic structure, carrier lifetimes, and other operating parameters of these NCs, a detailed atomistic model is necessary to capture the atomic scale inhomogeneities of the devices. Often, atomistic models of the NCs are severely size-limited, hindering a direct comparison of simulations with the experimental devices.

In this work, we carry out a computational study of the low-energy electronic states in dome-shaped Ge/Si core shell NCs using a full-band, $sp^3d^5s^*$ nearest neighbour empirical-tight-binding model including spin-orbit (SO) coupling as implemented in NEMO3D [3]. The strain due to the lattice mismatch between Ge and Si is calculated using the valence-force-field (VFF) model with Keating Potentials. The energy difference between the ground and excited first delocalized hole state is defined as the barrier height (Φ_b). Φ_b is calculated by analyzing probability densities ($|\Psi|^2$) of these states in the Ge core layer obtained from the tight-binding method. Using these barrier heights, the thermionic lifetimes (τ^{th}) that govern the overall retention characteristics are calculated as a function of capping layer and core layer thickness. In doing so, the height of the dome shaped QD is varied from 6.5 nm to 10 nm. The base size of the NC is maintained at 5 nm.

The energy gap (E_g) decreases from 1.125 eV for the 0.5 nm Ge core thickness and reached the bulk Ge bandgap value of 0.7 eV for 3 nm Ge core thickness. This reduction in the energy gap is mainly attributed to the increasing hole energy levels, where the electron energy levels remain unchanged. This behaviour is attributed to the TYPE-II band line up as shown in Fig.1.c. The quantum confinement energy (E_c) and the effective mass of the hole also show a strong dependency on the Ge core thickness, consistent with that found in other theoretical work [4, 5]. However, the effect of the capping layer thickness on these parameters is negligible. Similarly, the barrier heights and the thermionic lifetimes demonstrate a strong dependence on the core thickness. The lifetime reaches desirable lifetime of few microseconds when the Ge core thickness increases beyond 2 nm.

In conclusion, we have performed a comprehensive study on the effect of varying Si capping and Ge core layers on the carrier dynamics of the dome shaped Ge/Si core shell NCs using the atomistic tight-binding method including strain using the VFF model. Various carrier dynamic related parameters, such as confinement energies, bandgap, and effective masses, were also analyzed and these parameters match closely with the experimental measurements and follow intuition, showing that atomistic details of the devices are crucial to fully understand these devices. Our study also finds that the Ge core layer thickness dominates the carrier dynamics over the Si capping thickness, providing optimized design parameters for the devices.

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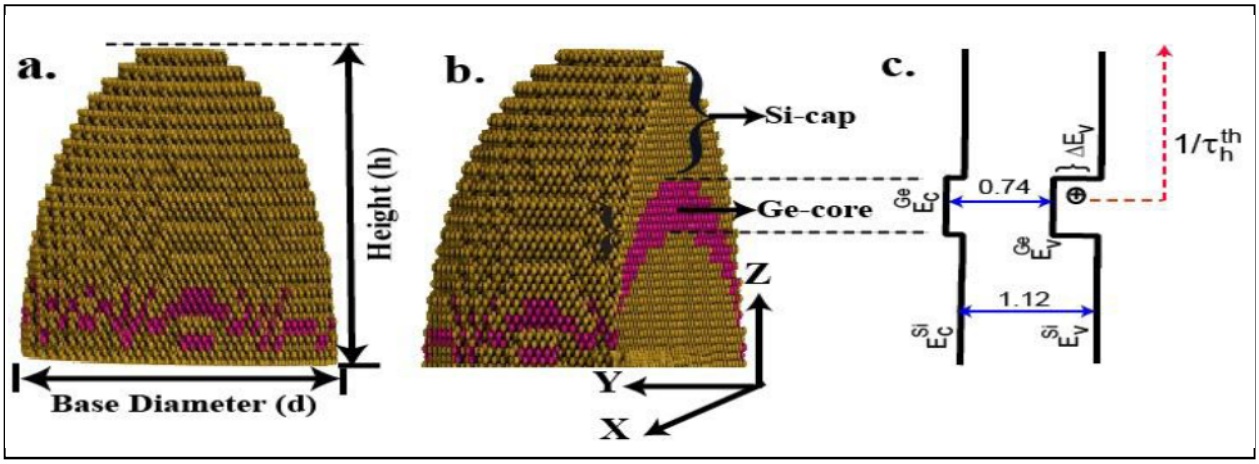

Fig.1 (a) Front view of the dome-shaped Ge/Si core shell NC with Ge core and Si cap thicknesses of 3 nm and 2.5 nm, respectively. The base diameter is maintained at 5 nm. (b) Dissected view of the same NC highlighting Si capping layer and Ge core layer. (c) Energy band diagram of Ge/Si TYPE-II heterostructure as formed by the combination of inner Si layer -Ge core layer- Si cap layer. The numerical values of 0.74 and 1.12 represent the bulk bandgaps in eV for Ge and Si, respectively. The $1/\tau^{th}$ is the thermionic escape rate of the hole from the Ge-region into the Si-region.

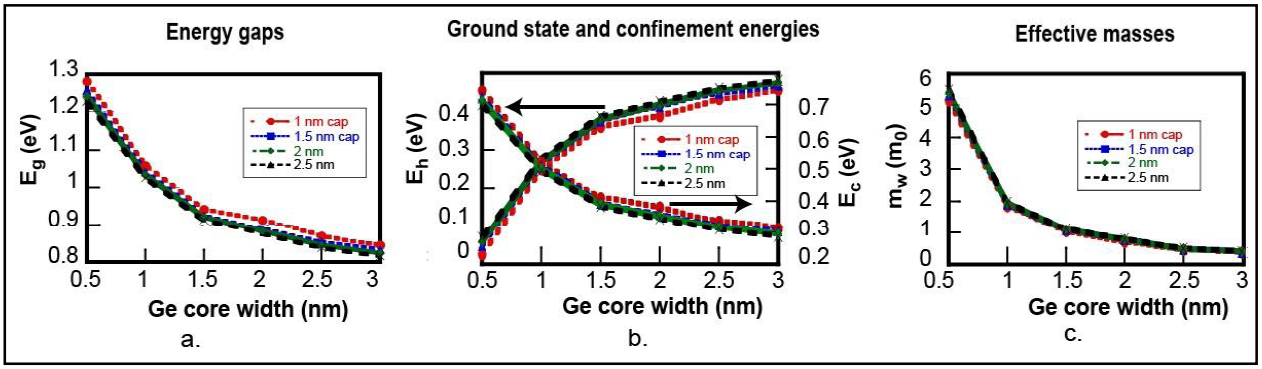

Fig.2 (a) Minimum energy gap (E_g) as a function of as a function of Ge core and Si cap thickness. (b) Ground state hole energy (E_h) and Confinement energy (E_c) as a function of Ge core and Si cap thickness. The confinement energy (E_c) is defined as $E_c = E_v$ (Ge) - E_h, where E_v (Ge) is the bulk valence band edge of Ge. (c) Effective mass of hole inside the Ge core layer.

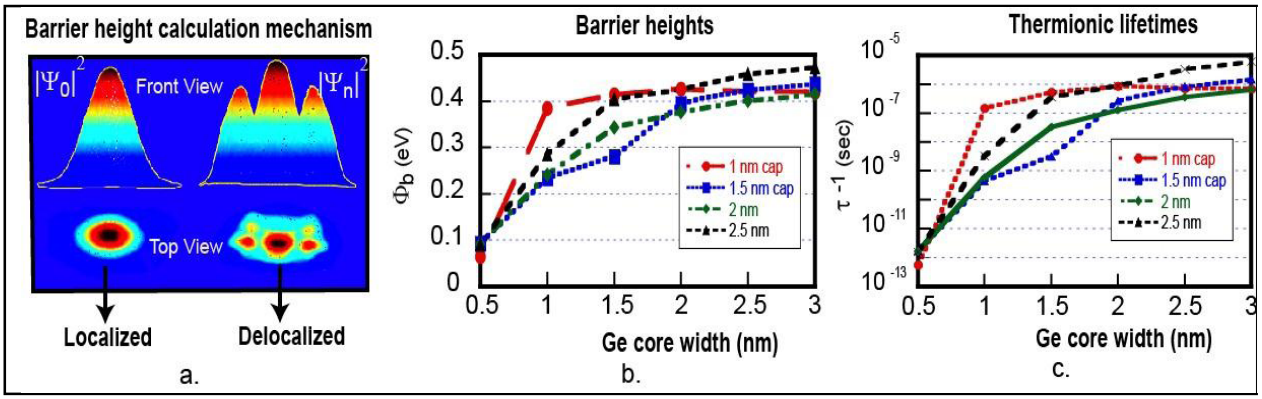

Fig. 3 (a) Probability densities ($|\Psi|^2$) of localized and first delocalized hole states in the Ge core layer of a dome shaped Ge/Si core shell NC with Ge core and Si cap thicknesses of 3 nm and 2.5 nm, respectively. The 'n' in the delocalized probability density represents the index of the first delocalized hole state. (b) The barrier height (Φ_b) i.e. $E_0 - E_n$, where E_0 is the ground state hole energy and E_n is the energy of the first delocalized hole states, as a function of Ge core and Si cap thickness.(c) Thermionic lifetime as function of Ge core and Si cap thickness