SIMULATIONS OF ION-BEAM INDUCED ATOM-MIXING OVER Si/SiO_2-INTERFACES FOR PREPARATION OF CONCENTRATION PROFILES

C. Fridlund, K. Nordlund and F. Djurabekova

Pietari Kalminkatu 2, P.O.B. 43, FIN-00014 University of Helsinki, Finland
email: christoffer.fridlund@helsinki.fi

The Internet of Things (IoT) have an ever-increasing demand for more power conserving components. Single Electron Transistors (SET) are very promising for reducing the energy consumption on electronic devices. Nanosized Quantum Dots (QD) are the working foundation of the SET, and the size is crucial for using them reliably at room temperature. To produce these transistors commercially, a reliable manufacturing method is needed. Previous research have proven, that it is possible to fabricate the desired size on the QD through controlled self-assembly during phase-separation in restricted volumes of meta-stable SiO_x.

Here, we present a computer simulation model, based Molecular Dynamics (MD), to assess the formation of SiO_x restricted volumes through ion-beam mixing of Si into a 7 nm thick SiO_2 layer embedded in Si. Systems with both one and two Si/SiO_2-interfaces have been used in the simulations. Atomic cascades, initiated subsequently by thousands of energetic Si^+ ions in a volume of approximately 20x20x7 nm^3, are needed to provide sufficient mixing of Si recoil atoms into SiO_2, for self-assembly of the 2-3 nm wide QD.

The ion-beam irradiation, for producing the meta-stable SiO_x volume over a single interface, was simulated in two independent series. One using a Tersoff-like Munetoh potential splined with a universal ZBL potential, and the other using a Stillinger-Weber-like Watanabe potential. One series of a bigger system with two interfaces, was simulated with a speed-up MD model. The system was connected to a heat bath by having a Berendsen thermostat controlling the border atoms during the cascades. The intermixing of Si into SiO_2 layer from the interfaces, related to forward scattering in the single interface system (forward- and back-scattering in the double interface system, was analyzed in detail during the development of the atomic cascades. The resulting concentration profiles of SiO_x from our MD model was used for phase-separation simulations by kMC model.

This work has been funded by the European Union's Horizon 2020 research and innovation program under grant agreement No 688072.