

Advanced Doping Processes in Group IV Semiconductors: Understanding and Modelling of Defects Formation and Dopant Activation

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In semiconductor technology, the various structural and electrical defects formed during the increasingly complex fabrication processes have a deleterious impact on the performances of the final devices. In most cases, such defects must be avoided or minimized. In practice, process optimization is achieved by combining thorough experimental investigations with physical modeling and predictive simulations in order to understand the underlying physics and identify the key parameters governing defect formation. Depending on the pursued degree of understanding, the required simulation methods may cover a very large range of size and time scales, from *ab-initio* methods to molecular dynamics, kinetic MC and continuum models. This is true in all phases of device fabrication, including the doping processes used for the fabrication of MOSFET source/drain regions, which will be discussed in this talk. In this case, the doping efficiency is intimately related to the formation and evolution of point and extended defects that form and grow during the dopant implant and annealing steps.

Two “historical” case studies, briefly resumed in the first part of the presentation, were the Transient Enhanced Diffusion phenomenon, and the incomplete dopant activation (i.e. below the equilibrium solid solubility) both occurring during annealing of ion-implanted dopants in silicon. Here, the perfect synergy between dedicated experimental and theoretical studies allowed to identify the nature and the energetics of the defects (self-interstitial or dopant-interstitial clusters) at the origin of the observed phenomena.

Today, the increased difficulties to maintain the transistor miniaturization pace have led to a diversification of both the basic device architecture and the fabrication processes. In particular, the recent advances in nanosecond laser annealing (NLA) have opened the way to solve a wide spectrum of difficult challenges in semiconductor technology, well beyond the “traditional” source/drain fabrication issues. In the second part of the presentation, we will therefore present some of our recent investigations on damage and strain evolution and their impact on dopant distribution and electrical activation during NLA of group-IV semiconductors. In one case, the successful collaboration between experimentalists and theoreticians has already provided an in-depth understanding of damage formation after NLA of ion-implanted silicon. Few other examples will be given where open questions persist, and a full understanding of the observed phenomena is still missing, such as the formation of surface hillocks at the early stages of the melt process and their impact on the final roughness of the liquid/solid interface.