UV Excimer laser processing of SiGe and SiGeSn: finite elements method numerical modeling

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During the years, Pulsed Laser Induced Epitaxy (PLIE) has always been the "alternative" for epitaxial formation of group IV alloys with great variety of intermixed components, ranging from SiGe¹⁻³, SiC⁴, SiGeC⁵⁻⁷ to GeSn⁸⁻¹⁰ and SiGeSn^{9,11,12}. First Abelson et al.¹ was able to overcome the drawback of PLIE, called "cellular" structure growth^{8,13} for SiGe and our group for GeSn⁹ (for the given bellow configuration), resulting epitaxial abrupt or tailored concentration Si/Ge/Sn layers. The process itself consists of ultra rapid (up to several hundred ns) pulsed laser heating/cooling of the alloy components previously deposited in form of a multilayer structure and a crystalline substrate followed by epitaxial growth and solidification of the mixture.

Numerical simulation of the laser/material interaction has been widely used, mainly in high power lasers processing, to predict and fine tune the optimal experimental conditions^{14,15}. Same approach was later transferred to PLIE processing of group IV elements¹⁶ and alloys^{10,12,17,18}. In general, it consists of Finite Elements Method (FEM) solution of the Heat Conduction Differential Equation (HCDE) for given boundary conditions and known heat gradient devoted from the Beer–Lambert law. The FEM analysis yields the values of the maximum melting depth (MMD) and melts duration (MD) for each mesh element. Those parameters can be extracted directly compared with experimental ones after sample characterization. MD or liquid phase monitoring, the so called Time Resolved Reflectivity (TRR), of the ultra rapid PLIE process yields essential experimental information correlated to the level of intermixing and thus composition^{1,9,19}. It can be easily obtained with the simple experimental setup shown on figure 1 (left). Fig. 1 (right) represents good agreement of the TRR signal with the data obtained from the FEM analysis of 4 nm Sn/100 nm Ge/Si(100) multilayer. This paper aims to represent our approach to FEM analysis of group IV elements PLIE processing in general and our latest results concerning GeSn and SiGeSn alloys.



Fig. 1 Experimental PLIE/TRR setup (left). Temporal evolution of the (a) interface temperatures, (b) depth of solid-liquid transition, and (c) reflectivity, caused by the first laser pulse of 200 mJ/cm^2 (right).

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