Experimental Studies of Dopant Diffusion in Strained Si and SiGe

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It is of crucial importance for modeling and simulation of physical processes, that reliable experimental information exists against which the models can be tested. Epitaxially grown semiconductor heterostructures are ideal systems for producing such information as a number of parameters can be varied such as e.g. chemical composition, and size and type of biaxial strain (tensile or compressive) [1]. The Si/SiGe epitaxial system constitutes such a system.

We have over the past 10 years studied atomic diffusion in the Si/SiGe epitaxial system using molecular-beam epitaxially grown structures containing well-defined narrow distributions of the tracer impurity or isotope under investigation. The atomic profiles were measured using secondary ion mass spectrometry (SIMS), and the structural quality of the samples and their possible strain relaxation by misfit dislocations during heat treatment were examined by transmission electron microscopy (TEM).

We have up to now studied the diffusion of four different elements in biaxially strained $Si_{1-x}Ge_x$ and strain relaxed $Si_{1-x}Ge_x$, namely the two interstitially assisted diffusers B [2, 3] and P [2, 4], the vacancy assisted diffuser Sb [5] and the mixed vacancy and interstitially assisted diffuser Ge [6]. For details on sample preparation, sample dimensions etc., we refer to the original papers. As concerns the studies of the strain relaxed systems, which is not the topic of this presentation, one of our goals is to follow the diffusion all the way from Si (x=0) to Ge (x=1). Up to now we have performed studies for $x \leq 0.5$. We are in particular concerned with an expected change-over from interstitially to vacancy assisted diffusion for B and P. In the case of diffusion in strained layers, strain relaxed systems of the same composition have been included in all are investigations in order to make it possible to separate the effect of strain from the effect of composition. During our recent studies of B diffusion in $Si_{1-x}Ge_x$ it became clear that in order to obtain accurate diffusion coefficients a protective capping of the surface layers is a prerequisite. As described in [3, 7], we have found a double layer of SiO_2 and Si_2N_3 adequate. The B results of [2] have been obtained using such coatings whereas most of the P results have been obtained with bare surfaces. Thus, the P results must be considered as being preliminary. It is nevertheless clear that compressive strain retards the diffusion of B and P, whereas tensile strain enhances the diffusion. This is in agreement with the prediction by Aziz [8]. The opposite is found to be the case for Sb and Ge. Thus, we conclude that the diffusion of interstitially assisted diffusers is retarded in compressive strain and enhanced in tensile, and that the opposite is the case for vacancy assisted diffusers. The activation energies for Sb diffusion are found not to vary with strain contrary to those of B, P, and Ge. Hence, the activation energy for vacancy assisted diffusion is apparently not strongly influenced by the strain unlike that of interstitially assisted diffusion, as also indicated from the formation energy calculations of [9].

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