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## LATTICE SITTING OF PLATINUM ATOMS IN DILUTED SiGe ALLOYS\*

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In this report we present high-resolution spectra obtained with a use of the Laplace transform deep level transient spectroscopy for platinum diffused into dilute (0–5% of Ge) SiGe alloys. Very significant changes are observed in the spectra associated with the transition metals as the germanium content is altered. We interpret these spectra in terms of the configurations of silicon and germanium atoms surrounding the transition metal. In order to explain the observed behaviour both the first and second nearest neighbour shells are considered.

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The microscopic scenario of the diffusion process of different elements in silicon has been studied in considerable detail (see, e.g., Ref. [1] for a review). In general, the diffusion of smaller than silicon atoms is promoted by the presence of self-interstitials, on the other hand, larger atoms diffuse faster when there are more vacancies. It is also known that metals in dislocation free silicon diffuse by the so-called kick-out mechanism, which is a combination of purely vacancy- or interstitial-driven processes. Namely, the metals diffuse via interstitial sites, however, they can also interchange site between interstitial and substitutional with a co-operation of a self-interstitial.

The above rules can be substantially altered when the diffusion process occurs in a silicon–germanium alloy. In general, the germanium atoms are larger than silicon ones thus one would expect that, from a purely elastic point of view, the diffusion process of smaller than silicon elements should be promoted, while those having larger than silicon atomic radius should be a poorer diffuser in the alloy

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than in the silicon crystal. One approach to investigate this hypothesis is to determine the lattice position of a metal diffused into the alloy and conclude whether the metal atoms have any preferences in terms of having more or less germanium atoms in their neighbourhood. A comparison of the observed probability of different configurations with the statistics of a truly random alloy can show whether specific sites are energetically favourable.

Point defects in the alloy can have different local environments resulting from the configuration of atoms in the vicinity of the point defect. As a result the electron or hole thermal emission process is slightly modified. In this case the capacitance transients measured by the deep level transient spectroscopy (DLTS) technique contain slightly different components whose number and amplitudes depend on the number of different atomic configurations and their concentrations in the neighbourhood of the point defect. In this study the site preferences of the point defect, in this case the platinum atom, are derived from the analysis of the high-resolution Laplace DLTS spectra. In this method, in contrast to the standard DLTS technique, it is possible to see a fine structure in the thermal emission [2]. The samples used for this study were grown by molecular beam epitaxy. The *n*-type epitaxial layers had between 0 and 5% of the germanium atomic content. The metals were diffused into the layers at 800°C for 24 hours.

The Laplace DLTS spectra of the platinum-related defect in silicon show, as reported previously [2], no structure with one peak. However, when the germanium content in the alloy is increased we observe additional features appearing in the spectra. These features, as for the case of gold in SiGe alloys [3], are seen in standard DLTS spectra as a broadening of the peaks. Our experience shows that when the germanium content in the crystal exceeds 5% then the number of the features on the spectra is too large to be observed by the Laplace DLTS method, thus the investigations are restricted solely to diluted SiGe alloys.

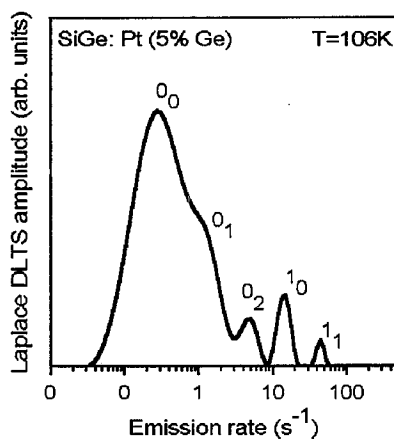


Fig. 1. The Laplace DLTS spectrum of the platinum-related centre in the SiGe alloy (5% of germanium). The figures and subscripts denote the number of germanium in the first and second nearest shell, respectively.

Figure 1 shows the platinum-related Laplace DLTS spectrum for a SiGe sample with 5% of germanium. In the spectrum there are five features not forming a series of lines. If one assumes that the distribution of germanium atoms in the first nearest shell is truly random then for four atoms in this shell one would expect to have five different configurations. However, in this case the probability of having more than three germanium atoms would be very low. In SiGe the influence of the local environment beyond the first shell is believed to be significant, therefore it is necessary to assume that the second nearest neighbourhood of atoms (an additional twelve) also influences the emission process. Consequently, features in the spectrum come from different configurations of atoms in the first and the second neighbourhood of platinum. A simulation of possible configurations, when two shells of atoms are considered, allowed us to assign the features on the spectrum to two groups of peaks, i.e., those having zero and one germanium in the first nearest shell. Within the group there are lines differing by a number of germanium atoms in the second shell and these atoms influence much less the emission process than those in the first nearest shell. The features on the spectrum have assignments where figures and the subscripts denote the number of germanium atoms in the first and second nearest shell, respectively. Although the pattern of peaks on the spectrum is similar to those obtained from the simulation procedure, the relative concentrations differ from the case where a random sitting is assumed. Basically, the configurations of atoms having more germanium in the first and/or in the second shell are observed in the spectra in larger concentrations than expected from the simulation procedure. Consequently, it seems that platinum prefers to occupy lattice sites closer to germanium atoms.

Similar experiments have been performed for the case of gold diffused into SiGe alloys by measuring electron emission from the gold acceptor. As in the case of platinum, peaks in the Laplace DLTS spectra, which we relate to the presence of germanium in the vicinity of the gold centre, have much higher relative amplitudes than one would expect if the concentration of germanium close to gold is the same as in the rest of the alloy.

Summarising, our results show that in the SiGe alloy the germanium atoms (which have a larger ionic radius than silicon) tend to increase the probability of the transition metal atoms (smaller than silicon) occupying adjacent sites as germanium and platinum (or gold) cause internal stress in the crystal of the opposite sign.

### References

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