Pseudomorph $Si_{1-x}C_x$ Films on c–Si to Enhance Nucleation of (100) Oriented CVD Diamond Films ◇

A. Bergmaier, G. Dollinger, and C. M. Frey

The outstanding properties of diamond such as wide band gap, high thermal conductivity and high dielectrical strength have raised particular interest in this material and its possible applications in the semiconductor industry. The chemical vapour deposition (CVD) technique has emerged as a well established method of depositing diamond films of good crystal quality on foreign substrates. In terms of future devices, using single crystal Si(001) wafers as substrates for diamond deposition has numerous advantages. One of the major difficulties to be overcome in the heteroepitaxial nucleation of diamond on Si substrates is the substantial lattice mismatch. The relation of the lattice constants of diamond ($a_{dia} = 0.3567$nm) and silicon ($a_{Si} = 0.5430$nm) is $a_{Si}/a_{dia} = 1.522$. Though the mechanism of heteroepitaxy of diamond on silicon is not finally understood yet, there are hints from high resolution electron microscopy pictures that a direct growth of diamond on silicon with orientation diamond[100]//silicon[100] is possible without any buffer layer [1]. That means, there exists nearly a 3:2 match of the lattices by a mismatch of 1.49%. The mismatch might be reduced by a suited buffer layer and, therefore, the nucleation of (100) oriented diamond should be enhanceable. Pseudomorph $Si_{1-x}C_x$ layers on monocrystalline silicon are suggested as buffer layers, because alloying silicon with a small amount of carbon reduces the lattice constant [2]. $Si_{1-x}C_x$ layers with carbon concentrations of $x < 10\%$ were grown on monocrystalline (100) silicon using solid source molecular beam epitaxy (MBE) [3]. In order to get exact information about the dependence of the lattice constant on the carbon concentration, the carbon contents in the films were quantitatively measured by means of high resolution elastic recoil detection (ERD) and the change of the lattice constant was determined using high resolution X–ray diffraction.

The ERD measurements were performed at the Q3D magnetic spectrograph, the experimental setup is described elsewhere [4,5].

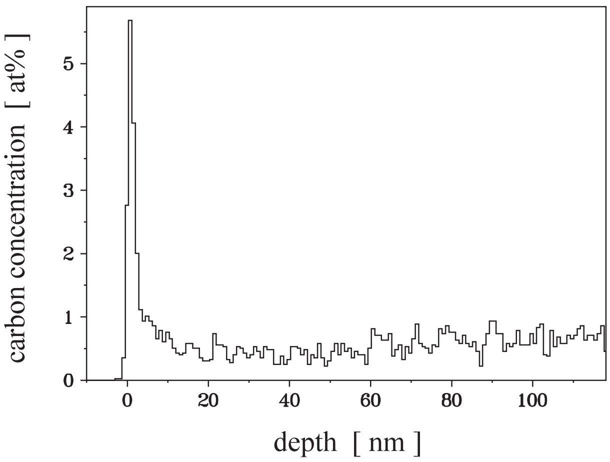

Fig. 1: High resolution carbon depth profile of a $Si_{1-x}C_x$ layer

High resolution depth profiling of carbon is important in order to get quantitative results even if strong surface contaminations would superpose the small carbon amount in the layers by low resolution analysis, e.g. the narrow peak at depth 0 in Fig. 1 stams from carbon contaminations on the sample surface. The spectrum shows a small increase with depth of the carbon concentration within the layer, while the average concentration is 0.61%.

For carbon concentrations $x < 2\%$ the $Si_{1-x}C_x$ layers were pseudomorphic with a smooth surface. For $x > 2\%$ the layers were highly twinned and had a surface roughness of about 20 nm. The as grown films show anisotropic lattice constants with no in plane relaxation. The distance of (100) planes parallel to the surface depends linearly on the carbon concentration and agrees quantitatively with Vegard's Law between Si and diamond (Fig. 2, solid line). The empirical law of Vegard says that the lattice constant of an alloyed crystal results from a summation of the weighted lattice constants of the pure crystals in the isotropic case. For comparison with Vegard's Law, the predicted change of the lattice constant according to Vegard's Law is transformed to the anisotropic case by elasticity theory using the elastic constants of Si. Using Si and SiC for Vegard's assumption, a linear dependence of lattice constant on C–content results in a stronger dependency (dotted line).

However, no in plane relaxation was found even after thermal treatment and, therefore, no enhancement of (100) oriented nucleation and growth of diamond was observed yet [6].

References

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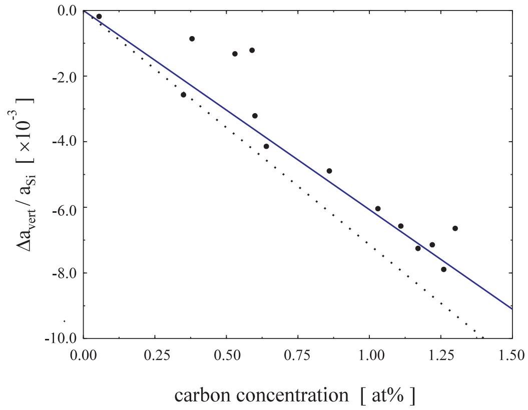

Fig. 2: Relative variation of the lattice constant of the $Si_{1-x}C_x$ layers versus carbon concentration measured by ERD.

◇in cooperation with T. Gutheit, Daimler–Benz AG, Research Center Ulm, D–89081 Ulm