ROBL-CRG	**Experiment title:** **Crystallisation of TaSi thin layers**	**Experiment number**: 20_02_IH3
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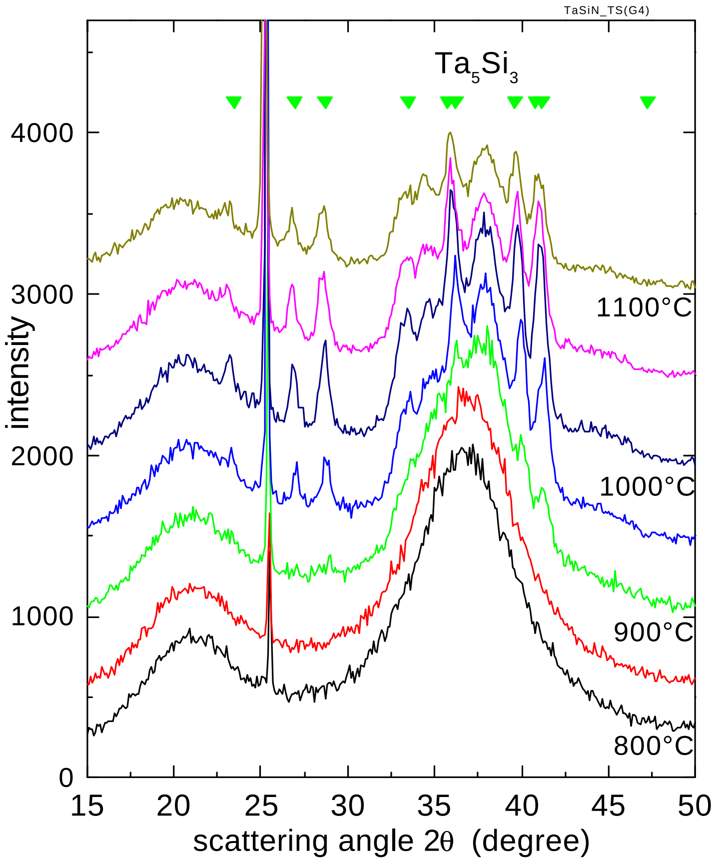
Report:

Tantalum or TaSi layers are promising materials for diffusion barriers in microelectronics circuits with copper conduction paths. It is known, that layers of 100 nm thickness show columnar crystals and that in such cases diffusion along grain boundaries plays a great role. Therefore, the suppression of crystallisation of Ta-containing layers is a way to improve the diffusion barrier. This crystallisation suppression should be guaranteed up to temperatures of 700°C in order to allow for the thermal processes during circuit production.
One way to destroy crystalline order is the ion irradiation of the layer, preferably with ions forming badly crystallising Ta compounds (e.g. N, O, B). For 100 nm TaSi layers the crystallisation of $TaSi_2$ was observed after annealing at 650°C for 1 h. After irradiation of the same film with $3x10^{17}$ N/cm^2 no crystallisation was observed up to 800°C [1].

In the actual study 50 nm TaSi layers on Si/SiO_2 substrate were compared with respect to thermal stability of the non-crystalline state for an as-deposited sample and another which was subjected to $1.5x10^{17}$ N/cm^2. For temperatures from 600 to 1100°C the diffraction was recorded in the high temperature chamber. A wavelength of 0.154 nm and an grazing incidence angle of 1° was used.

The initial diffraction pattern of both materials appears amorphous. With increasing temperature some Bragg-reflection of crystalline phases occur. For the **as-deposited TaSi-layer** at 900°C the first indications of crystalline Ta_2O_5 occur. Increasing the temperature up to 1100°C leads to a narrowing of the oxide peaks which is due to grain growth. The amorphous scattering contribution remains in the pattern up to 1000°C, which indicates the oxidation from the surface (vacuum in the chamber: $5x10^{-6}$ mbar). No other phases and no indication of the involvement of Si is detected.



The **nitrogen-implanted TaSi layer** remains amorphous up to 850°C (see figure on the left). Above this temperature the crystallisation starts and the compound is identified as Ta_5Si_3. The peak positions are indicated by triangle in the figure. Up to 1000°C there is a significant amor-phous scattering contribution indication a step by step crystallisation of the layer. The silicide peaks narrow up to 1050°C and than broaden again. The latter effect is regarded as the beginning dissolution of the crystallites.

The effect of nitrogen implantation in TaSi is not primarily the stabilisation of the amorphous state of the TaSi layer as expected from implantation into pure Ta [1]. The onset of crystallisation is only 50 K higher than for pure Ta. The mixing of Ta and Si obviously makes the formation of a tantalum silicide possible, since in the unimplanted sample no such compound occurs.

[1] E. Wieser, J. Schreiber, C. Wenzel, J. Bartha, B. Bendjus, V. Melov, M. Peikert, W. Matz et al., Proc. Adv. Metallization Conf. 99, MRS, Warrendale, PA (2000) p. 257