Plasma CVD of Si/C/N: Experimental and theoretical results

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Amorphous and crystalline silicon carbonitride materials have attracted great interest in recent years[1] due to outstanding oxidation resistance at elevated temperatures[2], high hardness[3] as well as excellent wear characteristics[4]. This study is focused on the synthesis of Si/C/N hard coatings on metal substrates for tribological applications. It is based on an interdisciplinary co-operation between four research institutes. Starting from single-source precursors, coatings were prepared using very similar PECVD devices at IPHT Jena and IFMS Darmstadt (Figs. 1 and 2). At Jena the CVD process is experimentally examined by laser assisted *in situ* mass spectrometry (Fig. 2). Quantum-theoretical calculations are used at RWTH Aachen in order to examine the species in the gas phase as well as surface reactions with the substrate and solid state structure-property relations. The mechanical and tribological characteristics important for industrial applications of the coatings and coating-substrate composites as well as the oxidation and corrosion behaviour (in particular at high temperatures) are examined at IfW. The overall objective of this joint research project is to gain a comprehensive understanding of the CVD process as a whole. First preliminary results are presented here.

Two single-source Si/C/N precursors, hexamethyl-disilazane (Me_3Si-NH-$SiMe_3$, HMDS) and bis(trimethyl-silyl)carbodiimide (Me_3Si-NCN-$SiMe_3$, BTSC) were used for deposition of the coatings by means of RF plasma CVD. Both compounds are colorless liquids with comparable volatility. Polished metallic substrates (e.g. $TiAl_6V_4$) and silicon wafers were used for the deposition of the coatings.

The experimental parameters are summarized in Table 1 and the deposition chamber is schematically shown in Figure 1. The structure, composition and properties of the coatings were experimentally investigated with FTIR, XRD, SEM, EDX, GDOES (glow discharge optical emission spectrometry), RBS, Auger spectroscopy, indentation hardness measurements and tribological testing.

All obtained coatings were homogeneous, smooth (SEM) and X-ray amorphous. FTIR and GDOES indicate relatively high hydrogen and oxygen contents. The chemical structure of the films strongly depends on the precursor and deposition parameters. Coatings with a thickness of up to 3 µm were obtained which showed hardness values around 30 GPa. Both the theoretical and the experimental results point to the fact that the hydrogen and oxygen content of the layers and the precursor structure have a very large influence on the entire property profile of the products.

Future work will be focused on correlating theoretically and empirically the type and characteristics of the gaseous species and surface processes as well as the relevant properties of the coatings in order to provide a deep and integral understanding of the selected PECVD process.

Table 1: Typical PECVD conditions

Precursor	HMDS	BTSC
T(substrate) [°C]	50 - 400	25 - 300
p [mbar]	0.1 - 5	1 - 15
RF power [W]	30	10 - 70
Carrier gas	Ar	Ar
t (deposition) [h]	1 - 2	0.5 – 2

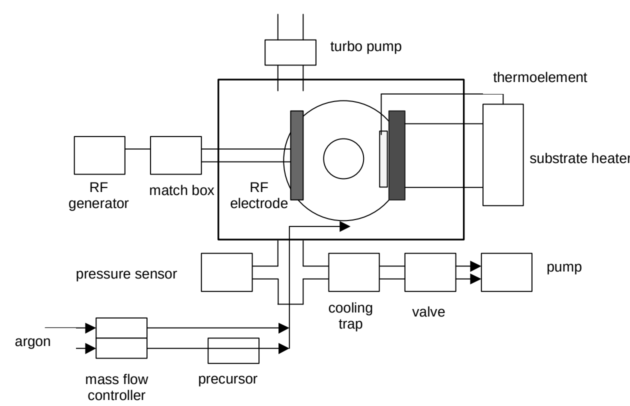

Figure 1: Scheme of PECVD apparatus

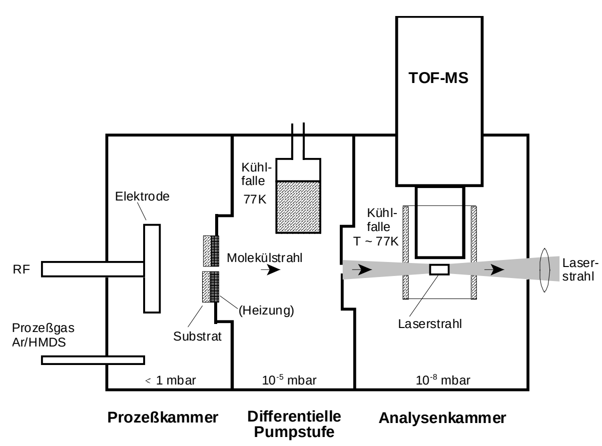

Figure 2: Scheme of PECVD apparatus with *in situ* mass spectrometry

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