

# Nanodiamond Surface Functionalization under Thermal Treatment in CCl<sub>4</sub>: Thermodesorption Mass Spectrometry Study

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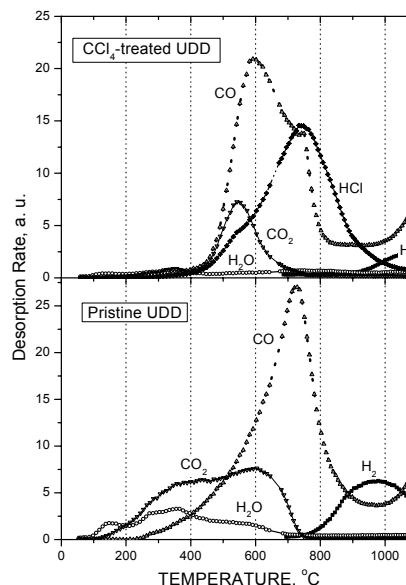
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**Introduction.** The behavior of ultradisperse detonation nanodiamond (UDD) in various environments is controlled by their surface properties which in turn depend on the details of detonation synthesis and chemical purification procedure [1]. As a rule the surface of commercially available UDD contains a number of functional groups of different composition and structure. The problem exists to unify and/or to modify the surface chemistry of UDD in an appropriate manner. One of the ways in this direction is the high-temperature treatment of UDD in CCl<sub>4</sub> [2]. We present the results of thermodesorption mass spectrometry (TDMS) study of UDD surface chemistry after this type of modification.

**Experimental.** UDD powder type UDA-SP produced and purified by "Sinta" was used as pristine material. Final chemical treatment was performed in the flow of CCl<sub>4</sub>/Ar mixture at 400°C for 1 and 5 hours. TDMS spectra were measured by quadrupole mass spectrometer under programmed heating (10°C/min) the sample up to 1100°C in vacuum.

**Results and discussion.** The main products of thermodesorption from pristine UDD were CO (400-800°C), CO<sub>2</sub> (200-700°C), H<sub>2</sub>O (100-600°C) and H<sub>2</sub> (800-1100°C) (see Figure). The complex shapes of thermodesorption profiles (especially in the case of CO<sub>2</sub> and H<sub>2</sub>O) indicate the presence of a number of surface H- and O-containing species of various configurations.

A substantial amount of HCl was found to release from modified sample (main peak at 740°C and a shoulder near 550°C). The HCl concentration increased with treatment duration and was comparable with the released amount of CO and CO<sub>2</sub>. At the same time CCl<sub>4</sub>-treatment caused the decrease in H<sub>2</sub>O (till the background level) and H<sub>2</sub> (tenfold decrease) abundance. The total content of CO<sub>x</sub>-yielded surface species was not changed too much though their configuration was modified noticeably as demonstrated by the temperature profiles of CO and CO<sub>2</sub> desorption. In summary, the thermal treatment of UDD in CCl<sub>4</sub> causes, besides drastic uptake of Cl-species, a substantial dehydrogenation (in the form of HCl) temperature lowering and some changes in the state of surface oxidation.



[1] D. Mitev et al. *Diam. Relat. Mater.* **16**, 776 (2007).

[2] B.V. Spitsyn et al. *Diam. Relat. Mater.* **15**, 296 (2006).