

1 Schematic representation of oxidation as initial step for further functionalisation.

2 Left: Non-functionalized Particles settle down immediately (sedimentation) Right: Functionalized Particles form a homogenous, stable mixture (dispersion) suitable e.g. for coatings.

## FUNCTIONALISATION AND COATING OF CARBON NANOMATERIALS

### Motivation

Nanocarbon materials are used as functional fillers to improve the properties of bulk materials and coatings. However, it is not possible to transfer all their superior intrinsic properties to the final composite. This is mainly caused by the complex processing of nanomaterials as well as the insufficient compatibility with the matrix material. In this regard, functionalisation is the key technology for the commercial usage of nanomaterials.

Functionalisation of filler materials improves the wetting properties and enhances the bonding to the matrix material. As a result, the filler material is much better dispersed and strongly bonded to the matrix. Furthermore, the protection from degradation caused by heat and/or strong mechanical forces during the production

process is another important usage for functionalisation.

### Fraunhofer IPAs approach

The objective of the Fraunhofer IPA is to develop economically feasible large-scale production methods for functionalisation, coating, purification and decoration of nanocarbon materials.

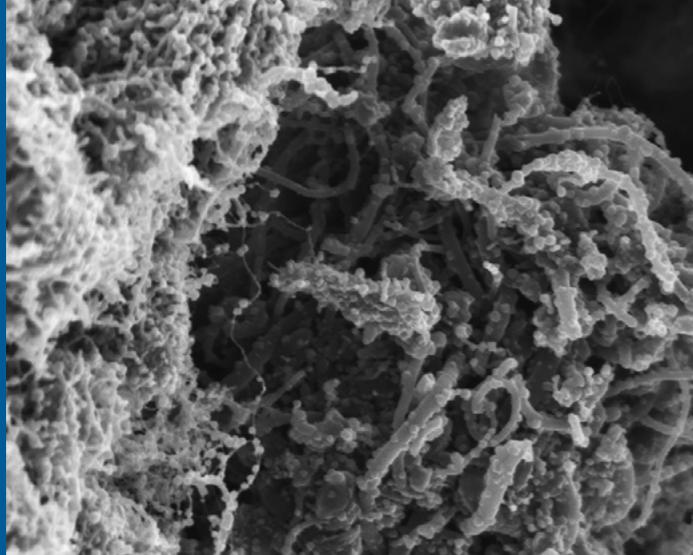
Purification of functionalised nanocarbons represents a complex problem, where the solution is never the same for two different products. Impurities and by-products consist of dissolved chemicals and various nanoparticles. High-performance physical methods are therefore used to separate products from the rest. Where standard processes could not be employed, Fraunhofer IPA develops alternatives according to customer demand.

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- Functionalisation of CNTs with carboxyl and fluorine-containing moieties: the generation of carboxyl-moieties and the covalent bonding of fluorine-containing groups allow for further functionalisation and, in this way, the further application by the customer.
- Coating of titanium/titania on CNTs: a coating of titanium/titania on CNTs can improve the further processing of CNTs in metal matrix composites. In this manner, a titanium/titania coating can be deposited on CNTs provided by customers or purchased from CNT manufacturers. Using high temperature procedures and chemical functionalisation, a thin titanium/titania coating can be partially applied on CNTs. Alternatively, bundles of CNTs can be coated. (CVD + Sol-Gel)
- Coating of nickel on CNTs: using electrochemical deposition, a coating of nickel can be applied on CNTs. This allows individual CNTs or bundles of CNTs to be used as starting materials.
- Other metallic coatings: using the technologies available at Fraunhofer IPA, metallic coatings other than those of titanium/titania or nickel can be deposited on CNTs. Particular requests will be first checked for feasibility.

All functionalisations are customer-specific. First, the requirements are stated and the synthesis route will then be determined, followed by the adjustment of reaction parameters. After an initial synthesis on a laboratory scale, customers will receive an estimation of the amounts and grades which could later be achieved on an industrial scale.

### Applications

Using a chemical blend of the nanocarbon materials with the matrix materials, composites with improved properties can be realised. This makes it possible to significantly increase their mechanical properties, such as tensile strength and E-modulus, and avoid defects within the composites, which result due to the agglomerates. In applications with ceramics and metals, improvements of the mechanical properties can be increased by several 100% compared to untreated nanocarbon materials.

Further developments deal with the cross-linking of functionalisation to improve the electrical and thermal properties of composites and thin layers.

### Benefits for customers

Our modified high-quality nanocarbon materials are designed to individually get the best processability as a filler material for composites or for coatings. These products have a range of uses, including:

- Barrier films
- Transparent conductive films
- Reinforced metallic and ceramic composites and structural materials
- Electrical conductive polymers

The functionalisations can be directly adjusted to the customer's manufacturing processes for composites and mean the best possible improvement of the material property can be achieved.

Developed final applications with our functionalisations demonstrate the following properties:

- Electrical conductivity of Al6061 alloys is improved by up to 20% with functionalised CNTs (no improvement with non-functionalised CNTs))
- Impact strength of Al6061 alloy increased by more than 250% (without functionalisation only 120%)
- Dispersibility of Ti-coated CNTs in several aluminium and aluminium oxide materials (without functionalisation, only possible with agglomerates)
- Transparent conductive layers with functionalised SWNTs and graphene nanoplatelets can be produced with high conductivity