

# Input to Materials Ontology Workshop

---

Michael Noeske: works at Fraunhofer IFAM since 2001 performing materials (surfaces) analysis and characterization

Main fields of his work that could contribute for elaborating materials ontology covering materials characterization:

- (1) **surface** science (thin films; time-dependent changes)
- (2) surface **analysis** (electron spectroscopy, scanning microscopy)
- (3) **probe** (electron, photon) / **matter interaction**

# (1) Surface science

## How to distinguish „between a given object and its surface“?

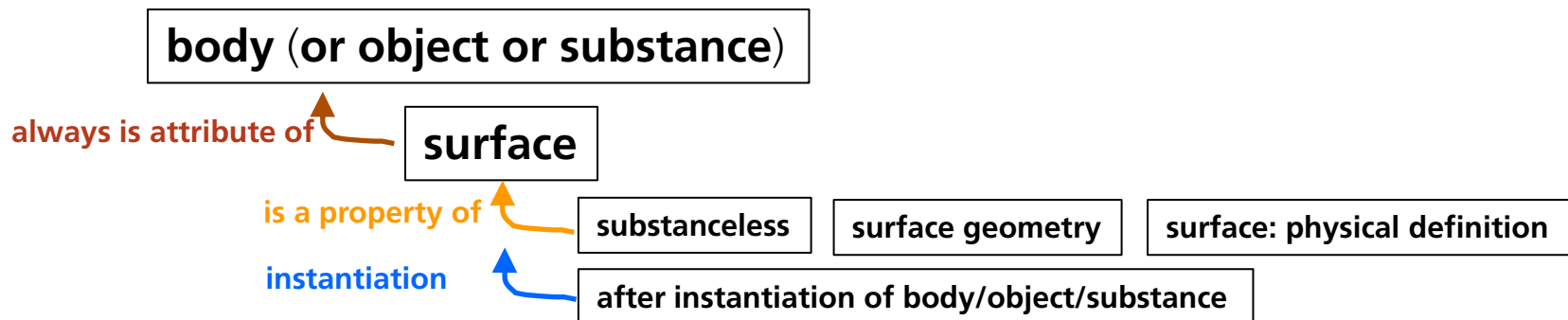
- geometrical distinction
- physical distinction
- ontological distinction

E. Paparazzo; „How old is surface science?“; Journal of Electron Spectroscopy and Related Phenomena 134 (2004) 9–24.

Aristotle (384 to 322 BCE):

Given a **body (or object or substance)**, its surface

- exists, as a mathematical and geometrical entity
- cannot be considered a substance
- is an accidental **attribute** of the substance to which it belongs
- can not be separated from it physically (only in thought)
- can not exist prior to the formation of the body.



# (1) Surface science

In IUPAC „Compendium of Chemical Terminology Gold Book“:

**Surface** is the boundary between two phases.

It is recommended *for the purpose of surface analysis* a distinction:

**Surface (in general)**

„outer portion“ of a sample

is a property of

undefined depth

is a type of

physical **surface**

in vacuum: that (one) **layer** „in contact with“ the vacuum

is a type of

experimental **surface**

during excitation with particles or radiation: that **portion** with which significant interaction (particles, irradiation) takes place;  
**Its volume is the larger one of the following two:**  
**1. volume** of the sample required for analysis OR  
**2. volume** corresponding to the escape for emitted radiation or particle

Michael's opinion: is a property of

information depth

adopted following <https://goldbook.iupac.org/html/S/S06154.html>

# (1) Surface science

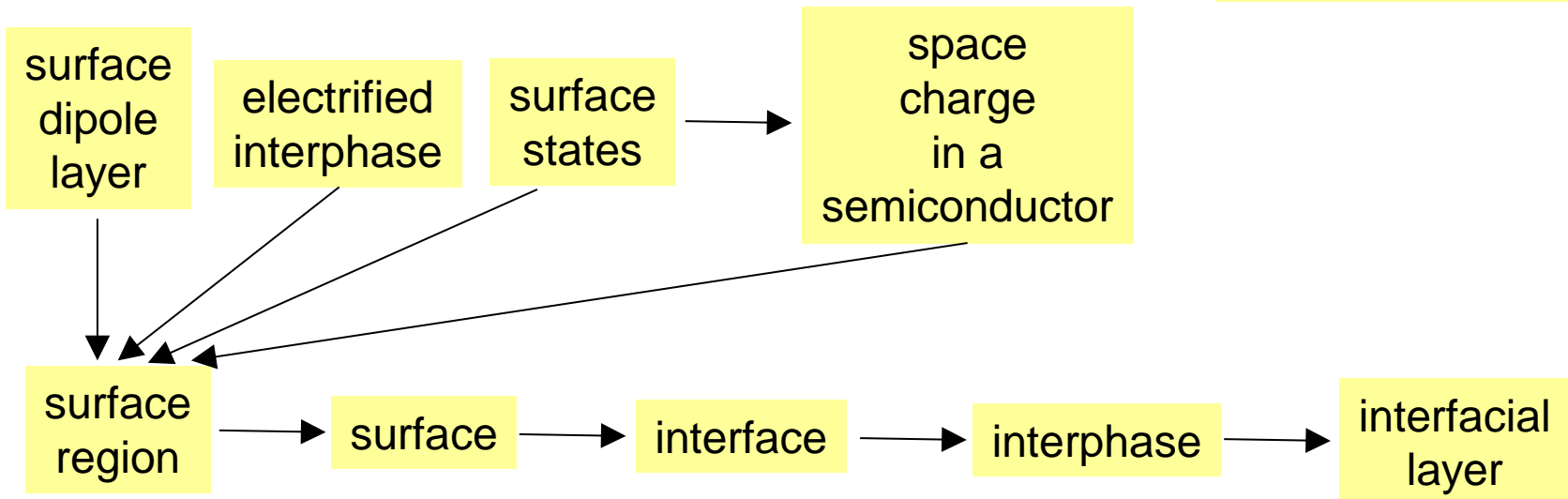
In IUPAC „Compendium of Chemical Terminology Gold Book“:

**Surface region** is the tridimensional region, extending from the free surface of a condensed phase towards the interior where the properties differ from the bulk.

The term **surface may also be used in this sense.**

Interactive link map

is related to

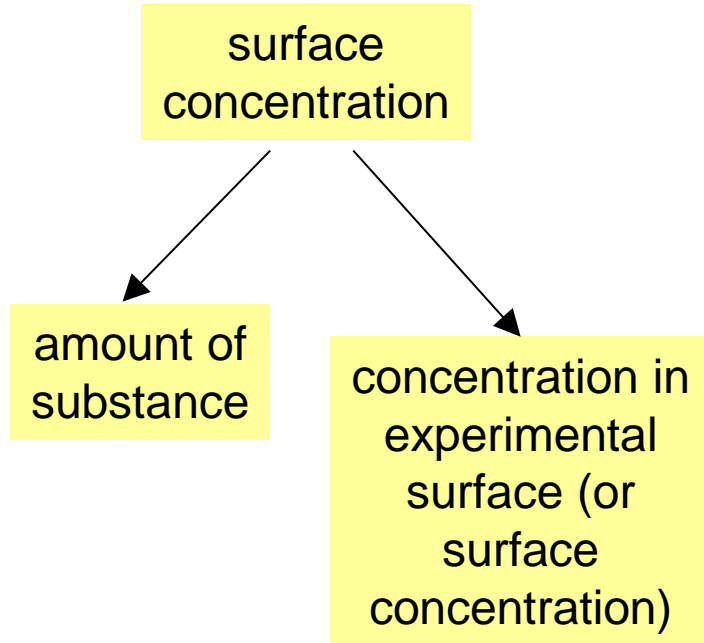


adopted following <https://goldbook.iupac.org/maps/S06154.3.map.html>

## (2) Surface **analysis**

**Surface** concentration (⇐ surface composition ⇐ surface characterization ⇐ materials characterization)  
⇐ comprises)

In IUPAC „Compendium of Chemical Terminology Gold Book“:



### **surface concentration:**

Amount of substance adsorbed on a surface divided by the surface area.

### **concentration in experimental surface (or surface concentration)**

The amount of the material of interest divided by the total amount of substances in the volume of interest.

**Concentration** may be defined in terms of

- numbers of atoms (particles) (ppma)
- weight ( $\mu\text{g/g}$ )

adopted following <https://goldbook.iupac.org/maps/S06162.3.map.html>

## (2) Surface **analysis**

### **Surface** analysis (**Methods / tools**)

X-ray Photoelectron Spectroscopy ( for determining **exp.** surface composition)  
Scanning Electron Microscopy ( for determining **exp.** surface structure)

X-ray photoelectron spectroscopy (XPS)

spectroscopy

adopted following  
<https://goldbook.iupac.org/maps/X06716.3.map.html>

optical spectroscopy

wavelength

Scanning Electron Microscopy (SEM)

back scattered electrons (BSEs)  
in in situ microanalysis

secondary electrons (se)  
in in situ microanalysis

adopted following  
<https://goldbook.iupac.org/maps/S05484.3.map.html>

## (2) Surface analysis

### Surface analysis (Methods / tools)

X-ray Photoelectron Spectroscopy (XPS)

tentatively adopted following <https://www.allotrope.org/allotrope-framework> and Allotrope Taxonomies Domain Model, suggested here as a base for discussion

