R&R Data Services 

The Description of Materials

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The Description of Materials

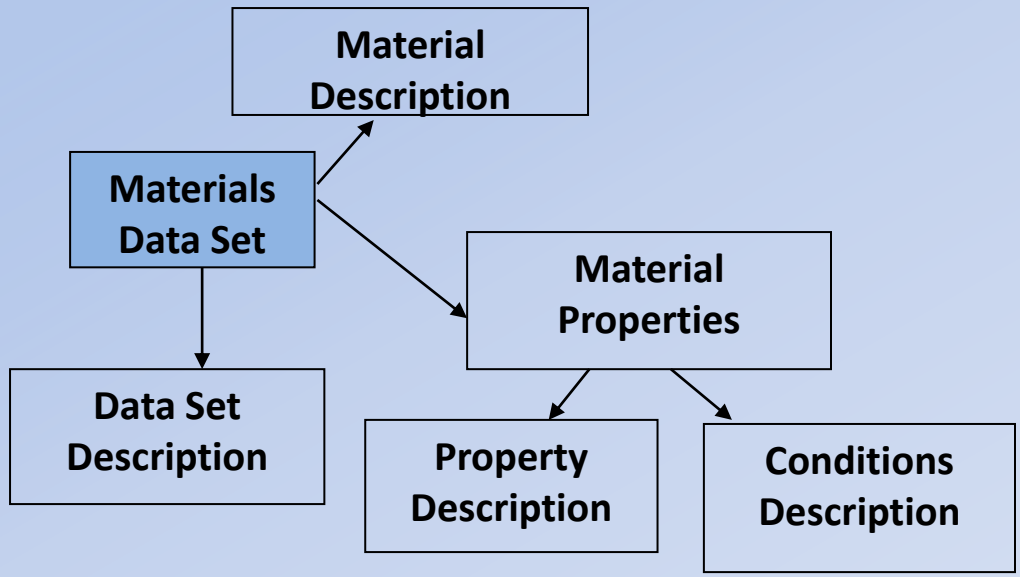
Today's Talk

- Status of materials description approaches today
- Differences between traditional materials and nanomaterials
- Challenges for the workshop

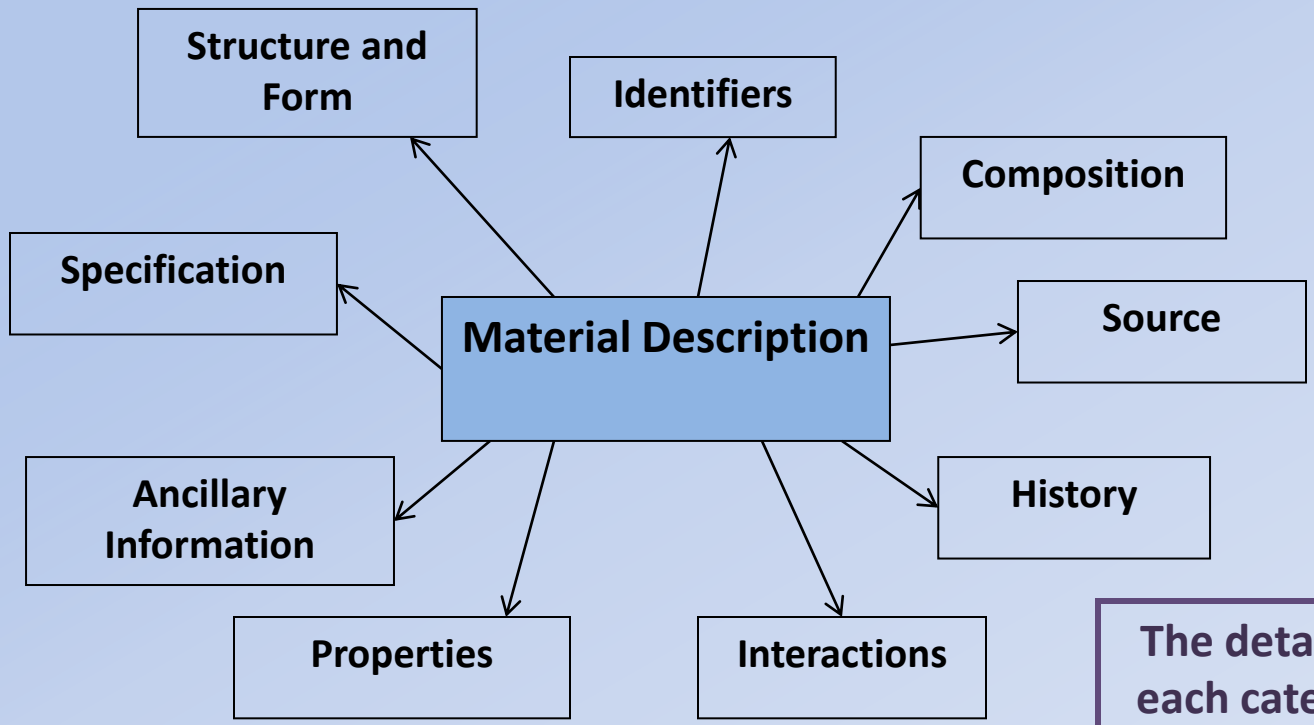
Goals on Material Description

- **Uniqueness**
  - To differentiate a material from every other material
  - To establish which particular material or instance of a material is being described
  - **"You know exactly what material you are talking about"**
- **Equivalency**
  - To establish that two materials or material instances are the same to some specified degree such that data sets can be combined
  - **"They are the same material"**

Materials Data



Components of Materials Description



The details of each category are obviously critical

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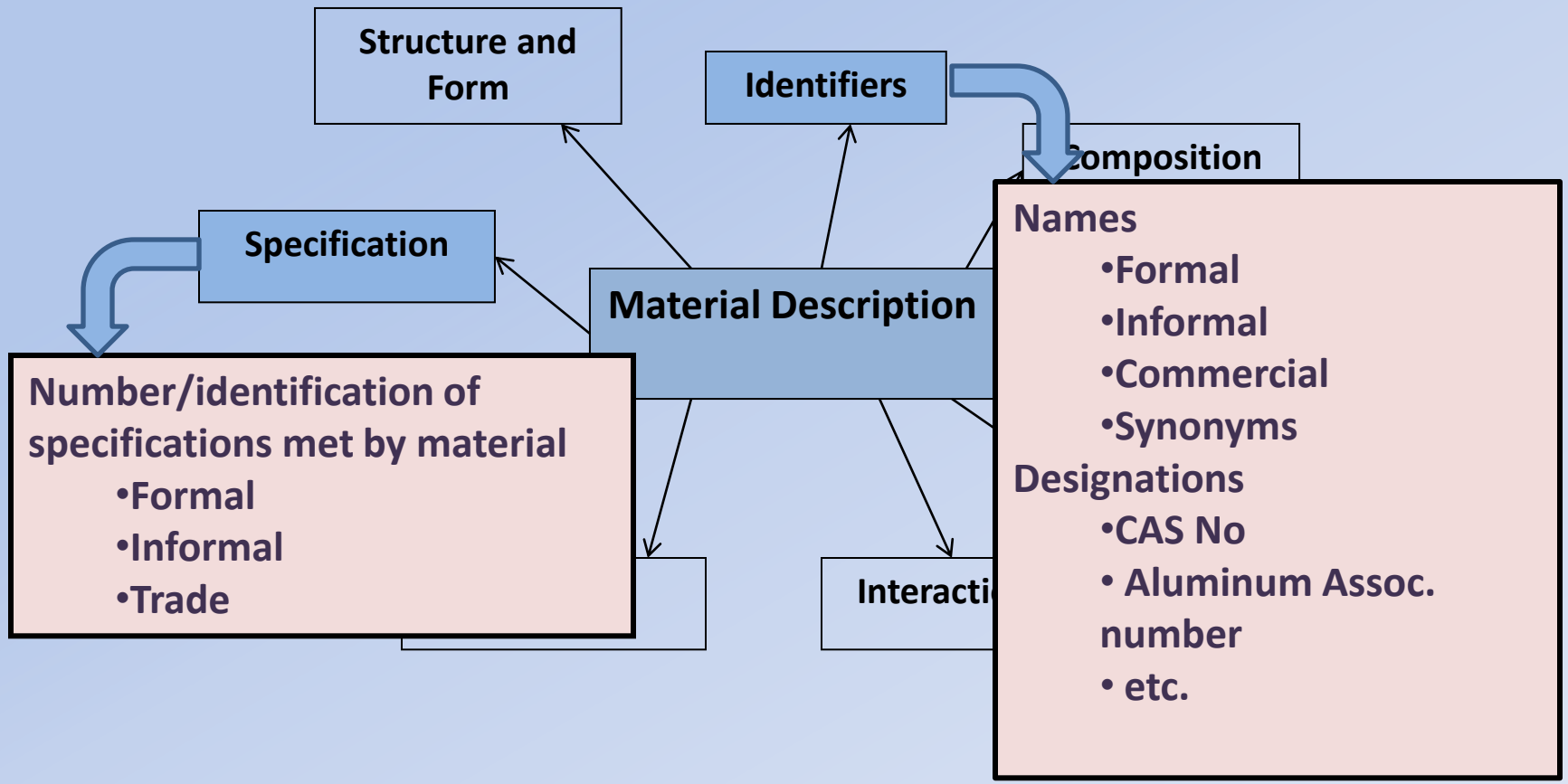

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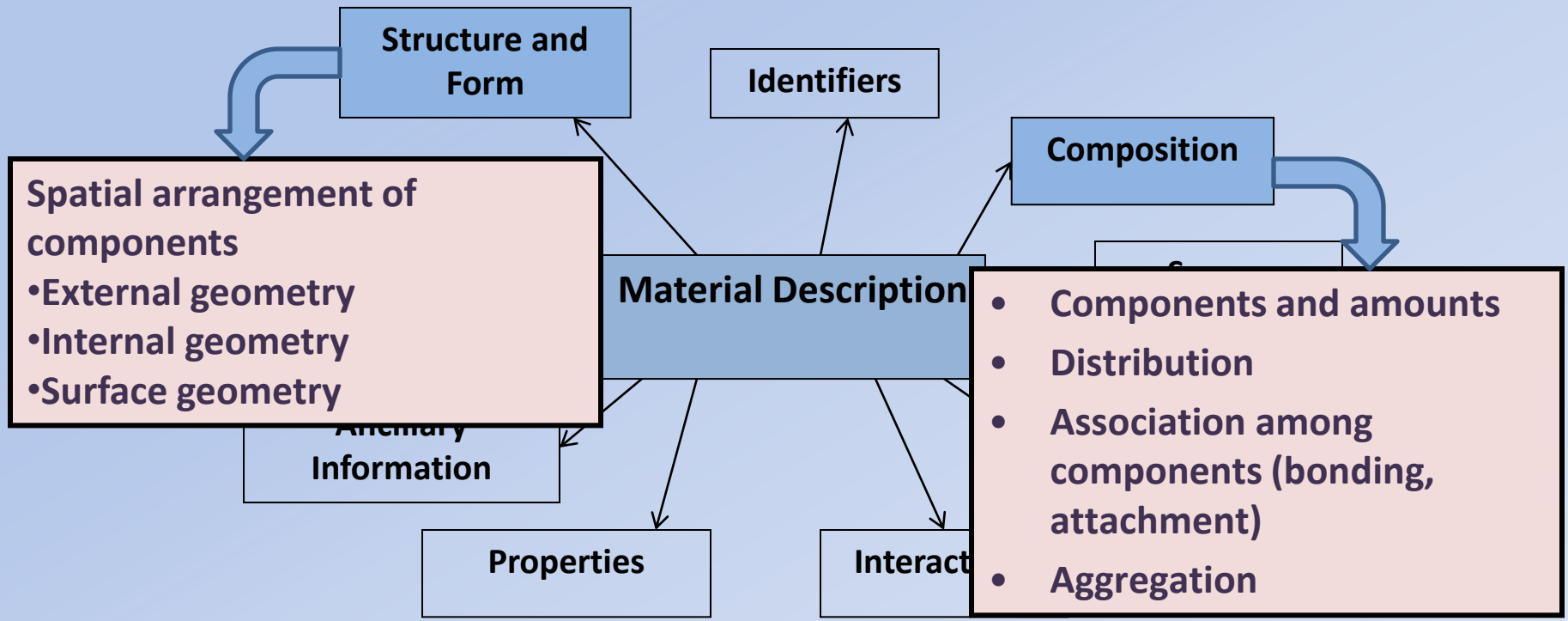

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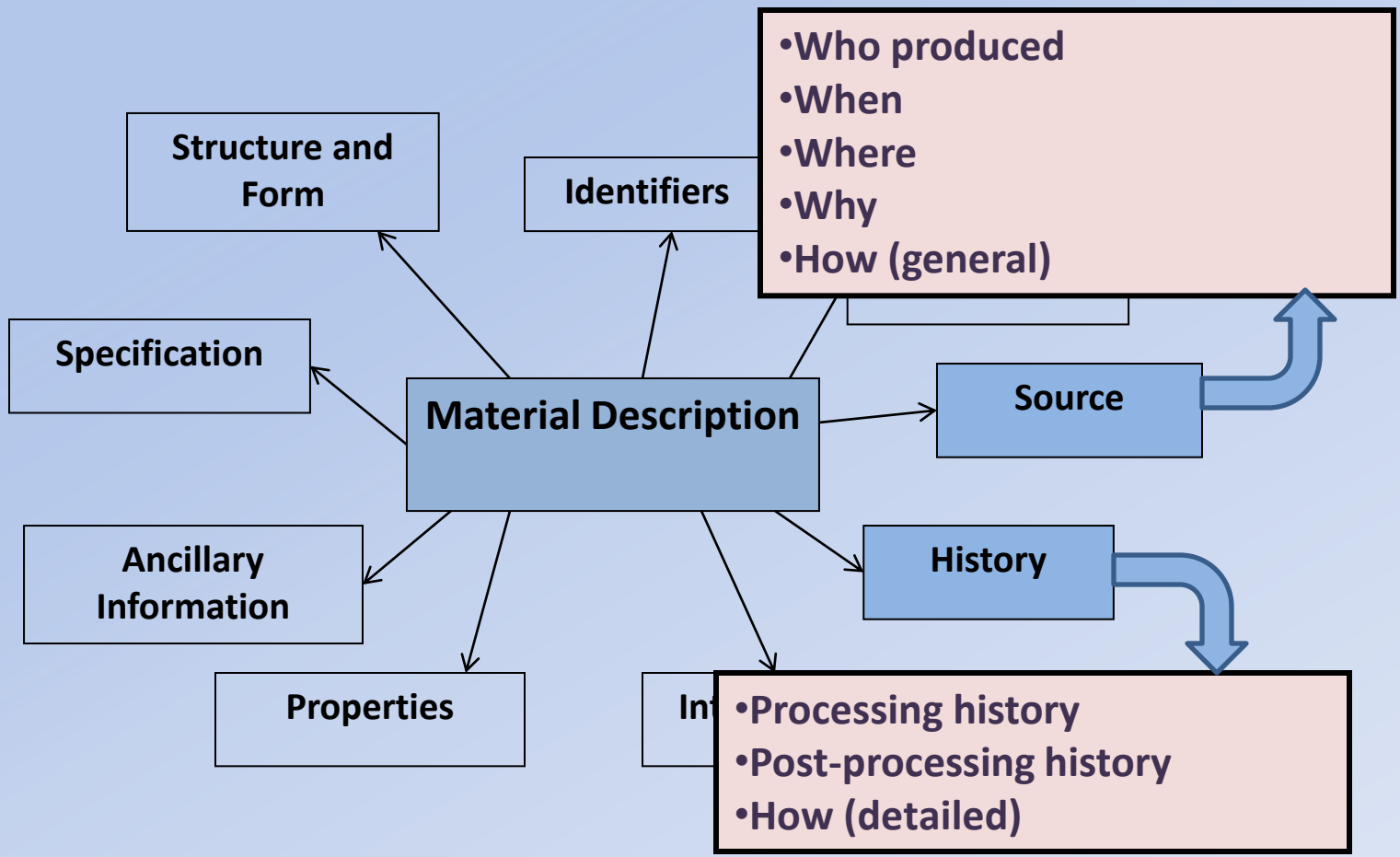

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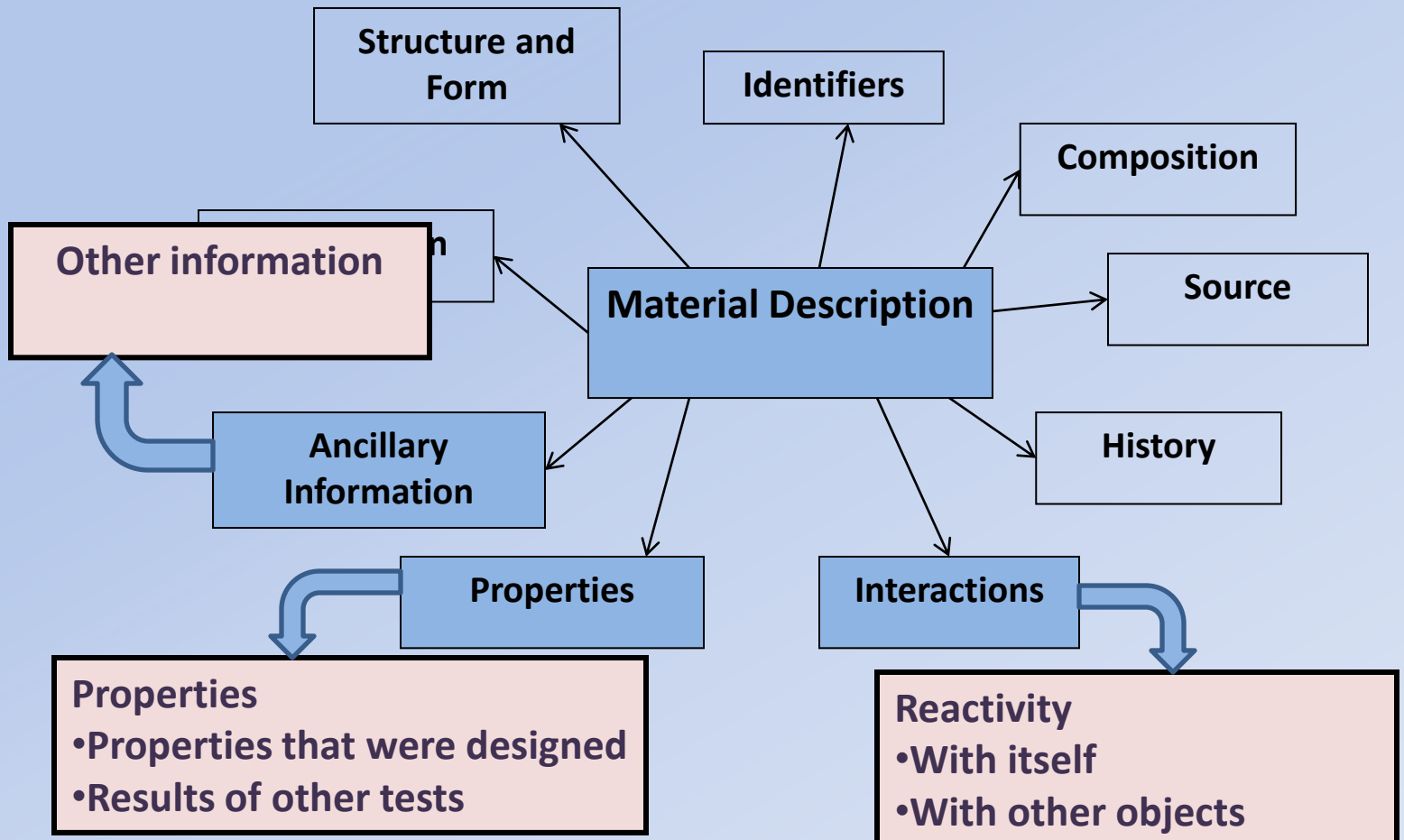

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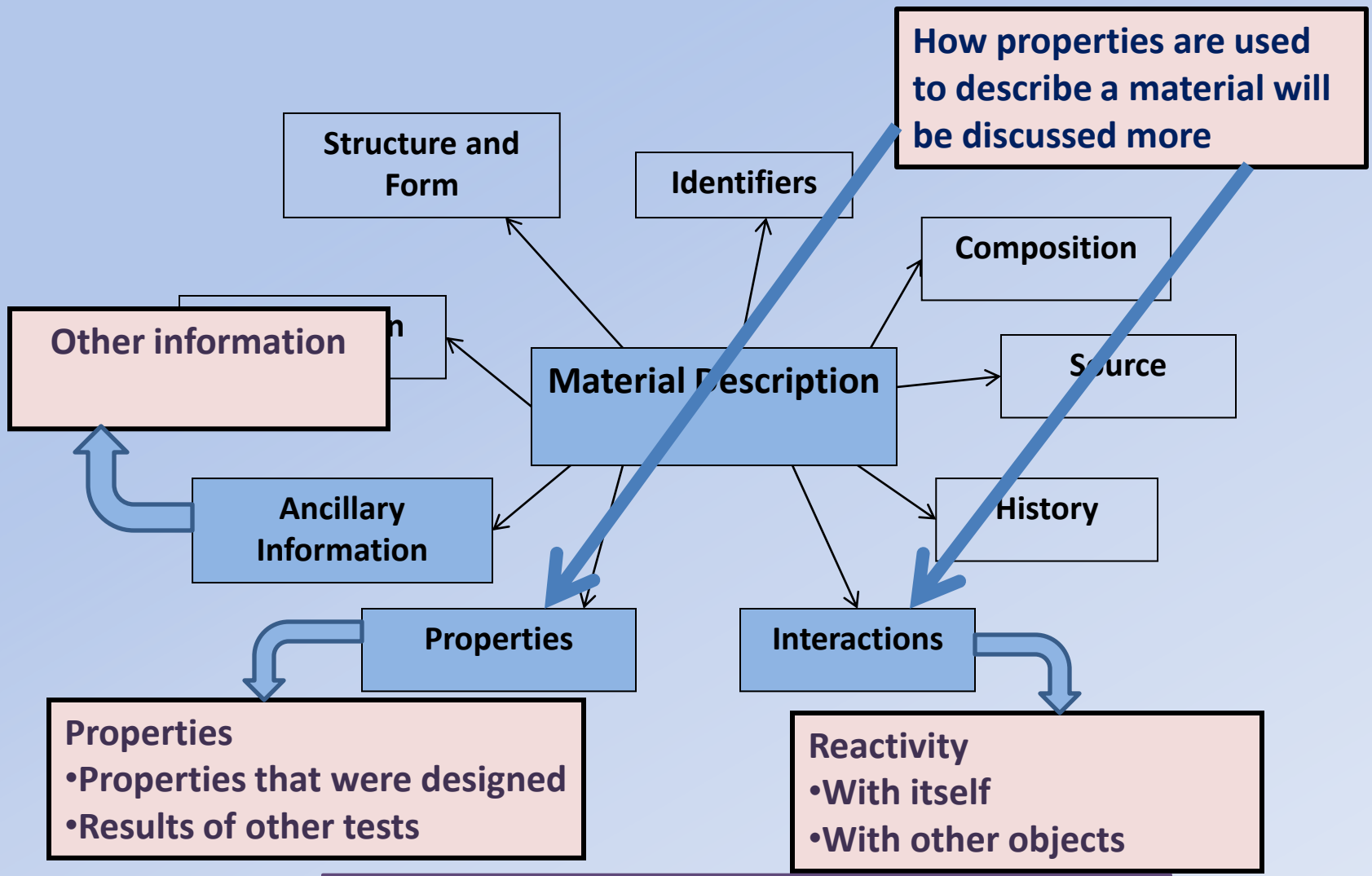

Are Properties Part of a Materials Description?

Two approaches

- A material is described without reference to its properties determined
  - The materials description is independent of the property description

- The description of a material includes its properties
  - The materials description contains all properties, but the properties are just one component of the description

Important implications for developing standards and regulations for nanomaterials

Existing Description Systems

• Molecules • Crystals	• IUPAC, Chemical Abstracts Service • IUCr and partners
• Metals and alloys	• Producer associations, national and international standards development organizations; hundreds of systems
• Polymers and ceramics	• Usually company specific, also producer associations, national and international standards development organizations

Existing Materials Data Exchange Systems

- MatML – at least two variations
- ISO STEP 10303 Part 45 and Application Protocol 235: Material and other engineering properties
- Weakly supported and not used often
- Part of larger STEP CAE standard

Both include a generic approach to materials description
Developed with great investment of time and money but have limited acceptance.
Still many semantic difficulties

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How are Materials Description Systems Used*

For

- Evaluation of properties
- Interactions with other materials
- Product design
- Materials selection
- Materials performance prediction
- Materials development
- Production engineering
- Product information systems
- Legislation
- Regulations
- Standards

*From VAMAS TWA 10: July 1987
Factual Materials Databanks The need for standards

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In these uses, what makes a nanomaterial different from other types of materials?

Steel W Type I-Beam W27/178

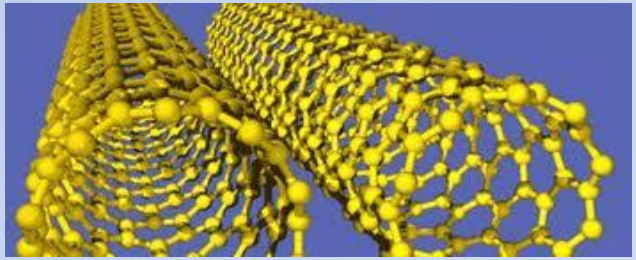
- 68.6 cm high
- 265 kg/m
- 12.1 m
- 3212 kg

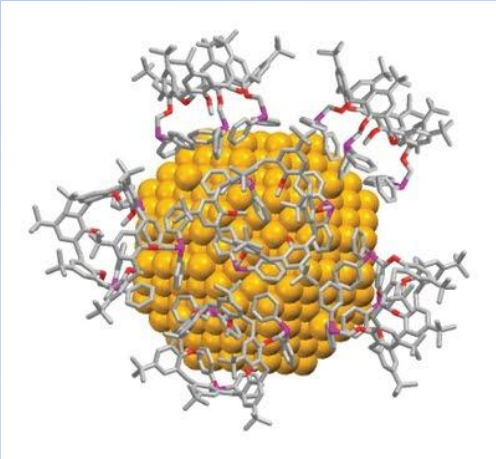
3.49 x 10^{28} atoms Fe (iron)

Carbon Nanotubes

- 0.5 nm to 10 nm diameter
- 3 nm to 10^4 nm long

10^6 to 10^{10}+ atoms C (carbon)





Nanoparticles

- 1 nm to 100 nm

10^3 to 10^9 atoms

Atoms are 0.10-0.15 nm, with Cs as large as 0.5 nm

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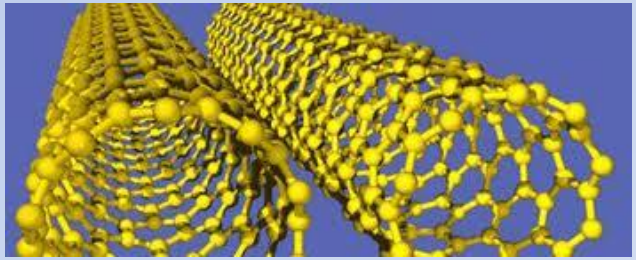
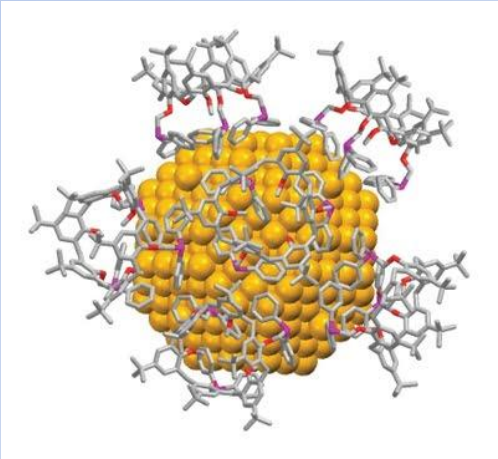




Nanoparticles

- 1 nm to 100 nm

10^3 to 10^9 atoms

Atoms are 0.10-0.15 nm, with Cs as large as 0.5 nm

Every instance of a nanomaterial is slightly different due to the complexity of processing, even for these small number of atoms

Goals of Nanomaterials Description

Uniqueness and Equivalency

- Are these goals still applicable for nanomaterials in the same way they are for materials?

- Yes, though the types of important information are different

Goals of Nanomaterials Description

- Can we simply define what makes a nanomaterial different from other materials?
  - Yes and No
- Nanomaterial (from ISO TC229):
  - Material with any external dimension in the nanoscale (approx 1 nm to 100 nm)
  - Or having internal structure or surface structure in the nanoscale
- Some materials have nanoscale internal structures

Exactly what makes a nanomaterial different ?

Differences

- Surface to volume ratio leading to changes from “bulk” properties (surface areas up to 1000 m^2 per gm)
- Different bulk and surface electronic structures
- Quantum size effects
- Dangling components on surface
- Chemical reactivity greatly different from more macroscopic forms (catalysis)
- New chemical forms (carbon nanotubes, titanium oxide, etc.)
- Small amount of impurities make big difference
- Self-assembly of ordered nanostructures

Exactly what makes a nanomaterial different ?

Consequences

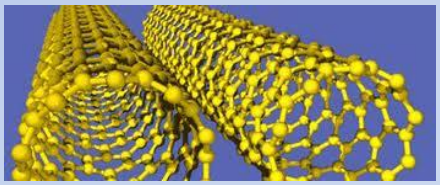
- Chemical reactivity different and not predicable from bulk properties
- Quantum size effects result in unique properties vis-à-vis macroscopic materials
- Difficult to predict and control unique collective effects and self-assembly
- Poor knowledge of mechanisms of action
- Difficulty in building a unified model of nanomaterials
- Need for new nano-focused test methods
- Need to develop experience in actual use and performance

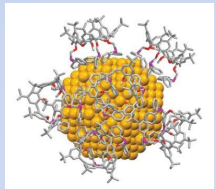
Amount of Information Needed

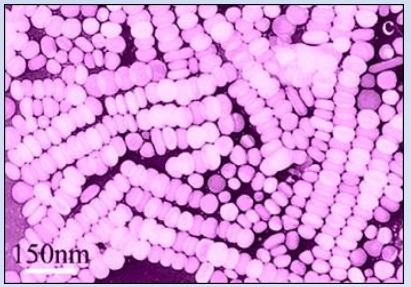
What is the minimum amount of information necessary to describe a nanomaterial completely?

1. **What is the information needed?**
2. **Can it be done without specifying properties?**
3. **If properties (or interactions) are required, which ones?**
4. **Is the amount of needed information independent of disciplines; e.g., chemistry, toxicology?**

- **Many different types of nanoparticles (nanomaterials): Are there many different minimum sets?**







Properties versus Measurements

- Properties are derived from multiple measurements and must include certainties
- Property values evolve over time as test methods improve and additional relevant independent variables are identified and controlled
- If a property value is used to define a nanomaterial, how good (reliable) is the test method? Are the uncertainties really understood?

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- **Challenges for the workshop**

Our First Set of Challenges

- **Do all uses have equivalent requirements for a description system?**
- **If not, can the different requirements be aggregated into a superset of requirements**
- **If not, which are most important needs for standardisation at this time?**

What is the minimum set of aggregated information needed?

Uses of Materials Description

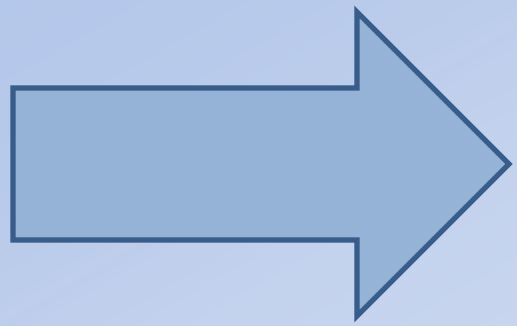
- Evaluation of properties
- Interactions with other materials
- Product design
- Materials selection
- Materials performance prediction
- Materials development
- Production engineering
- Product information systems
- Legislation
- Regulations
- Standards

Challenge Set 2

- **Is the problem the lack of a description system**

Or

- **i.e., Lack of unifying model of nanomaterials/ nanoparticles**



- **Lack of proven test methods**
- **Lack of experience in use**
- **Poor knowledge of mechanisms of action**

These are radically different issues

Challenge Set 3

- Chemistry
- Physics
- Materials science
- Food science and technology
- Nutrition science
- Toxicology
- Environmental and ecology science
- Medicine
- Biology

- **Do the description requirements vary from discipline to discipline?**
- **Do the testing methods requirements vary?**
- **Can an integrated set of requirements be developed for either?**

- **What is the minimal set of information needed?**

Overall Challenge

- Is our fear of the unknown forcing answers when not supported by our scientific knowledge?
- As we discuss these issues in this workshop, we must be mindful that standards codify knowledge, and if knowledge is lacking, the standards are meaningless
- Given the potential of nanomaterials, the standardisation process can and should drive the process of obtaining the needed knowledge