Characterizing the Minimal Information about Nanomaterials and Bringing Data Together to Accelerate Discovery

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ABSTRACT

There are ongoing efforts to understand the effects that nanomaterials have on biological and environmental systems, however sufficient understanding is lacking. The Nanomaterial Registry project curates characterization and biological and environmental study data on nanomaterials and dessimates infomation to the community via a public website (www.nanomaterialregistry.org). Using the Registry, researchers can access curated data records, share research, and work collaboratively to drive the discovery needed to understand the implications of nanomaterials.

The Nanomaterial Registry has established a minimal information about nanomaterials (MIAN). This MIAN includes 12 physico-chemical characteristics (PCC), the characterization techniques, the essential parameters for each of these techniques, and questions surrounding the scientific best practice during characterization.

Keywords: minimal information, nanoinfomatics, nanomaterial registry

1 INTRODUCTION

Nanomaterials are being used to enhance many products that are on the market today, from cosmetics to medicine. Consequently, nanomaterials, such as carbon nanotubes, nanosilvers and metal oxides are moving from research laboratories into products that are used in homes and other public environments [1]. As the use of applied nanotechnology grows, so does the need for a more comprehensive evaluation of the risks that these unique materials pose to human health and the environment [2-4]. Although risk assessment continues to be an area of overarching importance to the community, the diversity and complexity of nanomaterial properties and system interactions makes the understanding and regulation of nanomaterials a nontrivial task.

Critical knowledge gaps in nanotechnology need to be addressed so that the use of nanomaterials is not outpacing the understanding of the potentially risks of using these materials. A centralized body of integrated information is needed to enable researchers to gain knowledge from the growing body of research data.

NNI's Nanotechnology Signature Initiative (NSI) for a Nanotechnology Knowledge Infrastructure (NKI), includes a specific goal of enabling "a robust digital nanotechnology data and information infrastructure to support effective data sharing, collaboration, and innovation across disciplines and applications" [5]. The Nanomaterial Registry is an NIH-funded, publicly available tool that is being developed to serve this purpose. The Nanomaterial Registry archives curated nanomaterial data that are accessable via a public website (www.nanomaterialregistry.org). As multidisciplinary nanomaterial data is integrated and made usable to researchers -- the discovery of emerging trends and data gaps will be enabled.

The domain of the Nanomaterial Registry is physico-chemical characteristics of nanomaterials and biological, environmental, and ecological study data. Key concepts, such as minimal information set for nanomaterials, data compliance scoring, controlled vocabulary, and ontology, are being developed and applied by Nanomaterial Registry. The goal of the project is to support the continuum of understanding in nanotechnology, from data, to information, to knowledge and ultimately wisdom.

The purpose of this paper is to provide practical information on the archiving of data using the PCC MIAN, and to show the value proposition of this to researchers, those that guide research decision.

2 DATA AVAILABLE IN THE NANOMATERIAL REGISTRY

The data currently contained in the NR are curated from the following public data sources in broad stakeholder groups, percentages :

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- Biomedical Research (74% of records)
- Occupational Health & Safety (10% of records)
- Manufacturing: (8% of records)
- Regulatory: (4% of records)
- Environmental: (3% of records)
- Standards Organizations (1% of records)

Ongoing efforts in curation will incorporate strategic data sets for increased breadth (i.e. robust stakeholder group representation), and depth of information content (i.e. increased data records for target materials). For instance, future curation will target materials that have been identified by OECD's *Working Party on Manufactured Nanomaterials* (WPMN), which is comprised of 13 commercially relevant nanoscale materials, including MWCNTs, Silver NPs, and TiO2 [1].

2.1 Scope of a Data Record

The scope of data contained in a Nanomaterial Registry record includes physico-chemical characterization (PCC) and biological and environmental study data (Figure 1). This paper pertains to the PCC data and metadata, the study data are not discussed here.

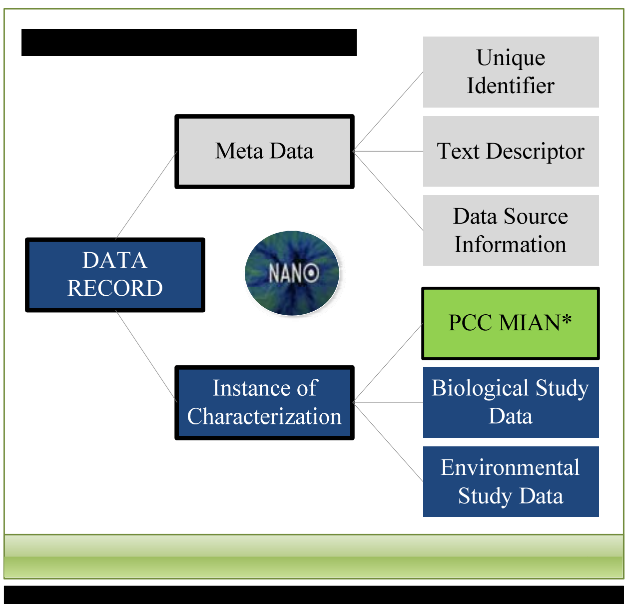

Figure1. The scope of data contained in a nanomaterial data record includes: metadata, and physico-chemical characterization (PCC) and study data. One or more instances of characterization can be contained in one data record, and each instance can have PCC and study data.

2.2 PCC MIAN Data

The scope of the PCC data is based on minimal information about nanomaterials (MIAN). The MIAN was created by the Nanomaterial Registry via leveraging efforts of community groups (such as the MinCharm Initaive, OECD Working Party on Manufactured Nanomaterials, and ISO Techical Comminty 229) and engaging an advisory board of nanomaterial experts with representation from private industry, academia, and governmental regulators.

There are 12 physico-chemical characteristics in the MIAN (Figure 2), as well as, protocols, parameters, and best practice questions for each PCC measurement (Figure 3).

Figure 2. There are 12 PCCs in the MIAN.

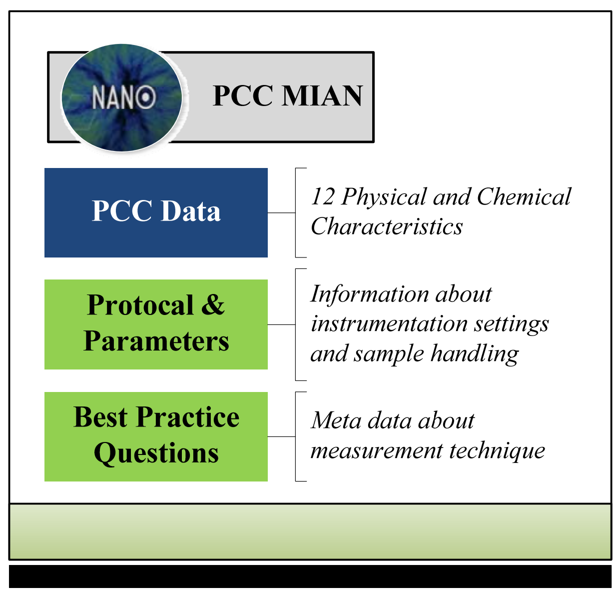

Figure 3. The PCC MIAN consists of characterization data (PCC data), information on protocols and parameters, and best practice questions. This data exists for each instance of characterization in a nanomaterial record.

The 12 PCC define "what" was measured, e.g. particle size; and the protocols, parameters, and best practice questions define "how" the measurement was made. This level of information supports validation and repeatability of research. The instance of characterization (IOC) defines

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the "when" or "where" a material was characterized, e.g. a time point or an environmental condition. The IOC concept is not discussed in detail in this paper, but is included in figure 1, and figure 4. The MIAN is applied in the Nanomaterial Registry data content, data model, and the website.

Nanomaterial PCC values are often method dependent. For example, consider the PCC "size" as reported by the National Institute of Standards and Technology (NIST) Report of Investigation for Reference Material (RM) 8011. The dependence of size on the measurement technique is apparent (table 1).

Table 1. Particle Size measurements in the Report on Investigation on the NIST Reference Material 8011.

Measurement Technique	Particle Size Reported
Atomic Force Microscopy	8.5 +/- 0.3
Scanning Electron Microscopy	9.9 +/- 0.1
Transmission Electron Microscopy	8.9 +/- 0.1
Differential Mobility Analysis	11.3 +/- 0.1
Dynamic Light Scattering	13.5 +/- 0.1
Small-Angle X-ray Scattering	9.1 +/- 1.8

The sample preparation and measurement process can also affect the measurement value, and fundamental factors must be considered for each technique. For these reasons, the Nanomaterial Registry MIAN is more detailed than a simple list of PCC.

It is worth noting that there are more than 70 (nano) reference materials, and the Nanomaterial Registry is committed to curating and archiving as much of this data as is available.

A portion of the data contained in the RM 8011 report, which was referenced in table 1 above, is shown according to the Nanomaterial Registry data structure (see figure 4). The record contains general metadata that allow the user to access the original report for validation and additional information. The gold nanoparticles were charaterized under three different IOCs, which pertain to different environmental conditions:

1. "As Received," particles in an aquous suspension,
2. "As Proccessed A," dried particles deposited on a substrate
3. "As Proccessed B," aerosolized particles.

Figure 4 shows details about the particle size measurement taken by dynamic light scattering (DLS), under the IOC "As Received" (in liquid suspension). Details include "Best Practice Questions" and "Protocols and Parameters." A similar level of information was curated for each of the 11 PCC shown in Figure 4. The full report on NIST RM 8011 (which is available online) has been curated and published in the Nanomaterial Registry

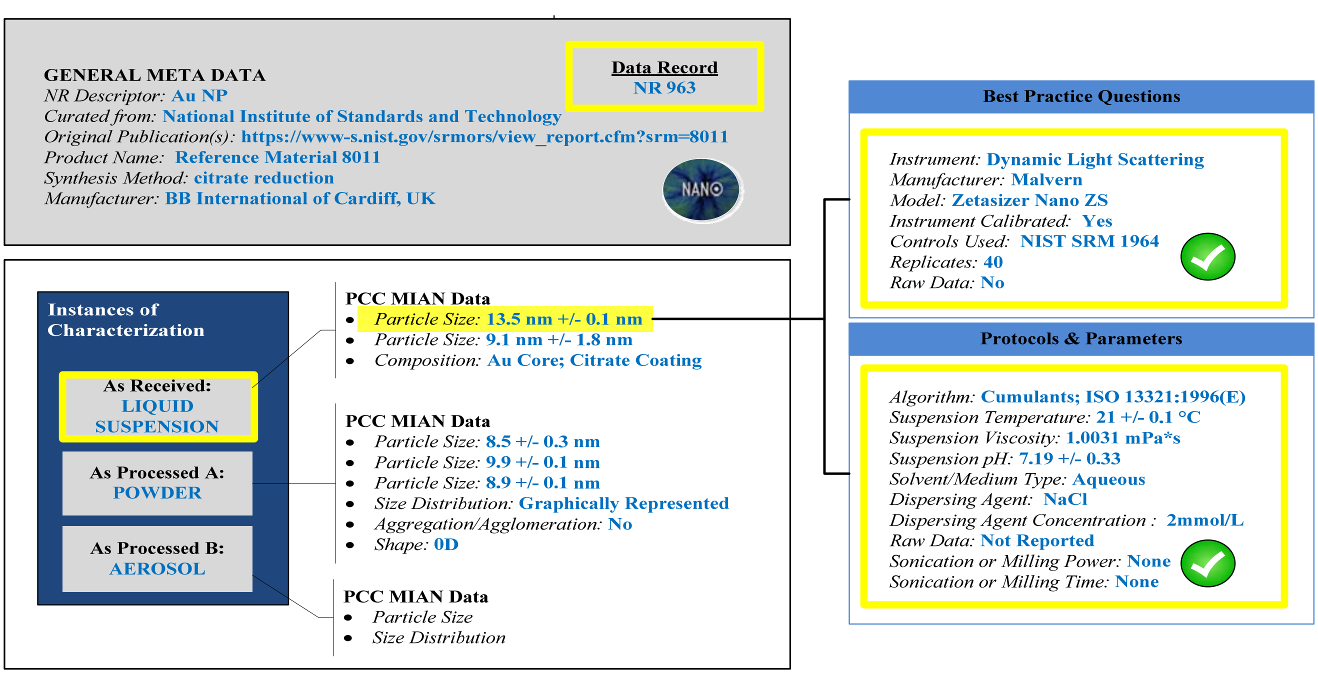

Figure 4. A portion of NIST RM 8011 data, as parsed out and reported by the Nanomaterial Registry. The entire record is available on line (https://www.nanomaterialregistry.org/NanomaterialDetails2.aspx?pid=963).

webiste. The data in the report has been parsed and archived according to Nanomaterial Registry data model

3. CONCLUSIONS

Data accessability and effective information sharing are critical to understanding the benefits and potential implications of nanomaterials. The Nanomaterial Registry has leveraged communuity efforts to create a MIAN, which is applied in order to normalize and archive nanomaterial research data. The data is publically available at www.nanomaterialregistry.org. Other concepts that are used in the project, but not discussed in this paper include standardized vocabulary and data formatting. Application of these information management concepts has created a repository of interoperable data sets that are searchable and usable in downstream analysis, and will drive knowledge creation in the diverse science of nanotechnology.

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