Metals & Alloys Structure Types in the PDF4+ - A Progress Report

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The ICDD Metals and Alloys sub file Working Group has for several years been editing the PDF's entries of the Metals & Alloys Sub file (MA) with the goal of assigning structure prototypes to nearly all entries in this sub file. At the inception of the review there were approximately 140,000 M&A entries. The Prototype Structures as defined by the Linus Pauling File were adopted and today have been entered for a large fraction of the M&A entries. The LPF Prototype Structure Type assigned to most phases in the LPF is based on a rigorous analysis of each atom's environment compared to that of the Prototype Structure.

Initially there were a large fraction PDF entries that did not have an associated prototype structure nor a crystal structure analysis so an "observationally-based Prototype Structure assignment approach was been adopted by the Working Group. For a PDF entry, if the structure type was not known or inconsistent with the LPF Structure Type then the Working Group compare the Pearson Symbol Codes, Space Group, lattice parameters, cell angels, and axial ratios as well as chemistry and formula to assign a Structure Prototype. A valuable consequence of doing this was the need to add to the PDF a standardized M&A formula, empirical formula and Z, which are based on the prototype structure. Along with the standardized Crystal Data standard cell, this standardized basis allows PDF users to use the PDF M&A subfile for (a) database mining based on prototype structures and (b) other structural parameters including atomic positions for use in structure analysis of a new phases.

The poster summarizes the editorial process, the current status of assigning LPF Prototype Structures to PDF M&A entries, and the developing tools users of the PDF can apply to help them solve their important research problems.