THE LINUS PAULING FILE (LPF) PROJECT

Jo Daams and Pierre Villars *
Daams Crystal Structure Consultancy (DCDC), Bombur 7, 5663 TC Geldrop, The Netherlands.
* Materials Phases Data Systems (MPDS), CH-6354 Vitznau, Switzerland.

The LPF consists of a data part; a data retrieval part and a newly developed software part for material science. The data part covers all non-organic (e.g. alloys, intermetallics, inorganic, ceramic, minerals, etc.) ordered solid state material systems. The relational database consists of crystal structure, diffraction, constitution, intrinsic property and bibliographic data. To have these four groups of materials data as numerical, factual and image data under the same computer environment is world unique. The LPF project is a long-term project (1996-2007) and it consists of a co-operation between JST, RACE and MPDS.
The database will have data coming from over 150.000 relevant publications and at the end of the project it will contain about 200.000 structure, diffraction and property data entries as well as about 35.000 constitution data entries (images) covering the world literature from 1900 to up to now.
As a starting point the following databases, JICST Crystal Structure, Pearson's Handbook 2nd edition, Structure Type Atlas, Massalski's Binary Alloys Phase Diagrams 2nd edition and Ternary Alloys Phase Diagrams (all published by ASM International) are used, but the LPF data are summarized from the original publication. The crystal structure data will be fully standardized with Structure Tidy. For each entry a calculated powder patterns with Lazy Pulverix will be included. Apart from that each entry is critical evaluated by the section editors and their remarks and/or comments will be included in the database. Furthermore new very sophisticated software has been developed to check each entry for all kinds of errors as well as to perform: model calculations, data visualization, pattern recognition, statistical considerations, etc.
In fact the LPF Material Data System will enable the scientists to build their own knowledge database system and the Discovery software included in the package can help the scientist to design new materials.
In our presentation we will show the first off-line product of the project and we will demonstrate that it can be used by the graduate student as well as the experienced material scientist. The on-line LPF product is already available (since the first of April) through the internet in Japan (by JST). We will shortly discuss the scope of the project and we will demonstrate the quality of the collected data and software on the binary compounds. This CDROM, called THE BINARIES, is already (or will be in a short time) available "free of charge" for the material scientist world.