Journal of
Applied Crystallography
ISSN 0021-8898

Received 29 June 2001
Accepted 12 October 2001

A database of incommensurate phases

Razvan Caracas

Université Catholique de Louvain, Unité PCPM, 1, pl. Croix-du-Sud, B-1348 Louvain-la-Neuve, Belgium.
Correspondence e-mail: caracas@pcpm.ucl.ac.be

A database of incommensurate phases is currently available at http://www.mapr.ucl.ac.be/~crystal/index.html. The present database offers a fast direct retrieval system for structural, physical and bibliographical data of incommensurate phases. The database contains data about inorganic, non-composite, non-magnetic and non-superconducting incommensurate phases only. Classification is according to the physical mechanisms responsible for the incommensurate phase transition. The main classes of incommensurate phases thus obtained are: the A_2BX_4 dielectrics family, zone-centre lock-in transition phases, cooperative Jahn–Teller incommensurates, tetragonal tungsten bronzes, charge-density wave systems and miscellaneous incommensurate phases. The latter class, because of the lack of available data, is classified on a chemical basis in several subclasses: silicates, perovskites, Mn-bearing oxides, other oxides, group VI compounds, intermetallics and other compounds. The database contains a brief description of the main physical, chemical and structural features of each phase, as stated in the literature. This description is very material- and bibliography-dependent and it is preceded by the phase transition sequence.

1. Introduction

During the past several years, the scientific community has shown a growing interest in incommensurate phases, as reflected in the Aperiodic Conferences Series, in the creation of the IUCr Commission on Aperiodic Crystals, the Special Interest Group on Aperiodic Crystals (SIG, 1998; http://www-xray.fzu.cz/sgip/aphome.html) and a structure-retrieving Internet database (Madariaga *et al.*, 2000), as well as in review articles (van Smaalen, 1995; Cummins, 1990), *etc*. As more and more incommensurate phases are being discovered, there is a need for a continuously updated repository of not only structural but also physical, chemical and bibliographical data of these phases. This is why a database of incommensurate phases has been created and is currently available on the Internet.

2. Database description

The database contains information about inorganic materials only. Organic and organic-bearing materials, composite materials, superconductors and spin-modulated materials are excluded for the time being.

The materials included in the database are classified as much as possible according to the physical mechanisms responsible for the incommensurabilities. Thus, first we separate the A_2BX_4 dielectrics class, further classified into a K_2SeO_4-type subclass, an Sr_2GeS_4-type subclass, an $ABCX_4$-type subclass, and a subclass of other less-studied compounds. Then we have cooperative Jahn–Teller incommensurates, tetragonal tungsten bronzes and charge-density wave systems. Because of the lack of information, a large class of miscellaneous incommensurate phases has been created, regrouping all the materials for which uncertainties still exist about the incommensurabilities. Within this group, the classification is performed on a chemical basis. We distinguish several subclasses: silicates, perovskites, Mn-bearing oxides, other oxides, group VI compounds, intermetallics and other compounds.

For each entry in the database, three kinds of information are available, as follows.

(i) Chemical formula and mineral name (if any). The chemical formula is provided, taking into account deviations from the stoichiometry. In the case of solid solutions, certain intermediate members of specific interest might be evidenced along with the end-member terms. In the case of minerals, both the formula and the mineral name are given according to the official IMA nomenclature (Mandarino, 1999).

(ii) Phase transition sequence and stability field of the polymorphs. The nomenclature proposed by the IUCr Working Group on Phase Transition Nomenclature (Tolédano *et al.*, 1998) is adopted. For each polymorph, where known, the stability field in terms of temperature and/or pressure, the structure/average structure symmetry, the modulation wavevectors, the number of molecular units in the unit cell/average unit cell, and the ferroic properties are provided.

(iii) Material description. The main physical, chemical and structural characteristics are briefly presented for each material. Special emphasis is placed on the mechanisms responsible for the existence of the incommensurabilities and for the phase transitions. This description is very material- and bibliography-dependent. Both theoretical and experimental results are reported.

The introduction of high-T_c superconducting oxides and spin-modulated systems should represent the next main step in the development of the database. The introduction of short descriptions of the common features for each class of incommensurate phase is also envisaged.

3. Availability

The database is actually available on the Internet at http://www.mapr.ucl.ac.be/~crystal/index.html.

A general PostScript file containing the entire database, a chemical index and a Bibtex-formatted file containing the bibliography are also available at the same address.

I kindly acknowledge H. Hochheimer for introducing me to the work of Cummins, all the authors who sent me reprints of their work, A. Janner for discussions about the list structure and content, G. Chapuis for discussions and for his great help in retrieving bibliographic information, M. Dusek for database searching, and X. Gonze for fruitful discussions.

References

Cummins, H. Z. (1990). *Phys. Rep.* **185**, 211–409.
Madariaga, G., Kroumova, E. & Luna, J. A. (2000). *Modulated Structures*, http://www.cryst.ehu.es/icsdb/index.html.
Mandarino, J. A. (1999). *Fleischer's Glossary of Mineral Species*. Tucson: The Mineralogical Record.
Smaalen, S. van (1995). *Crystallogr. Rev.* **4**, 79–210.
Tolédano, J.-C., Glazer, A. M., Hahn, Th., Parthé, E., Roth, R. S., Berry, R. S., Metselaar, R. & Abrahams, S. C. (1998). *Acta Cryst.* A**54**, 1028–1033.