s9.m31.p1 **A Computer Program for Transition Paths of Phase Transitions with No Group-Subgroup Relation Between the Phases.** C. Capillas, J.M. Perez-Mato, M.I. Aroyo, *Departamento de Física de la Materia Condensada, Universidad del País Vasco, 48080 Bilbao, Spain. E-mail: wmbcaloc@lg.ehu.es*

Keywords: Transition paths; Reconstructive phase transitions; Bilbao crystallographic server

In the last years there has been an increasing interest in structural phase transitions with no group-subgroup relations between the two phases. An essential step in the description of such transitions is the determination of the so-called *transition path* which includes the possible local atomic displacements and strains occurring during the transformation. Recently, we have developed a systematic procedure for the determination of possible transition paths between structures whose symmetry groups G_1 and G_2 are not group-subgroup related [1]. The transformation involves an intermediate "hypothetical" configuration described by a common space subgroup H of G1 and G_2 with specified indices. Although in general, there are a number of groups of the same space-group type Hi which are common subgroups with the required indices, for a complete analysis of the transition path $G_1 \rightarrow H \rightarrow G_2$ it is sufficient to consider only representatives of the conjugacy classes of H with respect to G_1 and G_2: It is to be expected that physically indistinguishable paths would result only for subgroups that belong to different conjugacy classes. Further important restrictions on the transition paths candidates are imposed by the symmetry constraints related to the occupied atomic orbits in the two initial structures. Additional structural conditions follow from the compatibility of both lattices. Our procedure is somehow similar to the one proposed in [2], but has specific features with respect to the symmetry search.

Here we report on the development of a computer program based on the described procedure using the tools provided by the Bilbao Crystallographic Server (www.cryst.ehu.es) [3]. Given the structures of the two initial phases specified by the symmetry groups, the lattice parameters, and the atomic coordinates in the asymmetric units, the program calculates the possible transition paths characterized by common subgroups H of G_1 and G_2. Using the available database on maximal subgroups of space groups, a modified version of the SUBGROUPGRAPH module [3] determines and classifies the set of subgroups Hi into conjugacy classes with respect to G_1 and G_2. The WYCKSPLIT module [3] checks the Wyckoff position splitting schemes for the pairs G_1>H and G_2>H. The transformed metric tensor components following the path $G_1 \rightarrow H \rightarrow G_2$ are related to the strains involved in the studied transformation.

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s9.m31.p2 **Design of a Graphical User Interface for the Control of a New X-Ray Parallel-Beam Powder Diffractometer via Internet.** Zunbeltz Izaola[a] and Gotzon Madariaga[a], [a]*Física de la Materia Condensada, Facultad de Ciencia y Tecnología, Universidad del País Vasco, Apartado 644, 48080 Bilbao, Spain. E-mail: wmbizazz@lg.ehu.es*

Keywords: GUI; Control; Diffractometer

Normally control and data treatment software is though as a proprietary black box system whose maintenance and enhancement is done by the instrument manufacturer, although many of its components belong to freeware repositories.

Open Software provides now a lot of robust resources which allow an extraordinary flexibility in the design of scientific software.

We have applied these ideas to control a X-Ray powder diffractometer developed in our Department in collaboration with TEKNIKER[1]. This task requires a good Graphical User Interface (GUI) for the control application that should be easy to use and flexible to achieve the highest efficiency. For this purpose the GUI and its environment (operating system, ...) must be as intuitive as possible for the user. To accomplish these basic objectives we have chose 1) to carry out the control via Internet and 2) to program the GUI in Python.

Internet allows us to connect computers regadless how much distance is between them. The diffractometer is controlled by a PC. Our GUI is connected to the control program of the PC by Internet connection (UDP sockets[2]), using a Client/Server model. Such a model permits, in the future, build other applications, like a remote monitoring program, to connect to the diffractometer. The use of Internet for remote control and other applications, such as, distributed computation and information management are being developed widely in the last years[3,4].

Python[5] is an powerful, multi-platform object-oriented interpreted programming language. Its dynamic nature makes it well-suited for rapid application development. Its multi-platform characteristic permits to run the programs in the mayor operating systems without changing, almost, any code line. A lot of scientific projects[6,7] are taking advantage of these and others capabilities of Python.

The combination of Internet and Python let us to build operation system independent and flexible GUI applications, which permit an easy interaction with many well tested crystallographic programs.

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