BAND_SYMM User's Manual

Content

1. INTRODUCTION

BAND_SYMM is a group of programs that analyzes the results calculated by PHASE / 0 [1] using group theory and identifies which irreducible ray representation the state belongs to. Moreover, a space group program called TSPACE [2] is employed during the group theory analysis of this package. This manual describes the preparation steps for using this package in Chapter 2, outline of the task in Chapter 3, details of the task in Chapters 4 and 5, and finally, utilization of this package in Chapter 6. An example can be given as follows to ensure a better understanding: The environment in which this package is to be used assumes that the external modules PHASE / 0, Fortran compiler, Perl, Gnuplot, and LaTeX are installed in a typical UNIX environment. See Section 7.1 for a detailed description of the used environment.

2. PREPARATION STEPS

This chapter describes how to unzip and build this package.

2.1. Decompression

First, create an appropriate directory (hereinafter referred to as the root) and unzip the archive file containing this package in that directory. The files and directories are created as shown below.

```
[mineo@azuma band_symm]$ tar xf band_symm.tar
[mineo@azuma band_symm]$ ls
band_symm.tar  make.inc  makefile  perl  readme.docx  sample  src  tspace
```

The files and directories that are included in this package are as follows.

1. make.inc

   This is the file that includes the makefile for creating band_symm. The Fortran compiler path and options are described, thus, you will need to modify the file according to your environment.

2. makefile

   The makefile for creating band_symm. This does not need to be changed, unlike make.inc.

3. src

   The directory that contains the source files for band_symm.

4. tspace

   The directory that contains the programs that come with TSPACE and makefile for building TSPACE.

5. perl

   The directory that contains the band_symm.pl script for band structure plotting.

6. sample

   The directory that contains various sample files for using this package.

7. readme.docx

   The user's manual (this document) for this package.

2.2. Building the Executable File band_symm

Execute the make command at the root to build the main program band_symm of this package according to the contents of the makefile. The following figure is an example of building (make) band_symm using GNU Fortran.

```
$ make
```

Abbreviation

```
gfortran -std=legacy -c -ffree-line-length-none  -cpp  main.F90
gfortran -std=legacy -o main main.o -I. commons.o phase_commons.o tspace_defines
.o tspace_commons.o container_commons.o container_lattice.o container_psicoef.o
degeneracy.o transd_vector.o character_table.o reduce_band.o compatibility.o cla
ssification.o ../tspace/tsp98.o
mv main ../band_symm
```

Abbreviation

```
$ ls
band_symm  makefile  make.inc  perl  readme.pdf  src  tspace
```

After the build is complete, ensure that the main program band_symm (shown in the figure above in green) is created at the root. In addition, you must go through the path to utilize band_symm and band_symm.pl.

When building with compilers other than GNU Fortran, it is necessary to rewrite make.inc provided in this package. The contents of make.inc are shown below. The compiler and linker can be changed by rewriting the compiler path in the 4th line and compiler options in the 5th line. Please adjust according to your environment. The following is part of the contents of make.inc. (The numbers at the beginning of the lines are meant to explain the content more clearly and do not appear in the actual file.)

Part of make.inc

1   ###

2   ###<< PLEASE CHANGE THE VARIABLES BELOW

3   ###

4   FC = gfortran -std=legacy

5   FFLAG = -ffree-line-length-none

```
6    ################################################################

7    ###<< PLEASE CHANGE THE VARIABLES ABOVE

8    ################################################################
```

3. OUTLINE OF THE TASK

The next page shows a flowchart that outlines the task.

See the following sections for details on each subtask.

   (a) PHASE/0 SCF calculation → Section 4.1

   (b) PHASE/0 band calculation → Section 4.2

   (c) band_symm → Section 5.1

   (d) band_symm.pl → Section 5.2

Precautions when performing the task.

-For subtask (b) shown above, band calculation is performed using PHASE/0, while ekcal is not used.

-The band_symm.pl in subtask (d) shown above may have the same function as band.pl, which has been provided so far, but how the options are specified may differ (see Section 5.2).
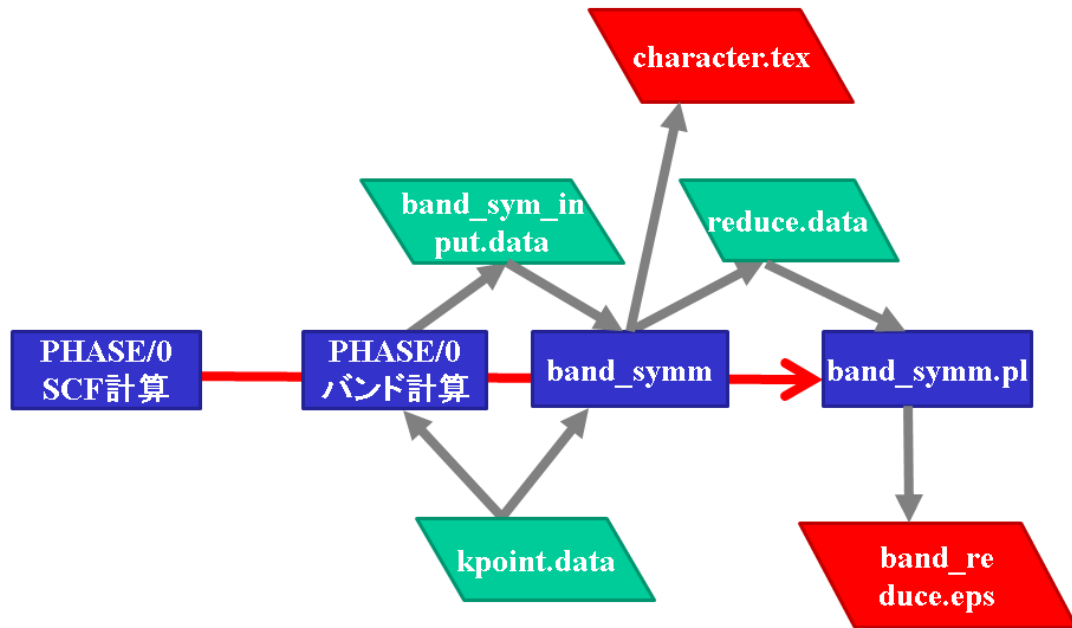
Figure 1: Flowchart of the task

4. ELECTRONIC STRUCTURE CALCULATION WITH PHASE/0

Next, calculate the electronic structure of the crystal using PHASE/0, and prepare kpoint.data and band_sym_input.data, which are input files for group theory analysis utilizing band_symm.

4.1. SCF Calculation

When performing the self-consistent calculation of the electronic structure (hereinafter referred to as SCF calculation), describe the input portion of the crystal structure in the input file as follows. Below is an example of the inputs used to calculate a crystal with a face-centered cubic structure (FCC).

```
1     structure{
2         unit_cell_type = bravais
3         unit_cell{
4             a = 10.26
5             b = 10.26
6             c = 10.26
7             alpha = 90
```

```
8            beta = 90
9            gamma = 90
10       }
11       symmetry{
12            method = automatic
13            tspace{
14                 lattice_system = facecentered
15            }
16       }
17       atom_list{
18            atoms{
19                 #default weight = 1, mobile = 0.
20                 #tag element rx ry rz
21                   Si 0.125 0.125 0.125
22                   Si -0.125 -0.125 -0.125
23            }
24       }
25       element_list{
26            #tag element atomic number
27              Si 14
28       }
29   }
```

Four factors to note.

1. In line 2, set the unit cell to the Bravais lattice.

2. Set the unit cell parameters to the Bravis lattice as shown in lines 4–9.

3. Enable automatic symmetry determination as shown in line 12.

4. Specify lattice_system as shown in line 14.

Because this example uses an FCC crystal, line 14 indicates FCC. For indications other than FCC, refer to the PHASE/0 manual. For other matters, follow the instructions provided in the PHASE/0 manual.

4.2. Calculation of Band Structure

After the SCF calculation, the band calculation is again performed using PHASE/0 (the band calculation is performed using PHASE/0 without using ekcal). First, create a file called kpoint.data

and state the information of the k-point per k-path. See the PHASE/0 manual regarding how to create this file.

```
1    Control{
2        cpumax = 2 hour
3        condition = fixed_charge
4    }
5    accuracy{
6        ksampling{
7            method = file
8        }
9        cutoff_wf = 25.00 Rydberg
10       cutoff_cd = 225.00 Rydberg
11       xctype = ggapbe
12       num_bands = 12
13       ek_convergence{
14           num_max_iteration = 500
15           sw_eval_eig_diff = on
16           delta_eigenvalue = 1.e-7
17           succession = 2
18           num_extra_bands = 2
19       }
20   }
21   Postprocessing{
22       sw_band_symmetry_analysis = ON
23   }
```

The following is an example input for band calculation. There are three factors to be considered.

1. In line 3, specify that the calculation with a fixed charge density should be executed.

2. In line 7, specify to enter the k-point described in kpoint.data.

3. In line 22, turn ON the option to output the space group and electronic structure data band_sym_input.data, which will be the input file of band_symm after the calculation is completed.

Additionally, there are no particular input restrictions other than those specified here, such as the number of bands and cutoff of plane waves. Therefore, describe them according to the PHASE/0 manual.

5. INSERTING IRREDUCIBLE RAY REPRESENTATIONS IN A BAND STRUCTURE

As explained in Chapter 4, after calculating PHASE p/0, create a band diagram that displays the irreducible diagonal line representation (hereinafter referred to as the irreducible representation). Before execution, to use band_symm and band_symm.pl described in Section 2.2, you must follow the path.

5.1.   Execute the Main Program band_symm

Use the main program band_symm created in Section 2.2. The purpose of this program is described as follows. Move to the directory containing kpoint.data and band_sym_input.data created in Section 4.2 and execute the following command. Moreover, this directory is referred to as the working directory as shown below.

band_symm kpoint.data band_sym_input.data > spacegroup.data

After running band_symm, ensure that reduce.data, character.tex, and spacegroup.data are generated in the working directory. See Section 7.23 for the algorithms used in this program.

5.2. Creating an EPS File Using band_symm.pl

Use band_symm.pl to plot the band structure specified through irreducible representations. From the outputs obtained in the previous section, reduce.data is required. By executing the command in the working directory, the encapsulated post script (EPS) format file band_reduce.eps for plotting a band diagram with irreducible representation is exported.

band_symm.pl reduce.data

Because band_symm.pl uses Gnuplot as an external module in addition to the Perl engine, EPS files cannot be adequately created unless Gnuplot is installed.

Below are some of the most commonly used options available in band_symm.pl. Some options require adding a string variable as a parameter, while others do not. Be sure to enter each parameter after each option with one or more spaces. The type of string variables that should be entered is indicated in the explanation of each option. In addition, the script will run without issues, even if you write the following options in a different order. See Section 7.2 for other existing options.

1.   –erange MIN, MAX: Records the energy range that displays the band. MIN and MAX indicate

the minimum and maximum values of the specified energy, respectively, and are set in eV units. If this option is not specified, the display range is determined from the maximum and minimum eigenvalues.

2. –with_fermi FILE: Specifies the Fermi level and uses it as the standard of energy. It also plots a horizontal dashed line at the zero energy marker. For the above parameter "FILE," specifies the file name referring to the Fermi level (default file name is nfefermi.data), which is exported from PHASE/0. If this option is not specified, the eigenvalue data reference will be the basis for the band diagram. In addition, the dashed line will not be plotted.

3. –h: Helps you run this script. This option does not require any parameters.

6. EXECUTION EXAMPLE

Using the sample file provided in this package, the irreducible representation classification band in Si2 (FCC) and GaAs (FCC) created through the steps described in Sections 4.1, 4.2, 5.1, and 5.2. The index table of each k-point indicates a conformance relationship.

1. The inputs for the SCF calculation used in Section 4.1 are as follows:
   sample / Si2 / SCF / nfinp.data

2. The input for band calculation used in the process of Section 4.2 is as follows:
   sample / Si2 / band / nfinp.data

3. In the execution of band_symm.pl in the process described in Section 5.2, the following is specified.
   band_symm.pl -linecolor red –erange -14,5 –with_fermi nfefermi.data –imrfont Helvetica, 20 –ticsfont Helvetica, 16 reduce.data
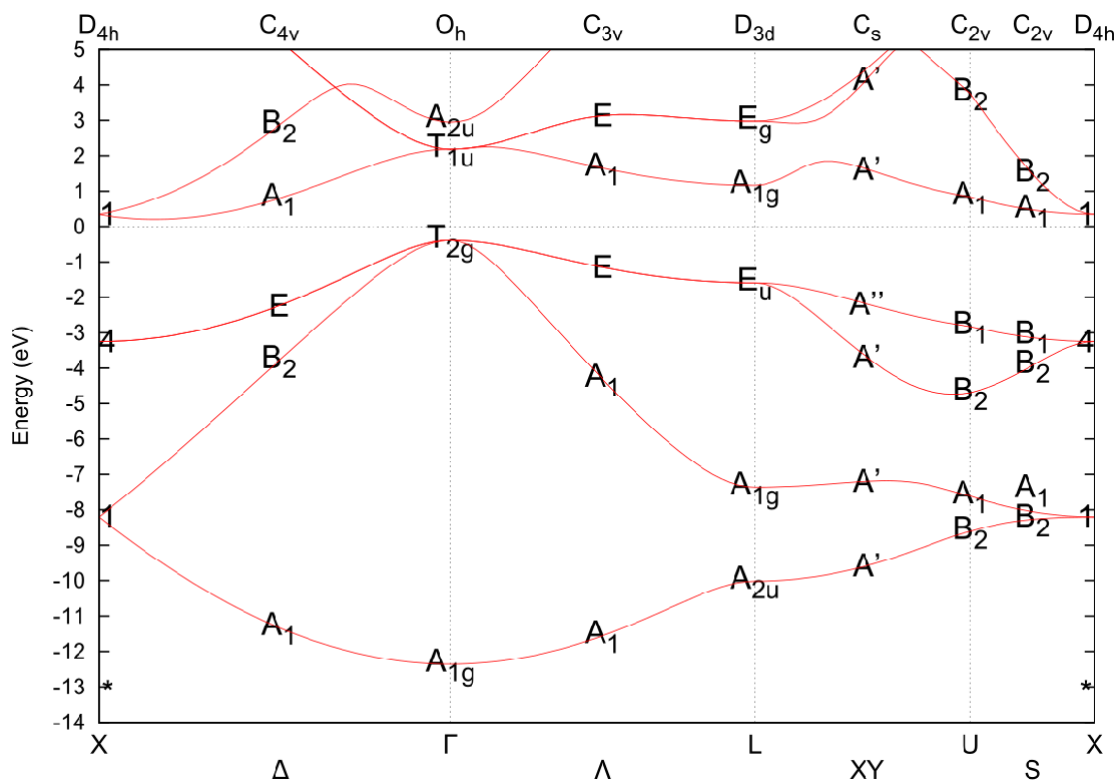   See sections 5.2 and 7.3 for details on options.

6.1. Si2(FCC)

Figure 2: Band structure plot of Si2 (FCC).

$\Delta(C_{4v}, 4mm)$	E	$C2X$	$2C4X+$	$2IC2Y$	$2IC2D$
$1(A_1)$	1	1	1	1	1
$2(A_2)$	1	1	1	-1	-1
$3(B_1)$	1	1	-1	1	-1
$4(B_2)$	1	1	-1	-1	1
$5(E)$	2	-2	0	0	0

Class	Operator
E	E
C2X	C2X
2C4X+	C4X+,C4X-
2IC2Y	IC2Y,IC2Z
2IC2D	IC2D,IC2F

Figure 3: Character table regarding the irreducible representation of each k-point in Si (FCC) (only a part is shown). Irreducible representations are indicated by numbers (1-5)

and Mulliken symbols (in parentheses).

2 Compatibility table

Γ	Δ	Γ	Λ
Γ_1^+	Δ_1	Γ_1^+	Λ_1
Γ_1^-	Δ_2	Γ_1^-	Λ_2
Γ_2^+	Δ_3	Γ_2^+	Λ_2
Γ_2^-	Δ_4	Γ_2^-	Λ_1
Γ_3^+	$\Delta_2+\Delta_5$	Γ_3^+	$\Lambda_2+\Lambda_3$
Γ_3^-	$\Delta_1+\Delta_5$	Γ_3^-	$\Lambda_1+\Lambda_3$
Γ_4^+	$\Delta_4+\Delta_5$	Γ_4^+	$\Lambda_1+\Lambda_3$
Γ_4^-	$\Delta_3+\Delta_5$	Γ_4^-	$\Lambda_2+\Lambda_3$
Γ_5^+	$\Delta_1+\Delta_3$	Γ_5^+	Λ_3
Γ_5^-	$\Delta_2+\Delta_4$	Γ_5^-	Λ_3

X	Δ
X_1	$\Delta_1+\Delta_4$
X_2	$\Delta_2+\Delta_3$
X_3	Δ_5
X_4	Δ_5

L	Λ	L	XY
L_1^+	Λ_1	L_1^+	XY_1
L_1^-	Λ_2	L_1^-	XY_2
L_2^+	Λ_2	L_2^+	XY_2
L_2^-	Λ_1	L_2^-	XY_1
L_3^+	Λ_3	L_3^+	XY_1+XY_2
L_3^-	Λ_3	L_3^-	XY_1+XY_2

U	XY	S	U	U	S
U_1	XY_1	S_1	U_1	U_1	S_1
U_2	XY_2	S_2	U_2	U_2	S_2
U_3	XY_2	S_3	U_3	U_3	S_3
U_4	XY_1	S_4	U_4	U_4	S_4

Figure 4: Compatibility relationship of k-path groups in Si (FCC).

7. APPENDIX

7.1. Details about the Utilized Environment

This package is intended for use in a UNIX environment with a 32-bit operating system. When used with a 64-bit operating system, we cannot guarantee that the package will be built and calculated correctly. In addition, the following external modules are required; only an overview of each module is provided here. Instructions on how to install each module are not available here; therefore, please refer to the user's manual of each module.

1. **PHASE / 0**

   This module calculates the one-electron state in a crystal using the first-principles calculation method. It allows the creation of band_sym_input.data, an input that describes the electronic structure and space groups of the crystal needed to run band_symm. In addition, some source code included in this module is quoted in the group theory analysis.

2. **TSPACE**

   This module is necessary to acquire the index of the irreducible representation of the k-group and

symmetry operation during the calculation present in the group theory analysis of this package. This module is already included in this package and does not need to be installed separately.

3. Fortran Compiler

    All programs and TSPACE included in this package are described using Fortran77 and Fortran90. Hence, a compiler for Fortran77 and Fortran90 must be installed on your system.

4. Perl

    The band structure plot script band_symm.pl is described in Perl. Therefore, you need to install a Perl engine on your system.

5. Gnuplot

    Inside band_symm.pl, a script for Gnuplot that plots a band structure that describes the irreducible representation from the k-path of the input band structure, eigenvalue of each state, and irreducible line representation (hereinafter referred to as the irreducible representation) are created and sent to Gnuplot. Therefore, you need to have Gnuplot installed on your system.

6. LaTeX

    By executing band_symm, you can obtain the index of the irreducible representation at each k-point of the k-path and character.tex that describes the conformity relationship between each k-point. This file is written according to the LaTeX notation, thus, if used, you can create the character table data that can be viewed by compiling this file using LaTeX.

7.2. Algorithm for the Electronic Structure Calculation Performed Through band_symm

In addition to the vector k in the wavenumber space, the electronic structure in the crystal is distinguished by the band index i.

$$\mathrm{H}\psi_i^k(r) = \varepsilon_i^k \psi_i^k(r)$$

The electron wavefunction ψ_i^k belongs to an irreducible representation of the k group corresponding to the given wavenumber k. The appropriate irreducible representation can be specified by using the projection operator P_k^l corresponding to the irreducible representation l (see Reference 3).

$$\mathrm{P}_k^l = \frac{1}{h}\sum_R \chi_k^l(R)^* R$$

$$\sum_i^{i+n-1} \int dr\, \psi_i^k(r)^* P_k^l \psi_i^k(r) = \delta_{l\,l'}$$

Here, R denotes the symmetry operator in group k, $\chi_k^l(R)$ is the index of the irreducible representation l in the k group, and h is the order of the group. Furthermore, l' is an irreducible

representation that the wavefunction belongs to. The above equation assumes that the energy of the wave function degenerates n-folds. In line 16 of the input example in Section 4.2, reducing the value of delta_eigenvalue improves the wave function accuracy as well as the evaluation accuracy of the above equation.

7.3. Options Available on band_symm.pl

Explanation of each option of band_symm.pl that was not explained in Section 5.2 is provided here.

1. -einc VAL: Sets the scale of the energy to be displayed. Specify the energy in eV units for VAL and scale set for each energy level. If this option is not specified, the scale is set from the maximum and minimum energy values.

2. -imrfont TYPE, SIZE: Specifies the font and size of the irreducible representation label. The specified font and size are valid only if they can be used with Gnuplot. Specify the font name in TYPE and font size in SIZE. The default TYPE is Helvetica and SIZE is 10.

3. -ticsfont TYPE, SIZE: This is the axis-label version of the abovementioned imrfont option. Change the labels on the X-and Y-axes. The default TYPE is Helvetica and SIZE is 10.

4. -imrcolor COLOR: Changes the color of the irreducible representation label. The color is specified according to RGB, and is set as COLOR = red or COLOR = blue. Similar to the fonts described in options 2 and 3, color is only valid if available in Gnuplot. The default setting is COLOR = black.

5. linecolor COLOR: Band version of the abovementioned imrcolor option. Changes the color of the band lines. The default value was COLOR = black.

6. -imrtype TYPE: Specifies the symbol type of the irreducible representation to be displayed. For TYPE, specify the name of the symbol of the irreducible representation. If this option is not specified, the default type the Mulliken symbol (Koster symbol in calculations that incorporate spin-orbit coupling). When TYPE is set to numerical, the name assigned to the program (hereinafter referred to as numerical notation) is described in the band diagram. Check the correspondence between the number notation and irreducible representation with character.tex output obtained from band_symm (see Figs. 3 and 9).

7. -nonecross: By default, bands with different irreducible representations are assumed to intersect when creating a band diagram. However, if the band is not displayed correctly, this feature can be disabled by specifying this option. This option does not require any parameters.

8. kgrouptype TYPE: You can specify the name of the group of k-points to be displayed on the X-axis. If TYPE = Schoenflies, the Schönflies symbol is used. If TYPE = Hermann Mauguin, the group name is displayed on the x-axis using the international symbol. By default, the plot is drawn using the Schönflies symbol.

The execution example and Si2 (FCC) band diagram plotted using the execution example are shown in (Fig. 6).

band_symm.pl ./reduce.data –erange -10,15 –einc 5 –with_fermi ./nfefermi.data -imrfont Helvetica,20 –ticsfont Helvetica,12 –imrcolor blue –linecolor red –imrtype number –kgrouptype HermannMauguin -nonecross

This execution example is carried out as follows:

- Set the energy display range from -10 to 15 eV and the energy scale every 5 eV.
- Specify the Fermi level and create a band structure plot based on it.
- Specify the font type of the irreducible representation label as Helvetica with a size of 20 pt, and the font type of the axis label as Helvetica with a size of 12 pt.
- Specify the color of the irreducible representation label as blue and color of the band line as red.
- Specify the symbol of the irreducible representation in numerical notation and symbol of the group of k-points in international notation.
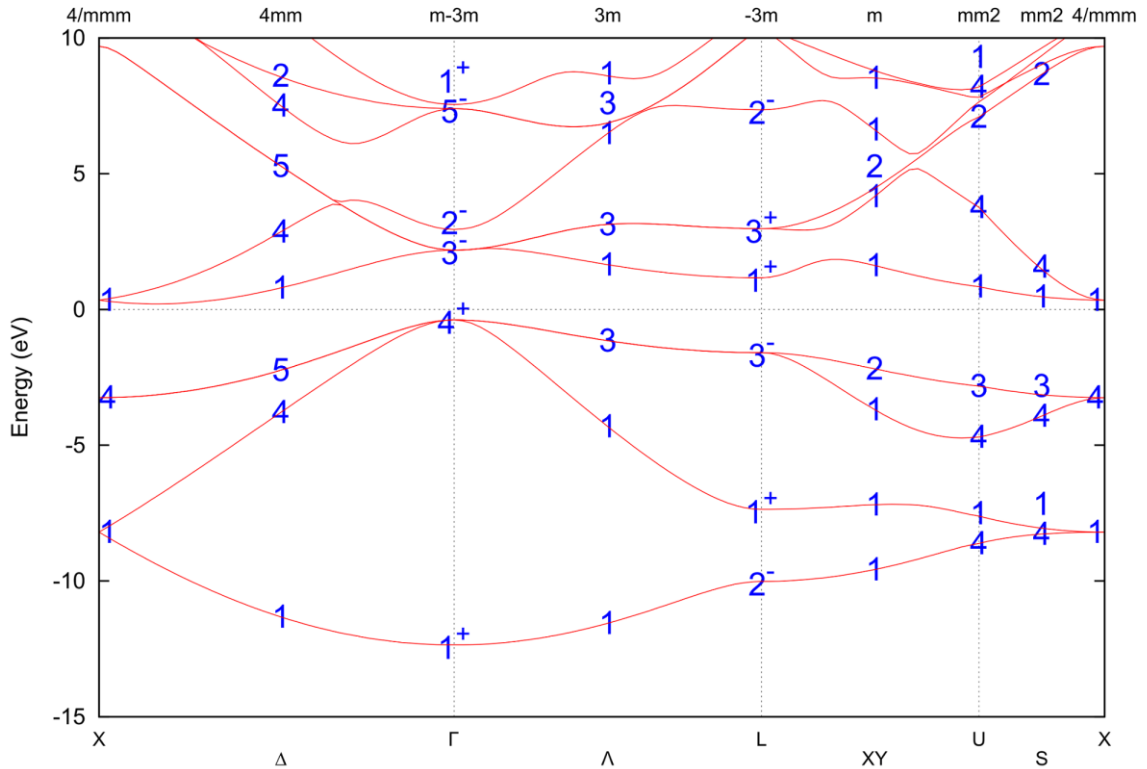- Do not execute the band crossing function.

Figure 5: Si2 (FCC) band structure plot.

7.4. Contents of spacegroup.data

In Section 5.1, the spacegroup.data output of executing band_symm includes the Jones representation of the all-symmetry operation regarding the calculated space group and accompanying translational vector, as well as the name for k-point and point group of that k-group. The name (Schoenflies and international symbols) is described. This file is originally output to the console when band_symm is executed to obtain spacegroup.data and redirect it. The following is an example of spacegroup.data found in an FCC crystal. The bold letters to the right of each line explain the meaning of the data in each line of spacegroup.data in this document and are not output in practice.

----- WELCOME TO TSPACE V4.1 1995/09/06 -----**String variables automatically output from TSPACE**

LATTICE CONSTANTS ARE SET AS

A= 10.26000   B= 10.26000   C= 10.26000 **Bravais lattice parameters (a, b, c)**

CA= 0.00000 CB= 0.00000 CC= 0.00000 **Bravais lattice parameters (cos(alpha), cos(beta), cos(gamma))**

#START OF SPACE GROUP   **Starting line in space group information**

FACE CENTERED LATTICE   **The name of the crystal system of the Bravais lattice**

GROUP ELEMENTS

1   1   E   X Y Z 0/1   0/1   0/1 **Symmetric index (1st and 2nd data from the left) and the name in TSPACE (3rd), Jones representation (4,5th, 6th), accompanying translation vector (7th, 8th, 9th)**

2   2   C2X   X -Y -Z 0/1   0/1   0/1

3   3   C2Y   -X Y -Z 0/1   0/1   0/1

4   4   C2Z   -X -Y Z 0/1   0/1   0/1

5   5   C31+   Z X Y 0/1   0/1   0/1

Omission

47   47   IC4Y- Z -Y -X 0/1   0/1   0/1

48   48   IC4Z- -Y X -Z 0/1   0/1   0/1

#END OF SPACE GROUP: **The last line in space group information**

#START OF K-POINTS   **The starting line in the information at each k-point**

1 X   82 0 0 82 D4h   4/mmm   2

The index of k-points (first data (1) from the left) and name given by TSPACE (second data (X)). Coordinates of the reciprocal lattice space are displayed as integers (third, fourth, fifth, sixth data (82,0,0,82)), of which the third, fourth, and fifth coordinates are the numerators x, y, and z,

and the sixth is the common denominator N of the coordinates. (The coordinates of the k-point are expressed as x/N, y/N, and z/N.). The name of the k-group (seventh and eighth data. The seventh denotes the Shane Fleece symbol (D4h), eighth denotes the international symbol (4 / mmm)), number of stars at the k-point (ninth data. When it is 1, this k-point is the first Brillouin zone). There is only one star in (hereinafter 1stBZ), which indicates that it is a point that exists inside 1stBZ. When it is two or more, multiple points are equivalent to this k-point in the 1stBZ, and they exist within the boundary. This proves that it is a point that exists in the environment. Omission

117 X   0   224   0   224 D4h 4/mmm   2

#END OF K-POINTS   **The last line in the information at each k-point**

7.5. Plotting a Band Structure in a Spin-Polarized System

When the spin-polarized system (sample input file is provided in sample/bccFe) is calculated using PHASE/0, band_sym_input.data is exported as a non-magnetic system. When this is used to execute band_symm, the up and down trajectories are individually reduced to a single representation. The list of identified irreducible representations is output to reduce_up.data and reduce_down.data. There are two ways to create an irreducible representation classification band for a spin-polarized system using these files.

1. Because reduce_up.data and reduce_down.data each have the same format as reduce.data has in a non-magnetic setting, by inputting these files separately into band_symm.pl, the upspin and downspin orbits become available to create the expression classification bands separately.

    band_symm.pl reduce_up.data

    band_symm.pl reduce_down.data

    However, the name of the EPS file output in either case of this command is band_reduce.eps. Therefore, if the commands are executed continuously, the EPS file for the downspin orbit will be overwritten to the upspin orbit. Thus, it is necessary to back up the EPS file for the first trajectory.

2. To plot the two trajectories in the same EPS file, execute the following command. In this case, only one EPS file is output.

    band_symm.pl reduce_up.data reduce_down.data

    However, using this function's band diagram output is more complicated than that presented in method 1. Therefore, it is recommended to use method 1.

Below are two plots of the spin-polarized band of Fe with body-centered cubic structure (BCC) created using method 1. The band_symm.pl option used was "-erange -9,26 -imrcolor blue -linecolor red -with_fermi nfefermi.data" for both upspin and downspin orbits.
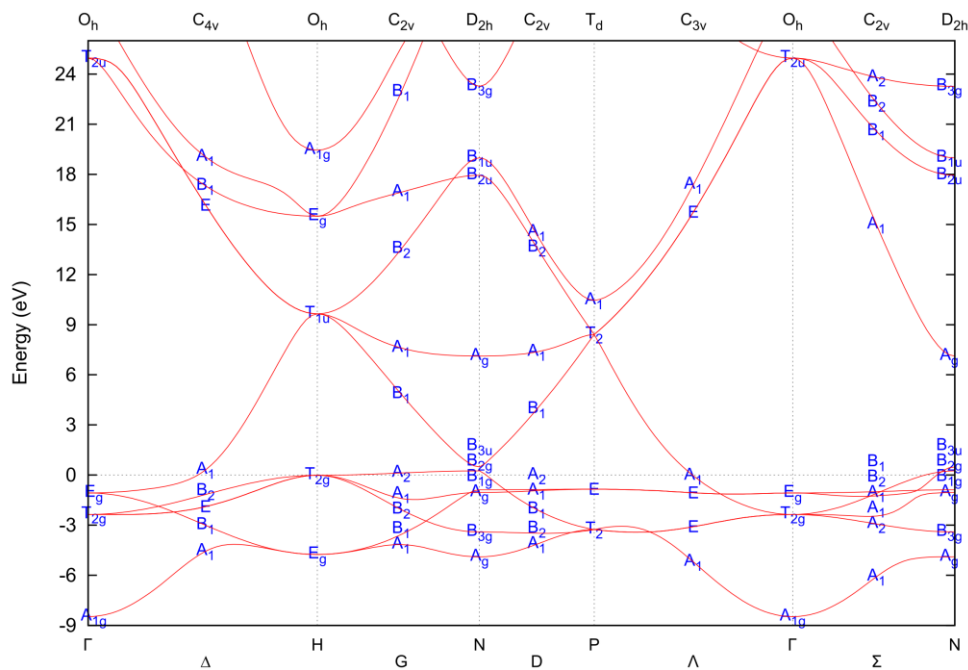

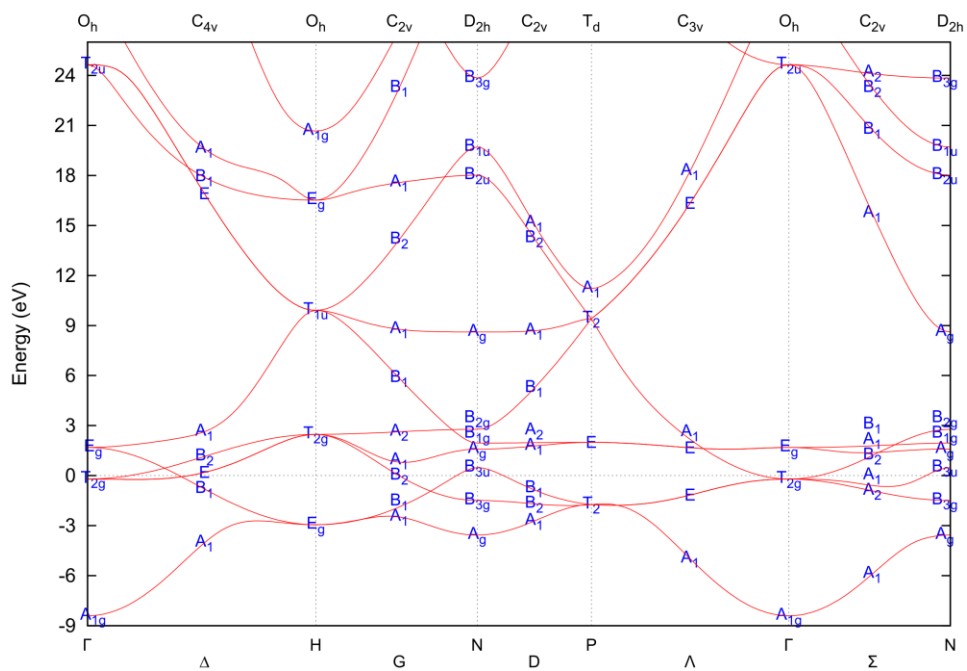Figure 6: Up-spin band structure plot of Fe (BCC).

Figure 7: Down-spin band structure plot of Fe (BCC).

7.6. Band Structure with Spin-Orbit Coupling

When the calculation is performed using PHASE /0 considering the spin-orbit interaction (the sample input file as that used in sample/bismuthene_soc), the band_sym_input.data is run when PHASE/0 is executed, same as the case where the spin-orbit interaction is not considered. If you execute band_symm as an input file, reduce_soc.data will be output.

Create Figure 8 by running band_symm.pl reduce.soc.data -with_fermi nfefermi.data -erange -13,2. By default, irreducible representations are written in the form of Koster symbols. For example, the number 5 at the Γ-point corresponds to the Koster symbol $\Gamma 5$. Refer reference four to see the relationship between Mulliken and Koster symbols. In Fig. 8, the k-point (S-C-Y line) indicated by * cannot be represented by a Koster symbol. This situation can occur at the end of the first Brillouin zone in a non-synchronous system. In this case, the default name assigned by the computer is used. The index of the irreducible representation written in this manner can be confirmed via the output of character.tex (see Fig. 9 for the S-point). At D-point, D_3 and D_4 are paired and have the same energy. The pairing information is output to spacegroup.data (see Section 5.1) (Fig. 10). **The numbers (1, 2) that appear in the output of this pairing correspond to D_3 and D_4, respectively, in the order of the irreducible representations that appear in the index table (Fig. 9).** Similarly, at S-point, S_1 and S_2, and S_3 and S_4 are paired (see Figs. 9 and 10).
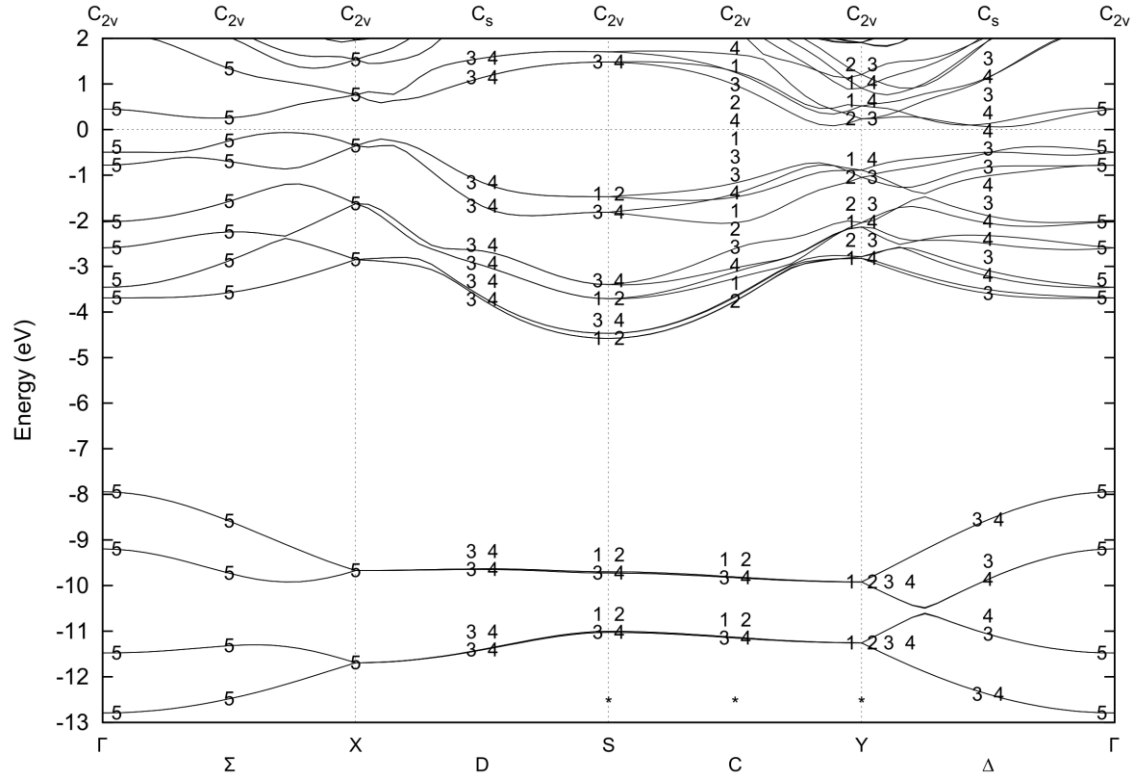
Figure 8: Band diagram of α-Bismuth (Considering spin-orbit coupling)

$D(C_s, m)$	E	$IC2Z$		Class	Operator
1(3)	1	$-i$		E	E
2(4)	1	i		IC2Z	IC2Z

$S(C_{2v}, mm2)$	E	$C2X$	$IC2Y$	$IC2Z$		Class	Operator
1	1	1	$-i$	$-i$		E	E
2	1	1	i	i		C2X	C2X
3	1	-1	$-i$	i		IC2Y	IC2Y
4	1	-1	i	$-i$		IC2Z	IC2Z

Figure 9: Character table (points D and S). In the character table at D-point, the numbers 3 and 4 in parentheses correspond to the Koster symbols D_3 and D_4, respectively. There is no Koster symbol corresponding to the irreducible representation of S-point (* appears above S-point in the band diagram in Fig. 8).

Figure 10: Partial spacegroup.data

8. CREATORS

The programs provided in this package were created, except for TSPACE, by Mineo Saito, Ryosuke Tomita, Itaru Sugita, Hiroyuki Oshima, Thomas Arisoca, Muhammad Y.H. Widianto, and Yuki Yamaguchi (Kanazawa University).

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