DMDW: A set of tools to calculate Debye-Waller factors and other related
quantities using dynamical matrices.

DMDW is a set of tools developed to calculate Debye-Waller (DW) factors and
other related quantities from a dynamical matrix (matrix of force constants
Hessian matrix) using the Lanczos recursive algorithm.[Refs.] This set inclu
a module integrated into FEFF, a standalone version that can be used
independently of FEFF and a Fortran module that can be integrated into
third-party programs. DMDW also includes conversion tools to generate the
required input files from different ab initio programs.

This document is divided into the following sections:

* Installing DMDW
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  ** Expected changes in dynamical matrix file format

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* Installing DMDW
  ** Installing as a FEFF module

The installation of DMDW within FEFF is straightforward. Please refer to the

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46 FEFF installation instructions. After the FEFF installation is completed a
47 module called "dmdw" should be located under the FEFF "bin" directory struct
48
49    ** Creating and installing the standalone version
50
51 Within the "src/DMDW" directory in the FEFF distribution, execute the follow
52 command:
53
54 make standalone
55
56 This will create a directory "dmdw_standalone" under "src/DMDW". Edit "Makef
57 inside the directory "dmdw_standalone/src". Change the "F90" variable to you
58 fortran 90 compiler of choice. Then execute the following commands:
59
60 make
61 make install
62 make examples
63
64 If everything worked correctly the reference results located in
65 "dmdw_standalone/examples/Reference_Results" should agree with those generat
66 in "dmdw_standalone/examples".
67
68    ** Using as a DW factor engine
69
70 [NOT WRITTEN YET]
71
72 --------------------------------------------------------------------------
73
74 * Using DMDW
75
76
77    ** Using dym2feffinp
78
79 Before explaining how to include dynamical matrix DW factors in EXAFS and XA
80 calculations, it is important that the user becomes familiar with some
81 constraints/limitations that are present in the current implementation. Thes
82 limitations stem from the fact that both the dynamical matrix and FEFF input
83 files contain structural information. These structures must match for the DW
84 values to be correct. Since FEFF internally sorts the atoms according to
85 distance to the absorber, special care must be taken to avoid mismatching th
86 structural information coming from the FEFF input with that from the dym fil
87 dym2feffinp is a utility that helps in the generation of FEFF input files wi
88 structures that match those in the dynamical matrix files. The usage of
89 dym2feffinp is as follows:
90
```

```
 91  dym2feffinp [Options] dymfile
 92
 93  where dymfile is the name of the file containing the dynamical matrix. This
 94  command creates two files, feff.dym and feff.inp, which contain correctly
 95  matched structures. (NOTE OF WARNING: If dymfile is named "feff.dym", then
 96  dym2feffinp will APPEND the updated dym information to it. We recommended th
 97  different name is used for dymfile. Future version will check that dymfile
 98  doesn't use the "feff.dym" name.)
 99
100  The default behavior of dym2feffinp can be modified with the following optio
101
102    --c  iAbs    Use atom iAbs as absorber
103    --f  fname   Write feff input to file fname
104    --d  dname   Write adjusted dym file to file dname
105    --j          Skip header and only write POTENTIALS + ATOMS cards
106    --s  spec    Write feff input for spec=XANES or spec=EXAFS
107
108  The --c options allows the user to choose different absorbers. The usual
109  approach of editing a FEFF input file and changing the potential type of a
110  certain atom to 0 will result in mismatched FEFF and dym structures. This sh
111  be avoided. It is recommended that different input files be generated using
112  --c option.
113
114  The --f and --d change the default output filenames from "feff.inp" and
115  "feff.dym" to fname and dname, respectively.
116
117    ** Using within a XANES or EXAFS calculation in FEFF
118
119  The inclusion of dynamical matrix DW factors in XANES and EXAFS calculations
120  analogous to the use of correlated-Debye DW factors in FEFF84. In the XANES
121  case, single-scattering DW factors are calculated for each pair of atoms in
122  cluster. For EXAFS calculations, the DW factors are calculated only for the
123  selected paths (for instance, selected with the RPATH card). For both cases
124  DEBYE card input is only slightly different than in previous versions:
125
126  DEBYE  Temp  Debye_Temp [DW_Opt [dym_File DMDW_Order DMDW_Type DMDW_Route]]
127
128  where:
129      Temp        Temperature at which the DW factors are calculated
130      Debye_Temp  Debye Temperature of the material
131      DW_Opt      Option that controls the type of DW factors used.
132              The possible values are:
133                  0   Correlated-Debye method
134                  1   Eqs. of Motion method
135                  2   Recursion method
```

```
136                      3   CL [?? Need to check]
137                      4   Read from "sig2.dat" file
138                      5   Dynamical-Matrix method
139                     <0   Do not calculate DW factors
140
141  Options 0-4 are explained in the FEFF manual. When DW_Opt=5, the following
142  parameters can be included:
143      dym_File    Name of the dynamical matrix information file. The
144                  default value is "feff.dym"
145      DMDW_Order  Lanczos recursion order to be used in the calculation.
146                  The default value is 2. Well converged results are
147                  usually obtained for DMDW_Order=6-10. For small size
148                  systems, these values might be too large. As a rule
149                  of thumb, DMDW_Order should be less than
150                  3*(Number of atoms)-6. Some paths, within systems with
151                  high symmetry, might require a lower DMDW_Order. The
152                  user should always check for convergence with this
153                  parameter.
154      DMDW_Type   Type of DW calculation.
155                  The possible values are:
156                      0   Parallel s^2
157                  [NOTE: the meaning of this parameter might change in a
158                  future release]
159                  The default value is 0.
160      DMDW_Route  Which paths to use in the dmdw module. These paths do
161                  not affect the path selection in the XAS calculations,
162                  they are used for the generation of an input file for
163                  the independent dmdw module.
164                  The possible values are:
165                       0  Skip dmdw module
166                       1  All SS paths from absorber
167                       2  Same as 1 + all DS paths from absorber
168                       3  Same as 2 + all TS paths from absorber
169                      11  All SS paths
170                      12  Same as 1 + all DS paths
171                      13  Same as 2 + all TS paths
172                  The default value is 0.
173
174    ** Calculating DW factors using the standalone version
175
176  Other capabilities of DMDW can be accessed by means of the "dmdw" module or
177  compiling the standalone version (which generates a "dmdw" module without
178  generating the rest of the FEFF code). All the details described below apply
179  the input used by both the "dmdw" module and the standalone version. During
180  execution of a normal FEFF run using ab initio DW factors, an input for the
```

```
181 "dmdw" module is automatically generated based on the options used in the DE
182 card. This autogenerated input can be used "as is" with the standalone versi
183 or further edited to access other capabilities.
184
185 The "dmdw" input is very simple, with the first three lines determining the
186 parameters of the calculation. The rest of the input depends on the content
187 these first lines.
188
189 Lanczos_Order
190 nT T_Min T_Max
191 DW_Type
192
193 where:
194
195 Line  1 — Lanczos_Order: Number of Lanczos iterations (integer).
196
197   This parameter is equivalent to the DMDW_Order parameter described above f
198   the DEBYE card. It corresponds to the number of Lanczos iterations to be u
199   in the calculation. Well converged results are usually obtained for
200   DMDW_Order=6–10. For small size systems, these values might be too large.
201   rule of thumb, this value should be less than 3*(Number of atoms)–6. Some
202   paths, within systems with high symmetry, might require a lower recursion
203   order. The user should always check for convergence with this parameter.
204
205 Line  2 — nT: Number of temperature values in grid (integer)
206           T_Min, T_Max: Minimum and maximum temperature values (real, in K)
207
208   Define a grid of temperatures in which to calculate the DW factors. This
209   option is very efficient in the generation of whole temperature curves sin
210   it performs the Lanczos procedure only once and then calculates the DW for
211   each temperature.
212
213 Line  3 — DMDW_Type: Type of DW calculation (integer).
214
215   This parameter is equivalent to the one described above for the DEBYE card
216   but more values are available.
217   The possible values are:
218     0   Parallel s^2
219     1   Vibrational free energy
220       2       Self Energy/Spectral function
221     3   Crystallographic u^2
222       4   Perpendicular s^2 (Not available yet)
223
224   The parallel s^2 is the usual mean–square relative displacement (MSRD) alo
225   path. The perpendicular s^2 is the MSRD orthogonal to a path. The
```

```
226    crystallographic u^2 is the mean-square displacement of a given atom with
227    respect to its stationary position. Finally, the vibrational free energy
228    associated with that crystallographic u^2 can also be calculated.
229
230    [NOTE: Options 1 and 4 are not fully activated in this release. Also notic
231         that the meaning of this parameter might change in a future release
232
233 The rest of the input depends on DMDW_Type. Here we list each possible case:
234
235 If DMDW_Type = 0 or 3, the rest of the "dmdw" input file should have the for
236
237 Filename
238 nPathDesc
239 PathDesc1
240 PathDesc2
241 .
242 .
243
244 where
245
246 Line  4 - Filename: Name of file containing the dynamical matrix (string)
247
248    The file must be present in the same directory as the DMDW input and be in
249    "dym" format (see below).
250
251 Line  5 - nPathDesc: Number of path descriptors (integer)
252
253    Define the number of path descriptors to use for the generation of paths.
254
255 Lines 6... - PathDescN: Nth path descriptor used to generate a list of paths
256                         (integer and real, see below)
257
258    A path descriptor has the following form:
259
260       nAt At(1)...At(nAt) Path_Length
261
262    where:
263
264       nAt: Number of atoms in the path (integer)
265       At(i): Index of atom that must be included in the path (integer)
266
267            These indices correspond to the ones used in the "dym" file. The
268            number 0 is a wildcard representing any atom in the structure.
269            For instance, the atom indices "1 0 2" represent a double
270            scattering paths starting at atom 1, ending at atom 2 and
```

```
271            passing through every other allowed atom in the system. The
272            paths are generated in such a way that no consecutive repeated
273            indices are allowed.
274
275       Path_Length: Effective path length cutoff (real, in Bohr)
276
277            This parameter helps fine-tune the generated path list, removing
278            paths that are longer than necessary.
279
280     If the number of atoms in the path is 1 (nAt=1), then only crystallographi
281     u^2 values are computed for the single atom in the path (for all cartesian
282     displacements of that atom). DMDW will skip any multi-atom path for u^2
283     calculations (DMDW_Type = 3) and any single atom path for s^2 calculations
284     (DMDW_Type = 0).
285
286   If DMDW_Type = 1 or 2, the rest of the "dmdw" input file should have the for
287
288   [Shauna, please include here the file format you use for the self-energy
289   calculations and VFE].
290
291     ** The "dym" dynamical matrix file format
292
293     A "dym" file contains the information required by the Lanczos algorithm. T
294     includes the atomic masses, structure and force constants. Two conversion
295     scripts are included in the "bin" directory to convert Gaussian 03 formatt
296     checkpoint ("fchk") files (fchk2dym) and Quantum Espresso dynamical matrix
297     files (dynG2dym) into our "dym" dynamical matrix format. The "fchk2dym"
298     command has been thoroughly tested, but the "dynG2dym" has not. The curren
299     format of the "dym" files is as follows:
300
301   Line 1 - dym_Type: Dynamical matrix file type (integer)
302
303     This value is for future use. Set to 1 for now.
304
305   [Shauna, please include here your modifications to the dym format.]
306
307   Line 2 - nAt: Number of atoms (integer)
308
309     Number of atoms in the system.
310
311   Lines 2..2+nAt - Atomic numbers (integer)
312
313     Atomic numbers of atoms in the system.
314
315   Lines 2+nAt+1..2+2*nAt - Atomic masses (real, in AMU)
```

```
316
317    Atomic masses of the atoms in the system.
318
319  Lines 2+2*nAt+1..2+3*nAt – Atomic coordinates (real, in Bohr)
320
321    Cartesian coordinates ("x y z") of the atoms in the system.
322
323  Lines 2+3*nAt+1..End – Dynamical matrix in atom pair block format (integer
324                          real, see below,in atomic units):
325
326    The force constants in the system are stored for each pair of atoms in th
327    system using the following block format:
328
329      i j
330      d2E/dxidxj d2E/dxidyj d2E/dxidzj
331      d2E/dyidxj d2E/dyidyj d2E/dyidzj
332      d2E/dzidxj d2E/dzidyj d2E/dzidzj
333
334    where:
335
336      i, j: Indices defining the atomic pair
337      d2E/daidbj: Second derivative of the energy (i.e. force constant) with
338                  respect to the a coordinate of atom i and the b coordinate
339          atom j, where a,b={x,y,z}.
340
341  ------------------------------------------------------------------
342  * Examples
343    ** Creating a FEFF input file from a dym file using dym2feffinp
344
345  Here we demonstrate how to convert a dym file, in this case created from a
346  Gaussian fchk file, into matched pairs of feff.inp and feff.dym files, for
347  different absorbing centers.
348
349  The dym file for a CO2 molecule (CO2.dym), converted from the formatted
350  checkpoint file looks like:
351
352  ##################################################################
353      1
354      3
355      8
356      6
357      8
358      15.99491460
359      12.00000000
360      15.99491460
```

```
361      0.00000000    0.00000000    2.20979482
362      0.00000000    0.00000000    0.00000000
363      0.00000000    0.00000000   -2.20979482
364        1    1
365    3.501599e-02 -7.311989e-13 -8.941376e-12
366   -7.311989e-13  3.501599e-02  3.206256e-11
367   -8.941376e-12  3.206256e-11  1.042343e+00
368        1    2
369   -7.001817e-02 -5.485621e-12  2.501278e-11
370   -3.211930e-12 -7.001817e-02 -2.341738e-11
371   -3.124223e-11 -3.615378e-11 -9.594793e-01
372        1    3
373    3.500217e-02 -8.681691e-13 -1.846564e-11
374    8.681691e-13  3.500217e-02 -1.245331e-11
375   -1.846599e-11  1.245327e-11 -8.286417e-02
376        2    1
377   -7.001817e-02 -3.211930e-12 -3.124223e-11
378   -5.485621e-12 -7.001817e-02 -3.615378e-11
379    2.501278e-11 -2.341738e-11 -9.594793e-01
380        2    2
381    1.400363e-01  1.883207e-12  2.058909e-11
382    1.883207e-12  1.400363e-01  4.005329e-11
383    2.058909e-11  4.005329e-11  1.918959e+00
384        2    3
385   -7.001817e-02  2.586772e-12  5.500370e-12
386    4.227571e-12 -7.001817e-02  3.602353e-12
387    3.495310e-11  1.591451e-11 -9.594793e-01
388        3    1
389    3.500217e-02  8.681691e-13 -1.846599e-11
390   -8.681691e-13  3.500217e-02  1.245327e-11
391   -1.846564e-11 -1.245331e-11 -8.286417e-02
392        3    2
393   -7.001817e-02  4.227571e-12  3.495310e-11
394    2.586772e-12 -7.001817e-02  1.591451e-11
395    5.500370e-12  3.602353e-12 -9.594793e-01
396        3    3
397    3.501599e-02  7.311989e-13 -8.940090e-12
398    7.311989e-13  3.501599e-02 -3.206153e-11
399   -8.940090e-12 -3.206153e-11  1.042343e+00
400 ##############################################################################
401
402 The dym files are not required to be sorted in any particular order, they r
403 the atom order of the program that generated the dynamical matrix. In this
404 the order is O, C and O, with the C atom at the origin. Since FEFF internal
405 sorts the atoms according to their distance to the absorber, if this dym fi
```

```
406  used as is to compute the EXAFS/XANES for the C atom, the results would be
407  incorrect. We can generate the appropriate FEFF input file and associated d
408  file with the following command:
409
410  dym2feffinp --c 2 --f CO2_C_feff.inp --d CO2_C_feff.dym CO2.dym
411
412  This creates the following CO2_C_feff.dym file:
413
414  ##############################################################################
415       1
416       3
417       6
418       8
419       8
420    12.000000
421    15.994915
422    15.994915
423     0.00000000     0.00000000     0.00000000
424     0.00000000     0.00000000     2.20979482
425     0.00000000     0.00000000    -2.20979482
426       1     1
427    1.400363E-01   1.883207E-12   2.058909E-11
428    1.883207E-12   1.400363E-01   4.005329E-11
429    2.058909E-11   4.005329E-11   1.918959E+00
430       1     2
431   -7.001817E-02  -3.211930E-12  -3.124223E-11
432   -5.485621E-12  -7.001817E-02  -3.615378E-11
433    2.501278E-11  -2.341738E-11  -9.594793E-01
434       1     3
435   -7.001817E-02   2.586772E-12   5.500370E-12
436    4.227571E-12  -7.001817E-02   3.602353E-12
437    3.495310E-11   1.591451E-11  -9.594793E-01
438       2     1
439   -7.001817E-02  -5.485621E-12   2.501278E-11
440   -3.211930E-12  -7.001817E-02  -2.341738E-11
441   -3.124223E-11  -3.615378E-11  -9.594793E-01
442       2     2
443    3.501599E-02  -7.311989E-13  -8.941376E-12
444   -7.311989E-13   3.501599E-02   3.206256E-11
445   -8.941376E-12   3.206256E-11   1.042343E+00
446       2     3
447    3.500217E-02  -8.681691E-13  -1.846564E-11
448    8.681691E-13   3.500217E-02  -1.245331E-11
449   -1.846599E-11   1.245327E-11  -8.286417E-02
450       3     1
```

```
451   −7.001817E−02  4.227571E−12  3.495310E−11
452    2.586772E−12 −7.001817E−02  1.591451E−11
453    5.500370E−12  3.602353E−12 −9.594793E−01
454       3     2
455    3.500217E−02  8.681691E−13 −1.846599E−11
456   −8.681691E−13  3.500217E−02  1.245327E−11
457   −1.846564E−11 −1.245331E−11 −8.286417E−02
458       3     3
459    3.501599E−02  7.311989E−13 −8.940090E−12
460    7.311989E−13  3.501599E−02 −3.206153E−11
461   −8.940090E−12 −3.206153E−11  1.042343E+00
462 ##############################################################################
463
464
465 This dym file is now centered on the C atom and the atoms are sorted correc
466 The associated CO2_C_feff.inp FEFF input file has the following structure
467 section:
468
469 ##############################################################################
470 POTENTIALS
471      0     6    C
472      1     8    O
473
474 ATOMS
475      0.00000     0.00000     0.00000     0    C  0.00000     0
476      0.00000     0.00000     1.16937     1    O  1.16937     1
477      0.00000     0.00000    −1.16937     1    O  1.16937     2
478 END
479 ##############################################################################
480
481 which is correctly centered and has the same structure as the dym file.
482
483   ** XANES and EXAFS calculations
484
485   A typical FEFF input file that uses ab initio DW factors in a XANES
486   calculation looks as follows:
487
488 ##############################################################################
489 * This feff9 input file was generated by dym2feffinp
490
491  TITLE absorbing atom:    0
492
493  EDGE        K
494  S02        1.0000
495
```

```
496 | *               pot      xsph      fms    paths   genfmt   ff2chi
497 | CONTROL          1        1        1       1       1        1
498 | PRINT            1        0        0       0       0        0
499 |
500 | *          ixc  [ Vr  Vi ]
501 | EXCHANGE      0
502 |
503 | *            r_scf  [ l_scf   n_scf   ca ]
504 | SCF          4.000
505 |
506 | *            kmax   [ delta_k  delta_e ]
507 | XANES        4.000
508 |
509 | *            r_fms      l_fms
510 | FMS          6.000
511 |
512 | DEBYE    500.0  1073.0  5 feff.dym  6  0  1
513 |
514 | POTENTIALS
515 |     0     8     O
516 |     1     1     H
517 |
518 | ATOMS
519 |     0.00000     0.00000     0.00000     0     O  0.00000     0
520 |     0.96141    -0.12674     0.00000     1     H  0.96972     1
521 |    -0.12674     0.96141     0.00000     1     H  0.96972     2
522 | END
523 | ###########################################################################
524 |
525 |   This input file results in the XANES O K edge spectrum of a single water
526 |   molecule. (If an EXAFS calculation is required, the same DEBYE card param
527 |   apply, but the XANES card should be substituted by the EXAFS one.) It use
528 |   initio DW factors at 500K and a dynamical matrix stored in the file
529 |   "feff.dym". The number of Lanczos recursion iterations is set to 6, the t
530 |   of DW calculation is to calculate parallel s^2, and it asks that all sing
531 |   scattering paths from the absorber be calculated independently in the "dm
532 |   module. The input generated for this module is:
533 |
534 | ###########################################################################
535 |     6
536 |     1    500.000    500.000
537 |     0
538 | feff.dym
539 |     1
540 |     2   1   0           3.20
```

```
541  ##############################################################################

542

543    The first line corresponds to the number of Lanczos iterations. The secon
544    defines the temperature, in this case a grid with a single point. The thi
545    defines the type of DW calculation and the fourth the name of the dynamic
546    matrix file. The fifth line declares that the input contains a single pat
547    descriptor, which is included in the next line. This descriptor defines a
548    single scattering paths from the absorber that are less than 3.2 Bohr lon

549

550    A dynamical matrix file for this calculation looks like this:

551

552  ##############################################################################
553        1
554        3
555        8
556        1
557        1
558     15.994915
559      1.007825
560      1.007825
561      0.00000000     0.00000000     0.00000000
562      1.81679640    -0.23950080     0.00000240
563     -0.23950080     1.81679640     0.00000240
564        1     1
565    5.398996E-01 -1.171079E-01  5.031484E-07
566   -1.171079E-01  5.399060E-01  9.690730E-07
567    5.031484E-07  9.690730E-07 -1.841479E-03
568        1     2
569   -4.941835E-01  3.022460E-02 -6.064138E-07
570    8.687800E-02 -4.571081E-02 -1.155657E-07
571   -6.583932E-07  7.894155E-08  9.207451E-04
572        1     3
573   -4.571614E-02  8.688332E-02  1.032683E-07
574    3.022992E-02 -4.941952E-01 -8.535212E-07
575    1.552287E-07 -1.048028E-06  9.207340E-04
576        2     1
577   -4.941835E-01  8.687800E-02 -6.583932E-07
578    3.022460E-02 -4.571081E-02  7.894155E-08
579   -6.064138E-07 -1.155657E-07  9.207451E-04
580        2     2
581    5.034834E-01 -7.711698E-02  6.431492E-07
582   -7.711698E-02  5.501543E-02 -7.759238E-08
583    6.431492E-07 -7.759238E-08 -8.716053E-04
584        2     3
585   -9.299924E-03 -9.761022E-03  1.524317E-08
```

```
586      4.689238E-02 -9.304625E-03 -1.349708E-09
587     -3.672524E-08  1.931636E-07 -4.913982E-05
588         3    1
589     -4.571614E-02  3.022992E-02  1.552287E-07
590      8.688332E-02 -4.941952E-01 -1.048028E-06
591      1.032683E-07 -8.535212E-07  9.207340E-04
592         3    2
593     -9.299924E-03  4.689238E-02 -3.672524E-08
594     -9.761022E-03 -9.304625E-03  1.931636E-07
595      1.524317E-08 -1.349708E-09 -4.913982E-05
596         3    3
597      5.501607E-02 -7.712230E-02 -1.185055E-07
598     -7.712230E-02  5.034998E-01  8.548785E-07
599     -1.185055E-07  8.548785E-07 -8.715942E-04
600 ###############################################################################
601
602    ** Calculating DW factors with the standalone version
603
604 [NOT WRITTEN YET]
605
606    ** Creating dynamical matrix files from third-party programs
607
608 [NOT WRITTEN YET]
609
610 --------------------------------------------------------------------
611 * Troubleshooting common problems
612    ** Structure problems
613
614 [NOT WRITTEN YET]
615
616    ** Lanczos problems
617
618 * If the code warns that there are less poles than Lanczos iterations, it
619   usually means that the iteration order is to high. Try with a smaller
620   number.
621
622 * When the structure associated with a dynamical matrix is not sufficiently
623   optimized, the program is likely to report that certain paths result in
624   poles associated with imaginary frequencies. The code currently ignores
625   these poles by setting their weight to zero. Usually this doesn't affect
626   results significantly, but they should be considered very carefully anywa
627
628 * The code checks the symmetry of the dynamical matrix. If isn't sufficient
629   symmetric, the results should be examined carefully.
630
```

```
631 ----------------------------------------------------------------------
632 * Future developments
633   ** Performance improvements
634
635 [NOT WRITTEN YET]
636 Parallelization of calculation of DW factors in XANES, if running under MPI
637
638   ** Expected changes in FEFF input format
639
640 [NOT WRITTEN YET]
641
642   ** Expected changes in DMDW input format
643
644 [NOT WRITTEN YET]
645
646   ** Expected changes in dynamical matrix file format
647
648 Inclusion of forces (to use with less than optimal structures)
649 Inclusion of a title (for bookkeeping purposes)
650
651 [NOT WRITTEN YET]
652
653
```