NLEM keyword reference

Keyword: REFLECTANCE

```
REFLECTANNCE { value [str] }
```

Value:

name of file

Description:

The file name which contains the reference data for the reflectance in a range of wavelengths (needed for fitting).

File format:

```
Wavelength [nm]      Reflectance
1200.0               0.29
1100.0               0.28
              .
              .
              .
```

Example:

```
 REFLECTANCE R_data
```

Keyword: MATERIAL

```
MATERIAL { value1 [str] value2 [double] value3 [int] }
```

Value1:

name of file

Description:

The file name which contains the refractive index for the material layer as a function of wavelength.

Value2:

thickness

Description:

Sets the thickness of the material layer in nanometers

Value3:

 0/1

Description:

Sets if the specified material will be fitted, i.e., 0: False, 1: True.

Example:

```
MATERIAL Air            0           0
MATERIAL SiO2        2000           1
MATERIAL Si             0           0
```

Keyword: FIT_LIMITS

Keyword1: **RUNS_NUM** { value [int] }

Value:

number of runs

Description:

Sets the maximum number of minimization cycles

Example:

FIT LIMITS RUNS_NUM   **10**

Keyword2: **ROUGH_LRS** { value [int] }

Value:

number of layers

Description:

Sets the number of layers for discretizing the rough surface into slices

Example:

FIT_LIMITS   ROUGH_LRS   **32**

Keyword3: **LAMDA_MIN** { value [double] }

Value:

wavelength

Description:

Sets the lower limit of the wavelength range in nanometers

Example:

FIT_LIMITS   LAMDA_MIN   **300.0**

Keyword4: **LAMDA_MAX** { value [double] }

Value:

wavelength

Description:

Sets the upper limit of the wavelength range in nanometers

Example:

FIT_LIMITS   LAMDA_MAX   **1200.0**

Keyword4: **LAMDA_NUM** { value [int] }

Value:

number of wavelengths
Description:
Sets the total number of wavelengths in range
`[LAMDA_MIN, LAMDA_MAX]`
Example:
`FIT_LIMITS  LAMDA_NUM   `**`1200`**

CAUTION Ordered Keyword (these should be specified in the following order)
FIT_PARAM ROUGH `{ value1[double] value2[double] value3[double] }` *# height*
FIT_PARAM ROUGH `{ value4[double] value5[double] value6[double] }` *# shape*

 # height
Value1:
Initial guess for height
Description:
Sets the initial guess for the roughness height to be used in the minimization
Value2:
lower bound for height
Description:
Sets the lower bound for the height parameter space
Value3:
 upper bound for height
Description:
Sets the upper bound for the height parameter space

 # shape
Value1:
Initial guess for shape
Description:
Sets the initial guess for the roughness shape to be used in the minimization
Value2:
lower bound for shape
Description:
Sets the lower bound for the height parameter space
Value3:
 upper bound for shape
Description:
Sets the upper bound for the shape parameter space

Examples:

Simultaneous prediction of height and shape may lead to optically similar rough morphologies (see accepted manuscript ...).

1. Only height as free parameter for the minimization
   (fixed shape i.e., value4 = value5 = value6):

```
FIT_PARAM ROUGH    30.0    12.0    62.0
FIT_PARAM ROUGH     1.0     1.0     1.0
```

2. Only shape as free parameter for the minimization
   (fixed height i.e., value1 = value2 = value3):

```
FIT_PARAM ROUGH    32.0    32.0    32.0
FIT_PARAM ROUGH     0.5     0.0     4.0
```

Keyword: EMT_PARAM

Keyword1: PMAX

Keyword2: GAMM

Keyword3: DELT

Keyword4: SEMI

Keywords 1-4 {fixed values}

These keywords correspond to the NLEM parametrization for the depolarization factor (see accepted manuscript)

Keyword: EMT_PARAM

Keyword1: BETA

Keyword2: ALPHA

Keywords 1-2 {fixed values}

These keywords correspond to the NLEM parametrization for the weight factor (see accepted manuscript)

Keyword: OPTION PRINT

```
OPTION { value [INT] }
```

Value:

0/1

Description:

Sets if info will be printed on screen, i.e., 0: False, 1: True

<u>Examples:</u>

```
OPTION PRINT    1
```