NAME

sts-y2xy − convert Digital Instruments NanoScope 4 TMSTS datafile from raw y to scaled xy format.

SYNOPSIS

sts-y2xy [−ahHdDivVz −er −b*bias* −c*center* −g*gain*] [−−] [−] [*filename*...]

It is possible to have whitespace between a command line option and its parameter.

DESCRIPTION

sts-y2xy is a program to convert Digital Instruments NanoScope 4 Atomic Force Microscope (Tapping Mode) / Scanning Tunneling Spectroscopy (TMSTS) datafiles from raw y to scaled xy format.

The single column datafile with raw current datapoints and with optional header lines is converted to one or two datafiles with both a sweep voltage column (x [V]) and a scaled current column (y [nA]). The header lines are stripped.

There are two types of sweeps:
1. extend: datafile contains one sweep, one output file: *filename*`xy.xy`
2. retract: datafile contains two sweeps, two output files: *filename*`xye.xye`, *filename*`xyr.xyr`

The conversion is controlled by the following parameters (with example values):

```
Sweep type retract  [y/n]: n
Sweep center voltage  [V]: 0
Sweep bias voltage    [V]: 1
Calibration factor [nA/V]: 0.1
```

This section is divided into the following subsections: Initialization, Options, Processing, Example NanoScope 4 TMSTS input file, Example sts-y2xy output file, Example sts-y2xy log-messages and Program exit status.

Initialization

When **sts-y2xy** is run, it starts scanning the commandline parameters. Then it requests for mandatory conversion parameters that not have been specified on the commandline. Next, processing of the input files specified on the commandline begins.

When no input files are specified, **sts-y2xy** issues an error message that no files have been specified. **sts-y2xy** does not behave like a filter program −process stdandard input, write to standard output− because it must be able to re-read the input file to determine the number of datapoints. This may not be possible with standard input.

Options

sts-y2xy can be executed with the following options:

−a print author information,

−h print overview of options,

−H print program description,

−d print debug information (−d: stdout, −D: stderr),

−dd print also number and value of each datapoint processed,

−i select files specified on commandline interactively,

−v verbose; print input filename and summary information (−v: stdout, −V: stderr),

−z suppress informative messages,

−e input file contains extended sweep only,

−r	input file contains both extended and retracted sweep,
−b *bias*	sweep bias voltage (half sweep amplitude) [V],
−c *center*	sweep center voltage [V], default 0,
−g *gain*	y-axis calibration factor [nA/V],
−−	end option section,
−	process standard input; cannot be used from a terminal, because input must be re-read.
filename	e.g. `*.txt` for all datafiles in the current directory.

Processing

sts-y2xy first checks if the length of the input filename without directory part and extension −the basename− is no longer than five characters. This is to enable the addition of `xy`, `xye` or `xyr` to the name. Next **sts-y2xy** checks if the input filename does not have a `.xy`, `.xye` or `.xyr` extension, because in that case you may be overwriting your input file. Then it determines the name(s) of the output file(s) and opens the output file(s). The filenames are constructed by removing the extension of the input filename and appending `xy.xy` for an extend-only sweep, or `xye.xye` and `xyr.xyr` for a retract sweep.

Next the total number of datapoints in the input file is determined by reading through the file. The number of header lines is of no importance, **sts-y2xy** looks for lines with datapoints, regular expression:

{whitespace}* [+−]?[0-9]+ .

Then the input file is re-read to obtain the data values and write the scaled values to the output file(s).

Finally the output file(s) is (are) closed and processing of the next input file can begin.

Calculation of sweep voltage for extend-only input file

The sweep voltage is calculated as follows from the sweep center voltage and the sweep bias voltage.

$$x_p = sweepCenterVoltage + sweepBiasVoltage\ \frac{p - 1 - \frac{n-1}{2}}{\frac{n-1}{2}} \quad [V]$$

where p is the number of the point (1. . *numberOfPoints*) and n is the *numberOfPoints*.

Calculation of sweep voltage for extend and retract input file

The calculation of the sweep voltage is broken into two parts, one for the data of the extended sweep ($p \le \frac{n}{2}$) and one for the data of the retracted sweep (the rest). The calculations are as follows.

Extended sweep, $p \le \frac{n}{2}$:

$$x_p = sweepCenterVoltage + sweepBiasVoltage\ \frac{p - 1 - \frac{n/2-1}{2}}{\frac{n/2-1}{2}} \quad [V]$$

Retracted sweep, $p > \frac{n}{2}$:

$$x_p = sweepCenterVoltage + sweepBiasVoltage\ \frac{p - 1 - n/2 - \frac{n/2-1}{2}}{\frac{n/2-1}{2}} \quad [V]$$

where p is the number of the point (1. . *numberOfPoints*) and n is the total *numberOfPoints* for extend plus retract sweep.

Calculation of scaled y value

The nanoscope current is calculated as follows from the y data.

$$y = calibrationFactor \frac{(\text{double})\ data}{65536} \quad [\text{nA}]$$

where *calibrationFactor* is the scaling factor as specified with option **-g** or entered for the `Calibration factor [nA/V]:` prompt and *data* is the integer value from the input data file.

Example NanoScope 4 TMSTS input file

An example of a part of a NanoScope 4 AFM (Tapping Mode) / STS datafile is shown below.

```
?∗Force file list
\Version: 0x04460200
\Date: 12:56:04 PM Mon Feb 05 2001
\Start context: ROL
\Data length: 20480
\∗Equipment list
\Description: MultiMode TMSTS
\Controller: IIIA
\Microscope: MultiMode
\Extender: None
snip
\∗File list end

    -212
     -96
    -160
    -188
    -101
snip
     160
     161
     163
     139
     107
```

Example sts-y2xy output file

Here is a snippet of the **sts-y2xy** extended output file for the inputfile shown above The following commandline was used: `sts-y2xy -v -r -b1 -g0.1 test3.txt`

```
-1              -0.000323486
-0.998045       -0.000146484
-0.99609        -0.000244141
-0.994135       -0.000286865
-0.99218        -0.000154114
snip
0.99218         0.000268555
0.994135        0.000306702
0.99609         0.000238037
0.998045        0.00025177
1               0.000369263
```

Example sts-y2xy log-messages

Here is an example of the **sts-y2xy** log-messages for the input file shown above, obtained with option `-v`.

```
sts-y2xy  version 1.5, May 21 2001  Convert TMSTS Y datafile to XY datafile(s).

Sweep type retract  [y/n]: y
Sweep center voltage  [V]: 0
```

```
Sweep bias voltage    [V]: 1
Calibration factor [nA/V]: 0.1

test3.txt: 2376 lines, 1024 datapoints written to .\test3xye.xye, .\test3xyr.xyr.
```

Program exit status

When a file cannot be found, or the file cannot be properly processed, the program stops and issues an error message. The failure to process a file is reflected in the programs exit status (see DIAGNOSTICS below).

ENVIRONMENT

No environment variables are used.

FILES

sts-y2xy uses and creates the following files:

filename.txt NanoScope 4 TMSTS raw input datafile with optional header lines,

*filename*xy.xy output file with scaled extend data for an extend-only sweep,

or

*filename*xye.xye output file with extend data for an extend plus retract sweep and

*filename*xyr.xyr output file with retract data for an extend plus retract sweep.

This naming scheme has been choosen to accomodate the use of Origin to create graphs of these files. Origin does not pay attention to the extension of a filename when importing files. Generally, *filename* is something like *ddd*, e.g. `012`. *filename* should not be longer than 5 characters to maintain compatibility with MS-DOS filenames (8.3).

DIAGNOSTICS

sts-y2xy can return the following exit values:

0 success: program execution has been successfully completed,

1 commandline error: an invalid option is specified,

2 processing error: a file could not be opened or closed, an error occurred while writing to an output file,

3 interruption: the user interrupted the program,

4 internal error: an unexpected situation in program behaviour occurred.

SEE ALSO

xy2xy(1), **xy2xyy**(1), **xyy2xy**(1).

NanoScope Version 4 information at:
http://www.weizmann.ac.il/surflab/peter/headers/index.html

EXAMPLE

1. Convert all .txt datafiles with extend and retract sweeps into *filename*xye.xye and *filename*xyr.xyr and record the messages into file alltxt.log. Bias is one Volt, conversion gain is 0.1 nA.

```
sts-y2xy -vr -b1 -g0.1 *.txt >alltxt.log
```

2. As above and collect normal *and* error messages into file alltxt.log (Windows NT).

```
sts-y2xy -Vr -b1 -g0.1 *.txt 2>alltxt.log
```

LIMITS

sts-y2xy cannot process files with lines longer than 200 characters.

BUGS

(to be determined.)

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