Documentation cp-tools

Version 1.0

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1 Introduction

The software bundle *cp-tools* is a set of Python classes and scripts that help to derive the thermophysical properties c_p, α, V and B as function of temperature according to the algorithm described by Zienert and Fabrichnaya (2018) [1]. In addition, several scripts are provided that can be used to extract necessary data from experimental datafiles.

1.1 About this guide

All written functions are excessively explained by comments in the source code. Therefore, no source code documentation will be given here. In the folder 'classes', you can find the core libraries of the software bundle. The cp algrorithm [1] is implemented in 'classes/class_debye.py'. The other three classes 'classes/class_consts.py', 'classes/class_datafile.py' and 'classes/class_math_helpers.py' defining sets of helper functions for dealing with experimental datafiles and doing certain mathematical calculations.

The 'examples' folder includes ready-to-use examples of how to use the core functions of *cp-tools*, especially how to call the cp-predicting algorithm. The folder 'scripts' bundles a set of helpful scripts that can be used to evaluate experimental data.

In this guide, the aim and usage of the scripts within the 'examples' and 'scripts' folders will be explained in detail.

2 Examples

2.1 cp-calc-auto.py

The script *cp-calc-auto.py* calculates the thermophysical properties using the c_p-predicting algorithm for all substances given in the main config file. If needed, you can use parallel computing.

CALL: *python examples/cp-calc-auto.py*

All necessary config variables are listed and descriped in table 2.1.

2.1.1 main config file

The input parameters for c_p calculation must be given in the main config file defined by *cfg_dir*+*cfg_file* (see table 2.1 for details). An example config file comes along with the software: 'cfg-cp-calc/data-cp-calc.cfg'.

The parameters must be given as tab separated values in the following order: **name**, **V0** in $^{cm^3}/_{mol}$, **B0** in GPa, **m** in $^{GPa}/_{K}$, **Theta_fit** in K, **Theta_calc** in K, **E_s** in $^{KJ}/_{g}$, **alpha_D** in $^{1e6}/_{K}$ and **T_m** in K, where Theta_fit is the calorimetric Debye temperature, Theta_calc is the calculated Debye temperature based on elastic constants, E_s is the specific energy, alpha_D is the volumetric thermal expansion coefficient at $T = \Theta_D$ and T_m is the melting temperature.

2.1.2 additional config files

For each substance defined by *name* in the main config file, an additional config file '*name*.cfg' can be created in the folder *cfg_dir*. In each line, an options can be given as '*option*=value'. Possible options are listed in table 2.2.

Table 2.1: Description of config variables used in *cp-calc-auto.py*.

name	description	type	value/options
		c_p Algorithm	
cp_variant	Sets how α_V at $T = \Theta_\mathrm{D}$ is selected.	string	***free***: α_V at $T = \Theta_\mathrm{D}$ is taken from config file ***prediction***: calculates α_V at $T = \Theta_\mathrm{D}$ from melting temperature.
TD_variant	Sets which Debye temperature is taken.	string	***fit***: use the calorimetric Debye temperature ***calc***: use the calculated Debye temperature based on elastic constants ***prediction***: estimate the Debye temperature using the *specific energy*-relation
		Change of input parameters (for evaluation purpose)	
PCT_vars	Sets which input parameters should be changed by *PCT_percents*	string list	***alpha***, ***B0***, ***m***, ***V0***, ***TD*** standard: PCT_vars=[] (no change of input parameters)
PCT_percents	Sets how much the parameters in *PCT_vars* should be changed.	float list	values in %
		Computational options	
CFG_compute_only_new	If a savefile already exist, should the calculation be redone?	boolean	***True***, ***False***

Continued on next page

Table 2.1 – continued from previous page

name	description	type	value/options
CFG_n_cpu	Sets the number of CPUs used for parallel computing.	int	Give the number of CPUs you want to use.
	General saving options		
cfg_dir	Sets the folder where the config files can be found.	string	Folder name can be relative or absolute.
cfg_file	Sets the name of the main config file.	string	The config file will be read as *cfg_dir*+*cfg_file*.
file_PREFIX	Sets the folder where the results will be saved.	string	Folder name can be relative or absolute.

Table 2.2: Description of additional options for ech substance used by *cp-calc-auto.py*.

name	**description**	**type**	**value/options**
		c_p Algorithm	
cp_T_end	Sets the highest temperature for calculation.	float	A temperature in K.

3 Scripts

3.1 calc-cp-cv-difference.py

The script *calc-cp-cv-difference.py* calculates the difference between the c_p of a material saved in *DATAFILE* and the calculated c_V for a given Debye temperature.

CALL: *python scripts/calc-cp-cv-difference.py DATAFILE*

The DATAFILE must contain tab separated T-c_p values. An example file can be found for silver in 'example-datafiles/data-Ag-cp-Furukawa1972.data' containing the values compiled by Furukawa et al. (1972) [2].

After calling, the script will ask for a Debye temperature in K and a filename to save the calculated values. In our example of silver, the calorimetric Debye temperature is 215 K.

3.2 debye-int.py

The script *debye-int.py* calculates values of c_V for a given temperature range and Debye temperature using Debye's equation [3] in steps of $\Delta T = 0.5\,\mathrm{K}$.

CALL: *python debye-int.py TD*

Here, *TD* is the Debye temperature in K that can be optional given as an argument. All possible config variables are listed and descriped in table 3.1.

3.3 debye-temperature-elast-const.py

The script *debye-temperature-elast-const.py* calculates the Debye temperature based on zero-Kelvin properties using the relations given by Debye (1912) [3] and by Anderson (1963) [4].

CALL: *python scripts/debye-temperature-elast-const.py*

The script will ask for the molar mass, number of atoms per formular unit, density, Poisson number and the bulk modulus. The calculated Debye temperatures and the value of the specific energy will be printed on the screen.

3.4 fit-m-from-B-T.py

The script *fit-m-from-B-T.py* calculates the linear slope m of $B(T)$ from a a least-square fit of a linear equation to given (experimental) data above the transition temperature T_B^{trans}.

CALL: *python scripts/fit-m-from-B-T.py* DATAFILE

The DATAFILE must contain tab separated values of T in K and B in GPa. An example datafile can be found in 'example-datafiles/data-Ag-11652-Wern2004.data' containing values for silver compiled by Wern (2004) [5].

The script will ask for the Debye temperature, the volumetric thermal expansion coefficient at the Debye temperature, and the values of volume and the bulk modulus at $T = 0\,\text{K}$. Using the c_p-predicting algorithm, the script determines the bulk modulus transition temperature and uses then all $B(T)$ values above this temperature for obtaining m.

3.5 fit-TD-from-heat-capacity.py

The script *fit-TD-from-heat-capacity.py* calculates the Debye temperature from a least-square fit of the Debye equation to experimental c_p values.

CALL: *python scripts/fit-TD-from-heat-capacity.py DATAFILE*

The DATAFILE must contain tab-separated values of T and c_p. An example file can be found for silver in 'example-datafiles/data-Ag-cp-Furukawa1972.data'.

The script will ask for the highest temperature that should be used for fitting. For best results, choose a temperature where $c_p \approx c_V$ is fulfilled. If your c_p values are from a multiphase sample, you can also give the mole fraction of each additional phase and its Debye temperature. Press ENTER if you do not want to add a further phase for calculation.

3.6 fit-TD-from-thermal-expansion.py

The script *fit-TD-from-thermal expansion.py* determines the Debye temperature from a least-square fit of Garai's equation [6] to (experimental) values of the thermal expansion coefficient.

CALL: *python scripts/fit-TD-from-thermal-expansion.py DATAFILE*

The DATAFILE must contain tab-separated values of T in K and α_V in $^{1e6}/_{\text{K}}$. An example file can found in 'example-datafiles/data-Ag-alpha-Kirby1972.data' using the data for silver compiled by Kirby et al. (1972) [7].

The script will ask for the highest temperature for fitting, which should be in the range of the calorimetric Debye temperature. After fitting, the script will print the Debye temperature and calculates for each given experimental value the estimated ones, which all are saved to a file named 'savefile-fit-te-*DATAFILE*'.

Table 3.1: Description of config variables used in *debye-int.py*.

name	**description**	**type**	**value/options**
	c_p Algorithm		
T	Sets the start temperature for c_V calculation.	int	Give a value in K.
T_end	Sets the end temperature for c_V calculation.	int	Give a value in K.
TD	Sets a Debye temperature that is used if no is given on the command line.	int	Give a value in K.
savefile	Sets the filename for saving the calculated values. The filename will be '*savefile-TD*'.	string	Give a name.

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