User's Guide

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Properties of solid materials

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Contents

Roadmap

Before you start

This manual is the reference user's guide for the standard solid material properties included in the CryoSoft programs, SOLIDS. SOLIDS is a set of routines that compute thermophysical material properties: density, specific heat, thermal conductivity, resistivity and critical surface of superconductors. It is called as a library by several CryoSoft programs, among which THEA and HEATER. The library is provided with a user interface that allows simple calculations of properties, table and plot generation. This manual gives a user-end explanation on the installation and working of the code, reference naming and usage of the material properties routines, instructions on the user interface, and a list of error messages.

How to use this manual

This manual is structured as follows:

- Chapter 1 gives a short description of the SOLIDS library, the wrapper and the user interface structure;
- Chapter 2 gives basic information on the installation, and explains how to start and run the SOLIDS user interface on a UNIX/LINUX workstation;
- § Chapter 3 contains the list of materials and material properties included in this version of SOLIDS;
- Chapter 4 contains information on the naming, indexing, calling protocol and variables used in the material properties routines;
- § Chapter 5 gives the main references to material properties and a general bibliography for documentation.

Beginners to SOLIDS should read chapters 1, 2 and 3 in sequence. They will make occasional cross reference to chapter 4 for detailed information. Experienced users will use chapters 3 and 4 for daily operation.

CHAPTER 1 **Introduction**

What is SOLIDS

SOLIDS is a set of routines to compute thermophysical material *properties* (e.g. density, specific heat, thermal conductivity, resistivity and critical surface of superconductors), as a function of a set of *state variables* (e.g. temperature, field and field angle, residual resistivity ratio, strain and operating current density). The routines are grouped in a self-contained library with a wrapper that facilitates the calling of single *properties* for a given material. The SOLIDS library is called by several of the CryoSoft simulation codes and provides a standard and homogeneous material database referenced to available sources and data from authorities in the field (see Chapter 5 References). The thermophysical properties of solid materials of common use in superconducting magnets that are included in SOLIDS have been obtained as fits to the data quoted, and are tailored as a balance of accuracy, execution speed and simplicity in the calling and returning protocol.

Building a material database is a delicate and labor-intensive matter, the SOLIDS library does not intend to substitute to existing databases, nor establishing a new reference. Overall errors on the properties of the order of 3 to 5 % can be expected with respect to published data and reference values for materials that are well established and extensively characterized (e.g. pure metals such as Cu, Al, W). Alloys and composites have a larger inherent variability, related to the variety of grades and details on the actual material nature. Accuracy in this case can be degraded to 10 to 20 %. In some cases, e.g. thermal properties of superconductors, the data sources are scarce or very scattered. In this case the material properties represent an average of data, representative values, sometimes obtained from theoretical limits, and cannot be taken as a true reference.

In addition to being a link-able library, the SOLIDS library comes with an application that allows to query directly the material properties. The user interface has a rather simple structure, and allows to compute *properties* for a certain value of the *state variables* (e.g. specific heat for a given temperature), build tables of *properties* as a function of the *state variables* in a certain range, or a plot of *properties* as a function of the *state variables* in a certain range.

All *property* routines are in the form of FORTRAN functions. The foundation of library is organized as a collection of *property functions*, one set of functions per material. The materials are categorized by classes:

- Pure metals
- Metallic alloys
- Insulating materials
- **Superconductors**

The *property* computed by each function is always a single value. The complete set of *properties* computed is the following:

whereby, depending on the class of the material, some of the above properties do not apply (e.g. superconducting properties only apply to superconductors, and electrical resistivity is not computed for insulating materials).

The complete set of *state variables* that needs to be provided as input can be as large as the following:

As for the *properties*, because of the variety of materials among the above classes, the *state variables* that need to be provided can be only a sub-set of above. This may also be true when a material *property* dependence on a specific *state variable* is not known. The result is that functions for the same property for different materials may have different calling protocols.

This is why we have added a *wrapper* for the routines whose function is to provide a homogeneous means to ask for a specific property of a specific material with the same set of state variables for all materials. The SOLIDS wrapper is a set of FORTRAN functions that act as interface from the calling program to the single material packages. A logical representation of the structure of the SOLIDS library is shown in Fig. 1. All properties are accessed through the wrapper, whose calling protocol is detailed later. Though the expert user can call directly the property routines of each single material, we recommend that the whole library is linked and the call is performed using the wrapper entries.

Finally, a user interface based on the SOLIDS library is provided with the standard installation. The user interface is a UNIX/LINUX program where the user can select a specific material, enter the state variables required for the calculation for the material, and have single properties computed for a specific set of state variables. Tables or plot can be generated by selecting ranges of state variables, instead of a single set.

¹ The angle is measured from the direction perpendicular to the current flow in the superconductor, i.e. normal to a LTS wire or aligned with the c-axis of an HTS wire. Applied field at zero angle is hence understood as transverse to the axis of current flow in the superconductor, while an angle of 90 degrees is understood as parallel to the axis of current flow. In the case of HTS no distinction is made between a field aligned along the a- or b-axis, i.e. an angle of 90 degrees is for field in the a-b plane.

Figure 1. Schematic view of the principle of the SOLIDS library. Single material properties functions are grouped in packages by material class. Though each property package can be called and reference separately, the properties are most conveniently called through a wrapper that provides a homogeneous calling protocol.

CHAPTER 2

Installing and Running SOLIDS

Platforms

SOLIDS is provided as a library developed for running under UNIX or UNIX-like (e.g. Linux) operating system. At the time when this manual is written, the platform where SOLIDS is developed is

Macintosh running MacOS-X (10.10.5 and higher) under XQuartz, $(2.7.8)$ gcc (5.1) with gfortran.

At different time of the development and production, the code has been installed and tested on the following platforms:

- Mac-OS X (10.2 and higher) operating system;
- GNU/Linux operating system (most distributions).
- INTEL PC's running RedHat Linux OS;
- IBM-RISC workstations running the AIX-V4 operating system and later;
- SUN-SPARC workstation running the Solaris OS operating system;
- DEC-ALPHA workstation running the OSF-1 operating system;
- HP workstations running HP-UX OS;
- Windows-2000 and Windows-XP operating system, with an installed CYGWIN environment (the reference version tested is CYGWIN 1.5.24-2).

Although UNIX obeys strict standards, the architecture of the operating and file system may vary from vendor to vendor. It is therefore possible that porting may require minor adaption of code and libraries. Contact us for advice.

In the following sections we assume here that you are running under a UNIX or UNIX-like operating system, and that you are familiar with UNIX commands, directory and file handling. Contact your system administrator for matters regarding UNIX commands and file system.

Although versions of SOLIDS have been ported to PC's running the Windows OS, at the time when this manual is written this is not a platform directly supported and part of the instructions provided below (i.e. how to run and post-process a case) may not be directly applicable.

Installation

SOLIDS is one of the standard libraries in the CryoSoft family of programs. You will have therefore received the CryoSoft package containing SOLIDS either as a tar-ball or in preinstalled form. Verify in the CryoSoft installation manual [6] the procedure to be followed for the proper installation of the complete package. A standard installation will generate the SOLIDS library by default when compiling any of the CryoSoft codes. The library generated by a standard installation is ~/CryoSoft/lib/solids.a and the executable code of the user interface is ~/CryoSoft/bin/solids (the symbol ~/ stands for your home directory).

How to link the SOLIDS library

The SOLIDS library generated by the compilation step described above can be linked as a static library using a fortran compiler such as GNU gfortran. As an example, the following command will link the library to a user program myprogram:

gfortran myprogram.f ~/CryoSoft/lib/solids.a -o myprogram

contact your system administrator for more explanations on how to link static libraries.

How to run the SOLIDS user interface

Start-up and properties queries To run the SOLIDS user interface you will need to launch the executable code. In the standard installation on a UNIX system described above SOLIDS is launched typing the command:

~/CryoSoft/bin/solids

The user interface has a simple menu structure that allows to select a specific material and choose one of the following queries:

- a single property value for a given set of state variables;
- generate a table of property values for a given set of state variables of which one has a define variation in a given interval;
- generate a plot of property values for a given set of state variables of which one has a define variation in a given interval.

The navigation through the menus is relatively simple. The material selection menu appears first, as soon as the user interface is launched. A screen-shot of the material selection is reported below. A given material is selected by entering the corresponding ID. A "0" entry closes the session. An incorrect entry (e.g. a non-existent ID, or a wrong format) causes the menu to loop and prompt for a correct entry. This principle applies to all menus.

Once the material is selected, the use has a choice of the type of query, i.e. single point, table or plot generation. A screen-shot of the query selection menu is also reported below. Note how the header indicates that the material selected is Copper. The user can return the material selection menu with a "0" entry.

In case the selected query is a single point property calculation, the user is asked to enter either a set of state variables as applicable for the particular material class. The result of the calculation is shown in the following screen-shot, where the corresponding thermophysical properties are printed to screen.

Material selection menu

Query selection menu

<<< Cu PROPERTIES >>> Enter Your Choice:			
		(3) Plots	(1) Inquiry (single point) (2) Table creation
			(0) Return to previous menu

Input of state variables for a single point property calculation (T=4.2 K, B=10 T, RRR=100)
 $\langle\langle\langle\,$ STATE VARIABLES $\rangle\rangle\rangle$

(free input format)

Example of single point property calculation for Copper (T=4.2 K, B=10 T, RRR=100)

Press <Return> to continue

As an alternative query, the user can select to generate either a table, or a plot. In this case the user is first prompted to select which state variable is the one specifying the range of variation in the table or plot. A screen-shot of this menu is reported below, followed by the corresponding prompts asking for the value of the *fixed* state variables, and the range of *running* state variable. This last is entered as an initial value, a final value and a step.

Example of state variable selection for running range

Example of state variable input (fixed T=4.2 K and RRR=100, running B in the range of 0 to 10 T with step of 1 T)

 $<<$ STATE VARIABLES \gg (free input format) Enter single value for: Temperature (K) $4,2$ Enter single value for: Residual Resistivity Ratio (-) 100 Enter range (begin, end, step) for: Field (T) $0\,$ 10 $\,1$

Tables As explained above, the SOLIDS user interface can generate tabulated properties as a function of the state variables in a range of variables and with a step chosen by the user. The table consists of the state variable selected as the independent variable, and the computed properties selected for calculation. The tables are found in the solids.txt file, which is found in the directory where the user interface is launched. The tables have a simple, tab-separated format, starting with a header containing the material name, a table header listing the keywords for the state variables and the properties calculated, followed by their physical units, and the tabulated values. This format allows for easy import in spreadsheet programs such as MS Excel or Matlab. Note that multiple tables generated in a single run of the user interface are appended in the same file.

Plots Similarly to the table generation, the SOLIDS user interface can be used to generate plots of properties as a function of state variables, The plots are generated in PostScript format, and are found in the solids.ps file, which is found in the directory where the user interface is launched.

CHAPTER 3

Materials

Materials of different types are included in the SOLIDS library. They are classed in four different types, describe below. For each type we give the list of state variables, and the properties computed by the library. Reference to sources and data are reported in Section 5.

Note While the state variables for each class of material is given by the complete set listed above, for some properties only a sub-set of the state variable is meaningful and used. As an example, the material density is computed as a function of temperature only, even in case of materials whose properties depend in general on other independent variables.

Pure metals These are selected metals of relatively high degree of purity, whose properties depend in general on temperature and magnetic field. The degree of purity is indicated by the residual resistivity ratio. The properties computed for pure metals are density ρ , specific heat c_p , thermal conductivity k and electrical resistivity η as a function of the state variables temperature, magnetic field and residual resistivity ratio, T, B, RRR.

The following pure metals are included in the present version of the SOLIDS library:

Metallic alloys These are alloys of metallic elements, indicated either by their composition in weight percentage of the various elements, or by a standard naming of the specific alloy in question. Alloyed material have a property dependence on temperature, but do not exhibit significant dependency on magnetic field (we neglect here magnetic anomalies). The residual resistivity ratio, depends on the alloy composition and is no longer an independent variable. The properties computed for metallic alloys are density ρ , specific heat c_p , thermal conductivity k and electrical resistivity η as a function of the only state variables temperature, T.

The following metallic alloys are included in the present version of the SOLIDS library (names in parentheses indicate conventional denomination of specific alloys, or close approximation to specific alloys):

Insulating materials Insulating materials and insulating composites are of a very wide variety. They span from polymers and plastics, composites, and ceramics. The range of thermo-physical properties (and their uncertainty) is comparably large. The properties of insulating materials are a function of temperature. The properties computed for insulating materials are density ρ , specific heat c_p , thermal conductivity k as a function of the only state variable temperature, T.

The following insulating materials are included in the present version of the SOLIDS library:

Superconductors Superconductors are the class of material with the highest complexity in terms of the description of the properties and their dependency on the state variables. Both LTS and HTS materials are included in the SOLIDS library. The properties of superconductors depend in general on temperature, magnetic field intensity and direction with respect to the crystallographic angles, and applied strain. We choose at this stage to limit the strain dependence to uniaxial strain in the longitudinal direction, i.e. along the conductor developed axis. The properties computed for insulating materials are density ρ , specific heat c_p , thermal conductivity k and normal state electrical resistivity η , critical field B_c, critical temperature T_c, critical current density J_c and current sharing temperature T_{cs} as a function of the state variables temperature, magnetic field intensity and direction, applied strain and operating current density, T, B, α , ε , J_{op} .

The following superconducting materials are included in the present version of the SOLIDS library (shaded entries in *italic* are presently only placeholder and will be updated in future releases):

Superconductors in the SOLIDS package have standard performance matching the critical surface of state-of-the-art industrial production. Below are the reference values used in this version of the SOLIDS material package.

Nb-Ti - The reference values for Nb-Ti are given below:

- $T_c = 9.5 \text{ K}$
- $B_c = 14.5 T$
- $J_c(4.2 K, 5 T) = 3000 A/mm^2$

 $Nb₃Sn$ - The reference values for Nb₃Sn are given below:

- $T_c = 16.73 \text{ K}$
- $B_c = 30.23$ T
- $J_c^{Non-Copper}(4.2 K, 12 T) = 1000 A/mm^2$

CHAPTER 4

Calling Reference

Materials referencing and calling protocol

As described earlier, SOLIDS consists of a set of material functions that are programmed in fortran and can either be called directly, or most conveniently using a wrapper, a unified interface.

Reference ID and names Materials are referenced in the wrapper by using a numerical ID, the *material index* (integer variable) that corresponds to a standard *material name* (string variable). In the tables below we report the correspondence between the materials presently available in SOLIDS, their standard internal naming, and the numerical ID used for referencing when asking for a property calculation.

Pure metals

Metallic alloys

Insulators

Superconductors

SOLIDS wrapper calling protocol A number of function entries are provided as part of the SOLIDS wrapper. These should be used as normal method to access material properties. In addition, functions are provided to convert from standard material names to material index and determine the type of material. The functions are listed below for reference.

character*72 function MaterialName(MaterialID)

convert a standard material index MaterialID (integer) into a standard material name MaterialName (character*72).

integer function MaterialID(MaterialName)

convert a standard material name MaterialName (character*(*)) into a standard material index MaterialID (integer).

character*72 function MaterialType(MaterialId)

return the type of material MaterialType (character*(*)) for a material identified by the index MaterialID (integer). The types of materials are Metal, Alloy, Insulator or SuperConductor.

real function Density(MaterialID,T)

return the density Density (real) of a material identified by the MaterialID (integer) at a temperature T (real). In the present implementation the temperature dependence is neglected.

real function Conductivity(MaterialID,T,B,RRR)

return the thermal conductivity Conductivity (real) of a material identified by the MaterialID (integer) at a temperature τ (real), field amplitude θ (real) and residual resistivity ration RRR (real). The direction of the field is neglected. In the present implementation field and RRR are only used for pure metals.

real function Resistivity(MaterialID,T,B,RRR)

return the electrical resistivity Resistivity (real) of a material identified by the MaterialID (integer) at a temperature T (real), field amplitude B (real) and residual resistivity ration RRR (real). The direction of the field is neglected. In the present implementation field and RRR are only used for pure metals. The value returned for an insulator is a default 1 G Ω m. In the case of a superconductor the value returned is the normal state resistivity, irrespective of temperature and field.

real function SpecificHeat(MaterialID,T,B,angle,eps)

return the specific heat SpecificHeat (real) of a material identified by the MaterialID (integer) at a temperature T (real), field amplitude B (real) applied at an angle angle (real) and applied strain eps (real). In the present implementation field, angle and strain are only used for superconductors.

real function CriticalTemperature(MaterialID,B,angle,eps)

return the critical temperature CriticalTemperature (real) of a material identified by the MaterialID (integer) at a field amplitude B (real) applied at an angle angle (real) and applied strain eps (real). This functions only applies to superconductors, and returns an error for other material types.

real function CriticalField(MaterialID,T,angle,eps)

return the critical field CriticalField (real) of a material identified by the MaterialID (integer) at a temperature T (real) in the direction with an angle angle (real) and applied strain eps (real). This functions only applies to superconductors, and returns an error for other material types.

real function CriticalCurrentDensity(MaterialID,T,B,angle,eps)

return the critical current density CriticalCurrentDensity (real) of a material identified by the MaterialID (integer) at a temperature T (real), field amplitude B (real) applied at an angle angle (real) and applied strain eps (real). This functions only applies to superconductors, and returns an error for other material types.

real function CurrentSharing(MaterialID,B,angle,eps,Jop)

return the current sharing temperature CurrentSharing (real) of a material identified by the MaterialID (integer) at a field amplitude B (real) applied at an angle angle (real), applied strain eps (real) and operating at a current density Jop (real). This functions only applies to superconductors, and returns an error for other material types.

Single materials functions

The wrapper described earlier in detail acts as the interface to the single material property functions. These last can be addressed independently from the wrapper, providing greater flexibility (e.g. modifying standard material performance parameters in superconductors). This however requires that the user is familiar with the material fits. For this reason in this manual we only provide a list of the single functions, which are generally contained in a source file per material. Contact us if you have questions on customization.

Pure metals

Metallic alloys

Insulators

Superconductors

CHAPTER 5

References

Data, reference and FORTRAN code can be found at the www repository: https://supermagnet.sourceforge.io/solids.html