Foundation for Virtual Experiments to Evaluate Thermal Conductivity of Semi- and Super-Conducting Materials

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Abstract Thermal conductivity of solids provides an ideal system for analysis by conducting numerical experiment, currently known as virtual experiment. Here, the model is a numerical model, which is dynamic in nature, as the parameters are interrelated. The present paper discusses the steps involved to conduct virtual experiments using Automated Reasoning for simulation to evaluate the thermal conductivity of Ge, Mg_2Sn semiconducting and YBCO superconducting materials, close to the experimental values.

1. Introduction

Computers can help human to be creative[1] in a number of ways e.g. providing a continuous interaction between the man and machine, requires an even deeper understanding of the subject concerned. AI techniques are required to put the efforts near to the actual experiment in most economical manner. However, its considerable applications have not been applied in the thermal science[12]. To execute the Virtual Experiment (VE), considering various parameters, a model has been designed. Using Automated Reasoning(AR) for simulation, we find the fitness proven to be a reasonable facsimile of real experimental values for the thermal conductivity of Germanium (Ge), Magnesium stannide (Mg_2Sn) semi-conducting and Yttrium Barium Cupric Oxide (YBCO) superconducting materials.

2. Foundation for Virtual Experiment

Belonging to different fields viz. Economics, Physics, Biology etc., simulated approach has been applied e.g. usefulness of simulation, using models of economic systems[13], is reported as "Simulation can be used to experiment with new situations about which little or no information is available, so as to prepare for what may happen". Which is also described[19] as the process of designing a computerized model to conduct experiments. This examines the nature of human intelligence by doing soft computing that mimic the intelligence behaviour[6]. In AR, programs are written to prove mathematical theorems and it has been used as a reasoning engine to discover the knowledge. Here, the propositional logic and an alternative representation for proposition clauses have been used.

2.1 - Applications of simulation

Reasons can be given in favour of the VE as [17] " Such refinements provide a better understanding of physical problems which can not be obtained from experiment". AI techniques are used in physical science e.g. phase transformation[14]; for predictions[16]; to identify the distillation process[18]; and to design the complex thermal system[15].
Due to their inherent peculiar properties, semiconducting and superconducting systems promise wide applications. The various models, needed to solve a complex problem are mentioned in Fig.2.1.

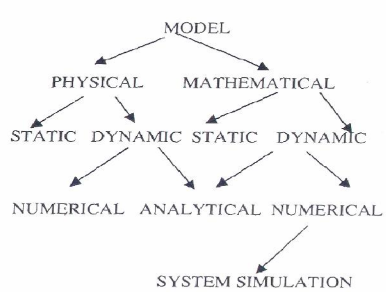

Fig.-1 : Types of Models

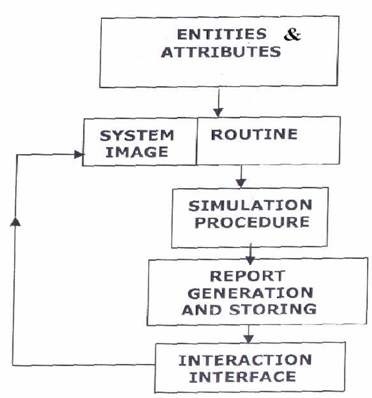

Fig.-2 :Flow Chart for Controlled Simulation

2.1.1 Stages for Simulation Task

There are mainly five stages mapped-out for preparing for simulation as shown in the Fig.2.1.1. An additional stage of interaction interface is being considered in the earlier 4 stages for simulation task[11]. This modification helps in controlling the simulation process. The first stage lists all parameters and activities. The second stage is to design the model by fitting the parameters and activities into the system image and routines separately to act like a model collectively. Thirdly, simulation algorithm is defined depending upon behaviour of the parameters. In the fourth stage, simulated responses are generated. In the fifth stage, interaction parameters are defined to provide a kind of feed back and help to retain the state of simulation and doing the repetitive process as required.

2.1.2 Automated Reasoning

Arithmetic and logical conditions have been applied and manipulated to decide whether the simulated results be accepted or neglected. The general format of the alternative representation for the propositional clause applied is :

IF < > THEN < > ELSE < >

During the simulation process, these conditions are applied and tested to get the best possible theoretical observations for fitting with the experimental values. The set of conditions as defined above are tested by using the logical AND operator. To gather the knowledge and to infer the simulated response for the fitness, rule-based systems has been applied as shown in the Fig.2.1.2 of the logic tree.

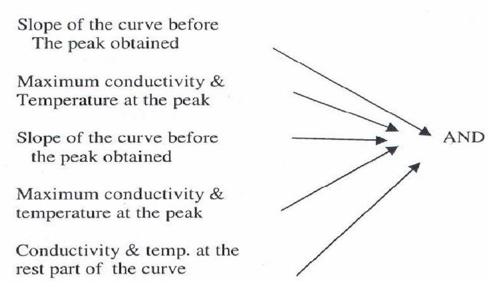

Fig. 2.1.2 : Logic Tree

2.2 - Applications of two dimensional arrays

By providing the feed back, interactively, appropriate values of different parameters are processed for the fitness of the hypothesis as shown in the Fig.2.2, the

self-explanatory diagram describing the interfacing algorithm. The preliminary development of this approach has been partially reported elsewhere[3].
The values for the conductivity (K) have been generated in the form of a 2-D matrix/arrays as RESS(I,J), for a set of parameters, while the value of one of them has been altered. For a set of constant values of parameters - A, γ, α, β and, $\in$ and altered parameter δ, a 2-D array of temperature v/s δ is shown in Table 2.2.

Table 2.2 : Storage of responses

Temp/δ	200	210	220	230
50	4.92	4.77	4.64	4.51
100	4.30	4.15	4.00	3.86
120	3.94	3.79	3.65	3.52
160	3.29	3.15	3.02	2.91

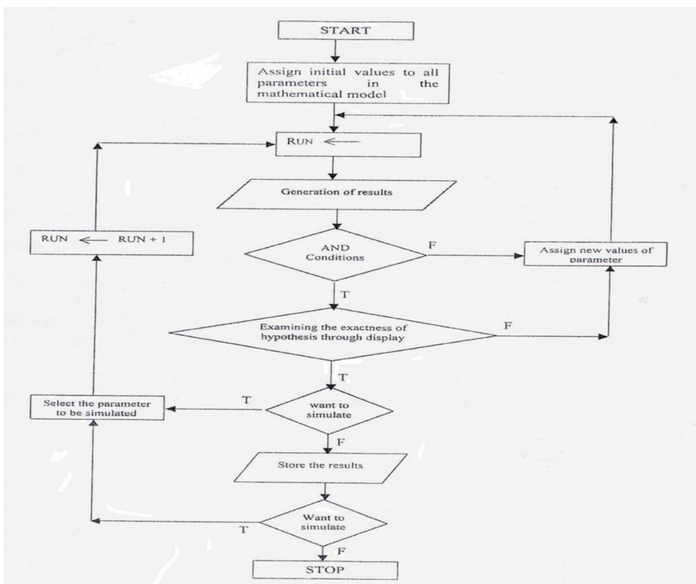

Fig. 2.2 : Interfacing Algorithm

3. Mathematical Model and Virtual Experiment

The problem of integral calculations occurs very often in thermal science, where many parameters are involved to understand the nature of various scattering processes, operating at different temperatures simultaneously. To evaluate the thermal conductivity, theoretical model (numerical) of Callaway[7] has been considered.

3.1 Rule for Numerical Integration

The functions in the theoretical physics besides being continuous are usually one or more times differentiable. Therefore, to increase the accuracy of the numerical integration for an equal number of mesh points, the Simpson rule[8] is applied. The mesh width of each interval between a and b, can be defined as, h =(b-a)/n, n(even) is the sub-subintervals where a=.00001, b=20.0 and n=100 have been taken into account. The error is only of the order of h^4, so precision is under controlled.

3.2 Algorithm For Virtual Experimentation

Logic is developed to execute the desired work and a computer program is developed accordingly as shown in the Interfacing Algorithm diagram. To compute speedily and to overcome the repetitive programming steps, subroutines are preferred. DO statement is extensively applied for various reasons, especially for arrays and subroutine handling. The computer program is developed in the FORTRAN-77 language[9].

4. Test for different cases to evaluate thermal conductivity

We have executed the above discussed logic on the proposed model, for instance, for the Ge, a semi-conducting material. After successfully testing its conductivity results in the temperature range from 2^o K to 10^o K, we have proceeded further for detailed computations for the conductivity analyses for Ge & Mg_2Sn semi-conducting and YBCO superconducting samples.

4.1 Test for Germanium(Ge) Semiconductor

In analyzing the phonon conductivity of germanium, following equation for the thermal induced phonon relaxation rate is required,

$$\tau^{-1} = v/FL + A\,\omega^4 + (B_1+B_2)\,\omega^2\,T^3 + D\,\omega^3\,T \qquad (4.1)$$

Here v is the sound velocity, T is the temperature and other symbols are the various parameters needed to test a particular theory. Values of different parameters used in the calculation for a preliminary test are taken from the earlier work[10], wherein the use of a computer program for achieving fitness in the wide range of temperature has been insisted. The set of values are :

$v=3.5x10^5$ cm/s; L=.24 cm' F=.8; $\theta_D=376$; $A=2.4x10^{-44}\ s^5$

$B_1+B_2=2.77x10^{-33}$ sec K^{-3}; $D=1.203x10^{-33}\ s^2\ K^{-1}$.

Test shows accuracy with the experimental results for the temperature 2 °K, 4 °K, 6 °K, and 10 °K, which are .474 , .261 , .504 , .791 and .985 $W/cm^{-1}K^{-1}$, respectively. Due to fitness of test, it is further carried up to the temperature of 40° K. The Table 4.1.1 illustrates the different values of the parameters and their simulated inferences for the conductivity values are shown in the Table 4.1.2.

Table 4.1.1 : Parameters and Values for Ge

Parameters ↓	Values →			
	I	II	III	IV
v($x10^5$ cm/sec.)	3.5	3.5	3.5	3.5
L	.24	.24	.24	.243
F	.80	.77	.77	.77
θ_D	376	376	376	376
A (x 10^{-44} sec.^{3})	2.4	2.4	2.4	2.4
B_1+B_2('x 10^{-23}sec.K^{-3})	2.77	3.43	3.43	3.43
D (x 10^{-33}sec.$^3K^{-1}$)	1.203	1.433	3.423	3.334
Max. Conductivity($x10^7$)	21.50	18.61	12.62	12.83
(at Temp.°K)	17	16	18	18

Table 4.1.2 : Thermal Conductivity measures for Ge

Re-sponse	K ($x10^7$) ↓	Temp 2 →	4	8	10	15	20	25	30	35	40
I	Cond.	.49	3.17	1.20	1.58	2.10	2.10	1.26	1.58	1.32	1.10
II	Cond.	.47	2.98	1.09	1.42	1.80	1.80	1.52	1.32	1.05	0.91
III	Cond.	.45	2.52	7.79	0.97	1.20	1.24	1.09	0.97	0.80	0.70
IV	Cond.	.46	2.56	7.93	0.99	1.22	1.26	1.11	0.98	0.81	0.71

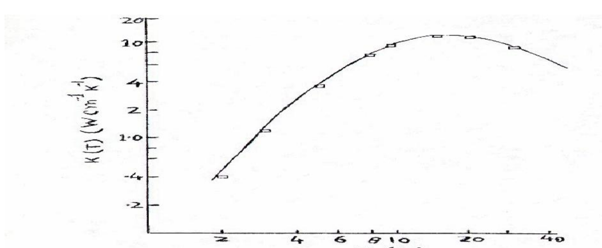

Fig. 4.1 : Ge

These four inferences for thermal conductivity measurements are closely examined and the values shown against the IVth observations (marked with *) are found fit, graphically depicted in the Fig. 4.1, where circle shows the experimental point and the present analysis has been shown as the curve-line.

4.2 Test for Magnesium Stannide (Mg_2Sn) Semiconductor

We consider the following expression for relaxation time,

$$\tau^{-1}(\omega)= (v/FL)+A\omega^4+[B_1+B_2\exp.(-\Theta/aT)]\omega^2T^3+D\omega^3T \qquad (4.2)$$

It has been a usual practice, to generally neglect the exponential temperature dependence of the parameter B_2 for the conductivity calculation, representing Umklapp phonon-scattering and both B_1 (normal phonon scattering parameter) and $B_2$are lumped into a single parameter B, assumed to be independent of T. Therefore, B_2 is taken to depend upon T, exponentially, in the analysis. Table 4.2.2 shows four simulated response against the values of different parameters as shown in the Table 4.2.1.

Table 4.2.1 : Parameters and Values for Mg_2Sn

↓ Parameters	Values →			
	I	II	III	IV
v(x10^5 cm/sec.)	**359**	**359**	**359**	**359**
L	**.11**	**.11**	**.10**	**.10**
F	**.54**	**.54**	**.54**	**.54**
$\propto$	**2.0**	**2.5**	**2.5**	**2.5**
θ_D	**154**	**154**	**154**	**154**
A (x 10^{-44} sec.^{3})	**6.3**	**6.3**	**6.3**	**6.3**
B_1(x 10^{-23}sec.K^{-3})	**7.0**	**7.0**	**7.7**	**7.7**
B_2(x 10^{-23}sec.K^{-3})	**4.7**	**4.7**	**4.7**	**4.7**
D (x 10^{-33}sec.^{3}K^{-1})	**2.75**	**2.75**	**2.75**	**2.95**
Max. Conductivity(x10^7)	**6.483**	**6.398**	**6.088**	**5.909**
(at Temp.^{o}K)	**16**	**14**	**14**	**14**

Table 4.2.2 : Thermal Conductivity measures for Mg_2Sn

Re-sponse	**K ↓ (x10^7)**	**Temp 2 →**	**6**	**8**	**10**	**14**	**20**	**26**	**30**	**36**	**40**
I	**Cond.**	**.96**	**2.37**	**3.89**	**5.16**	**6.45**	**5.74**	**4.08**	**3.15**	**2.15**	**1.69**
II	**Cond.**	**.96**	**2.37**	**3.89**	**5.16**	**6.39**	**5.47**	**3.71**	**2.79**	**1.87**	**1.46***
III	**Cond.**	**.89**	**2.21**	**3.65**	**4.87**	**6.08**	**5.25**	**3.57**	**2.70**	**1.81**	**1.42**
IV	**Cond.**	**.68**	**2.17**	**3.57**	**4.74**	**5.90**	**5.10**	**3.49**	**2.64**	**1.78**	**1.40**

The corresponding results for thermal conductivity are examined and the values of the II observations(marked with *) are found fit, shown by the curve-line in Fig.4.2 where the experimental data is shown as circle-points.

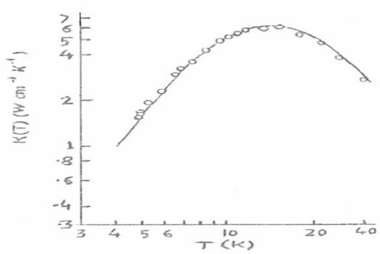

Fig. 4.2 : Mg2Sn

4.3 Test for Yttrium Barium Cupric Oxide (YBCO) superconductors

In computing the thermal conductivity of YBCO superconductors, behaviour has also been examined by earlier workers [2]. We have considered the Callaway's model, which is also used by Tewordt et.al.[20] in a modified form-

$$K = A\, t^3 \int x4\, e^x / [(e^x - 1)^2 . F(t, x)]\, dx \qquad (4.3.1)$$

$$F(t,x)=[1+\alpha x^4 t^4+\beta x^2 t^2+ \gamma t x g(x,y)+ \delta x^3 t^4+(\in x^2 t^5] \qquad (4.3.2)$$

A, α, β, γ, δ and $\in$ are scattering strengths due to boundary scattering, point defect scattering, sheet like fault, electron-phonon scattering, interference scattering and three phonon scattering. Corresponding maximum conductivity values are shown in the Table 4.3.1.

Table 4.3.1 : Thermal Conductivity measures for YBCO

Response	Max.Cond.	Temp	A	α	β	γ	δ	$\in$
I	**3.50**	**70**	**4**	**15**	**50**	**50**	**210**	**.01**
II	**3.82**	**60**	**4**	**25**	**50**	**50**	**210**	**.01**
III	**4.14**	**60**	**4**	**15**	**50**	**50**	**210**	**.01**
IV	**3.81**	**70**	**5**	**15**	**50**	**50**	**210**	**.01**

Table 4.3.2 : Thermal Conductivity measures for YBCO

Re-sponse	**K ↓ ($x10^7$)**	**Temp →**								
		10	**20**	**30**	**40**	**80**	**100**	**120**	**140**	**160**
I	**Cond.**	**.68**	**1.67**	**2.35**	**2.73**	**3.03**	**2.95**	**2.82**	**2.68**	**2.54**
II	**Cond.**	**1.39**	**2.73**	**3.40**	**3.70**	**3.70**	**3.49**	**3.24**	**2.99**	**2.75**
III	**Cond.**	**1.43**	**2.87**	**3.63**	**3.98**	**4.03**	**3.80**	**3.54**	**3.27**	**3.02**

IV	Cond.	.86	2.09	2.93	3.41	3.79	3.68	3.53	3.35	3.17

We have found positive results in the temperature range from 10-160 °K and fitness(shown as curve-line) with the experimental results (shown as circle-point) from the IV observations of Table 4.3.2, as shown in the Fig.-4.3.

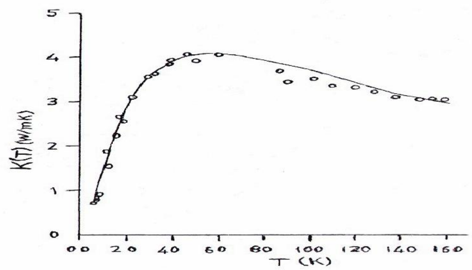

Fig. 4.3 : YBCO

5. Model Validation

The model has also been validated in two cases. First case of the semiconducting material Ge, shows[5] a good agreement between theory and experiment in the temperature range 2 to 100 °K.. For the second case, similar approach also enables to analyse the three different samples of YBCO superconductors[4] in the temperature range 0 to 260 °K and the interference scattering & exponential temperature dependence lead to a good agreement with the experimental data.

6. CONCLUSION

It emerges that the VE has immense capabilities to yield good results, within the prescribed automated reasoning and the interface algorithm,. In performing VE over the different models for these materials (Ge, Mg and YBCO) , the various parameters have been considered so as to search for the unusual features or properties might provide a background for understanding the mechanisms.

7. ACKNOWLEDGEMNT

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