Modeling Materials through a Phase Transition: Using COMSOL Multiphysics and Applying Physics First Principles Techniques

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Abstract: This paper presents a new phase transition model that is easily created and runs rapidly. It is designed so that the modeler can determine immediately the relative accuracy of the end result by use of physics first principles. Phase transitions are readily observable in many commonly utilized engineering materials. In fact, most modern devices and/or tools employ a phase transition in their manufacture. This model demonstrates the ease of use that is inherent in COMSOL model development. This model builds on earlier COMSOL phase transition modeling examples.

Examples are presented here of variations in the model parameters by using four different eutectic metal alloys in separate model runs. Such alloys are commonly employed to achieve both a strong mechanical contact and a high conductivity electrical contact. Variations of this model will allow the tracking of the phase boundary as a function of time.

Keywords: phase transition, soldering, brazing, electrical contact, mechanical contact

1. Introduction

The COMSOL Multiphysics model developed and presented in this case is a 2D axially symmetric model of a hollow metallic disk with quasi-static radial material flow outward from the axis. This model is used to demonstrate how the correct position of the phase boundary can be determined by inspection through the use of physics first principles. It also shows how these results are related to the geometry and the boundary condition of the model. This model was developed through reference to the modeling techniques developed in the Continuous Casting Model in the Heat Transfer Module Guide [1].

1.1 The Materials Modeled

The metallic materials [2] chosen as examples for use in this model are listed in Table 1 below: {(E) indicates a eutectic alloy}

Solder	Bi	In	Sn	Pb	Zn
	%	%	%	%	%
BiPb(E)	55.5	0	0	44.5	0
BiSn(E)	58	0	42	0	0
In	0	100	0	0	0
SnPb(E)	0	0	63	37	0
SnZn(E)	0	0	91	0	9

Table 1 Lead Free Eutectic Solders, Indium, Tin Lead and Bismuth Lead Eutectic Solders

These particular metallic phase change example materials were chosen for use in this model because they are widely used in electronic and mechanical industrial processes.

1.2 The Physics

In a phase change transition, all of the properties of the material in question change, some by a small amount, others significantly. The most obvious material property change is the liquid-solid or solid-liquid transition and the related structural and mechanical property changes. Less obvious and possibly less familiar property changes are those phase change related differences that are exhibited in the thermal and electrical characteristics of such materials. These property changes are induced by the order-disorder transition that occurs in the solid-liquid or vice versa in the liquid-solid phase transition. Knowledge of such phase change induced structural, mechanical, thermal, electronic and related property changes and their associated shifts in the related magnitude and temperature (T) dependence are critically important for the formulation of accurate FEA models.

Both the heat capacity and the thermal conductivity of the eutectic metal alloys in the range discussed in this paper (380K- 480K) are dominated by electron energy transport. Experimentally, in this temperature range for these materials, the heat capacity can be expressed as:

1. $C = \gamma T + AT^3$

where γ and **A** are material specific constants [3] and the phonon contribution (AT^3) is very small compared to the electron contribution.

The thermal conductivity (**K**) is related to the heat capacity per unit volume as:

2. $K = \frac{1}{3} C v \ell$

where **C** is the heat capacity per unit volume, v is the electron velocity and ℓ is the mean free path [4].

1.3 The Materials

The materials chosen as examples in this model are four eutectic alloys and one pure metal (In). A eutectic alloy [5,6] is a mixture of two or more materials that when combined have the lowest possible melting point for that composition. All the alloys chosen for this model are binary (two components) alloys.

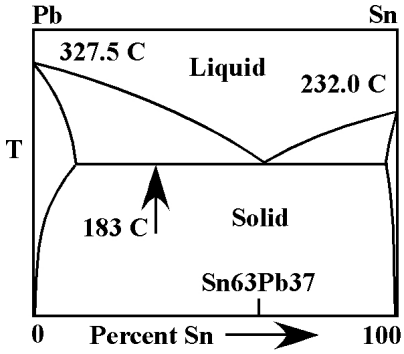

Figure 1. Tin-Lead Phase Diagram (after [5])

Also, that unique eutectic alloy composition transforms directly from a solid to a liquid or vice versa, without passing through a mixed composition (solid/liquid {mushy}) phase, as shown for Tin-Lead in Figure 1 above.

The lack of a mushy phase at the eutectic point results in a more abrupt transition. However, for ease of modeling in an FEA based system and to achieve rapid convergence, the eutectic materials and the metal in this model are treated as if they each have a narrow liquid-solid transition zone.

2. The Model

This model is configured in COMSOL Multiphysics as a 2D axisymmetric model with a phase change transition.

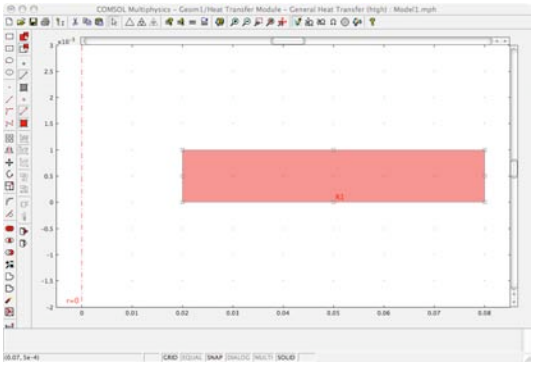

Figure 2. 2D Axisymmetric Phase Transition Disk Model

Figure 2 above shows the COMSOL modeling window, as configured for the 2D Axisymmetric Phase Transition Disk Model.

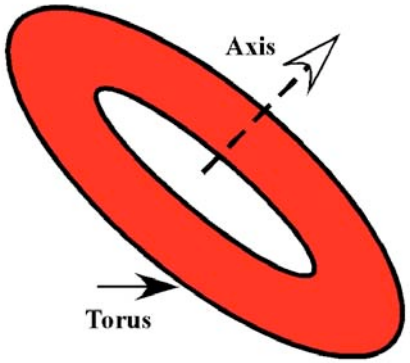

Figure 3. Toroidal Disk Modeled

Figure 3 above shows an off-axis view of the modeled flat toroidal disk.

The radial location of the phase transition is a function of the transition temperature (T_trans) of the particular binary eutectic alloy or metal

and the temperature differential between the inner radial boundary and the outer radial boundary

2.1 Setting Up the Model Constants

The model window, as shown in **Figure 2** above, is established by opening the **Model Navigator** and clicking the **New** tab. In the **Space dimension** list, select **Axial symmetry (2D).** From the list of application modes, select the **Heat Transfer Module>Fluid-Thermal Interaction>Non-Isothermal Fluid-Thermal Interaction>Steady-state Analysis** and then click OK (after [1]).

Open the **Options** menu and select the **Constants** window. The column values associated with each metal in the following tables are entered as a group in separately created copies of this model for each unique material.

The first model was built using the BiSn material and thus the bisn subscript. When a model is run for a different material, the subscript can remain the same and only the name of the model needs to be changed, to avoid confusion in analyzing the results.

Solder	BiPb	BiSn	In
Variables			
T0	300	300	300
T_in	480	480	480
T_out	380	380	380
dT	0.5	0.5	0.5
dH	20.9[J/g]	44.8 ‡	28.47 ‡
Cp_bisn	0.126[J/g*C]	0.167 ‡	0.243 ‡
rho_bisn	10.44[g/cm^3]	8.56 ‡	7.31 ‡
T_trans	397.15	411.15	430.15
u_cast	1e-5	1e-5	1e-5
eta_bisn	0.01	0.01	0.01
k_bisn	0.04[W/cm*C]	0.19‡	0.86‡

Table 3 Constants for the First Three Phase Transition Materials (in the case of omitted units, they are the same ‡ as for the first member of the row; otherwise they are the default SI units).

Figure 4 below shows an example of the **Options** > **Constants** window as filled in for the Bismuth (Bi58) – Tin (Sn42) solder.

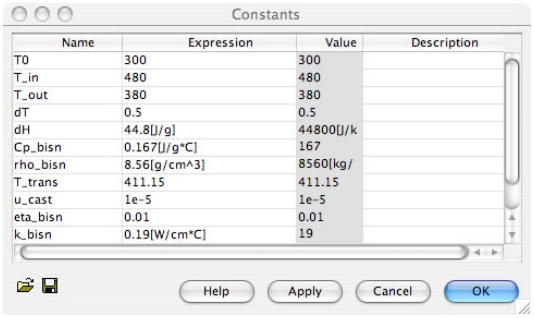

Figure 4 Options > Constants window for Bi58Sn42 Eutectic Solder

Solder	SnPb	SnZn
Variables		
T0	300	300
T_in	480	480
T_out	380	380
dT	0.5	0.5
dH	45.0[J/g]	71.2[J/g]
Cp_bisn	0.167[J/g*C]	0.239[J/g*C]
rho_bisn	8.4[g/cm^3]	7.27[g/cm^3]
T_trans	456.15	472.15
u_cast	1e-5	1e-5
eta_bisn	0.01	0.01
k_bisn	0.50[W/cm*C]	0.61[W/cm*C]

Table 4 Constants for the Last Two Phase Transition Materials (units are as shown; otherwise they are the default SI units).

2.2 Setting Up the Model Scalar Expressions

Figure 4 Scalar Expressions Window

Open the **Options** menu and select the **Expressions > Scalar Expressions.** Once filled in as shown in **Table 5** below, it will appear as shown in **Figure 4** above.

Variable	Expression
D	exp(-(T-T_trans)^2 /(dT^2))/sqrt(pi*dT^2)
B	(T-T_trans+dT)/(2*dT)* ((T<=(T_trans+dT))* (T>=(T_trans-dT))) +(T>(T_trans+dT))
Sr	(1-B)^2/(B^3+1e-3)*1e5* (u-u_cast)
Sz	(1-B)^2/(B^3+1e-3)*1e5*v
Cp1	Cp_bisn+dH/T_trans*H
H	flc2hs(T-T_trans,dT)

Table 5 Scalar Expressions

The expressions in **Table 5** are the same as shown in the Continuous Casting example [1] for D, B and H. The expressions for Sr, Sz and Cp1 have been modified as shown. In the case of Cp1, Cp_bisn replaces the value "380". That substitution allows value changes to be required only in the Constants window in order to explore the use of different materials in the same physics model.

2.3 Setting Up the Model Geometry

As shown in **Figure 2** above, the model geometry is relatively simple.

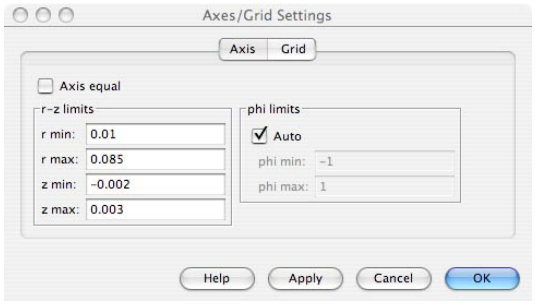

Figure 5 Axis/Grid Settings Window

Open the **Options** menu and select the **Axis/Grid Settings.** Unselect the **Axis equal** button and enter the values shown in **Table 6** below.

R min	0.01
R max	0.085
Z min	-0.002
Z max	0.003

Table 6 Axis/Grid Values

From the **Draw** menu, select **Specify Objects > Rectangle** and enter the values shown in **Table 7.**

Object	R1
Width (R)	0.06
Height (Z)	0.001
Base	Corner
R	0.02
Z	0

Table 7 Geometry Specifications

2.4 Setting Up the Physics Subdomain Settings

In the **Multiphysics > Model Navigator** select **Non-Isothermal Flow**. Move to the **Physics** menu and select **Subdomain Settings > Subdomain** 1. From **Table 8** below, enter the parameters as shown under the **Physics** menu button. **Figure 6** shows the **Non-Isothermal Flow Physics Subdomain Window** with the entered parameters.

Parameter	Expression
ρ	rho_bisn
η	eta_bisn
k_{dv}	0
F_r	$-S_r$
F_z	$-S_z$

Table 8 Non-Isothermal Flow Physics Subdomain

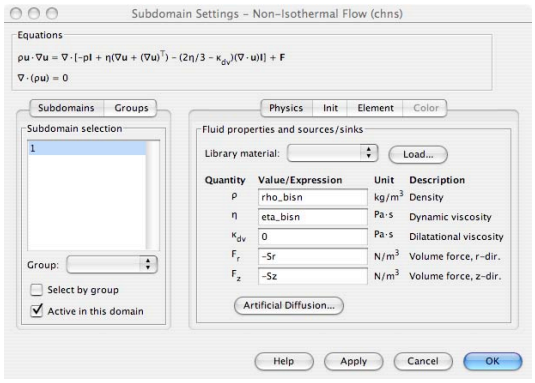

Figure 6 Non-Isothermal Flow Physics Subdomain Window

Next, click the **Init** button of the same window and enter u_cast in the $u(t_0)$ space, as shown in **Figure 7** below. Click **OK.**

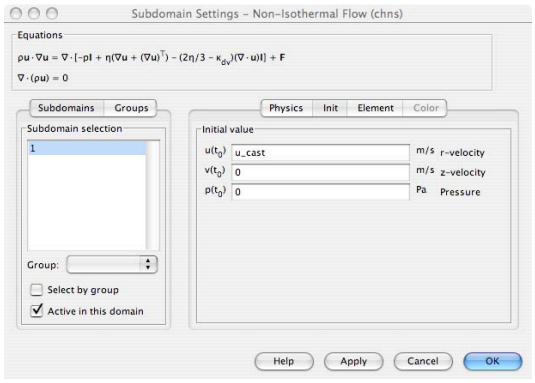

Figure 7 Non-Isothermal Flow Physics Subdomain Window with the Init button clicked.

Open the **Multiphysics > Model Navigator** select **General Heat Transfer**. Move to the **Physics** menu and select **Subdomain Settings > Subdomain** 1. From **Table 9**, enter the parameters as shown under the **Physics** menu button. **Figure 8** below shows the **General Heat Transfer Physics Subdomain Window** with the entered parameters.

Parameter	Expression
k	k_bisn
ρ	rho_bisn
Cp	Cp_bisn+D*dH
Q	0

Table 9 General Heat Transfer Physics Subdomain

Click the **Init** button and enter T_in in the $T(t_0)$ window. **Figure 9** below shows configured **Init** window.

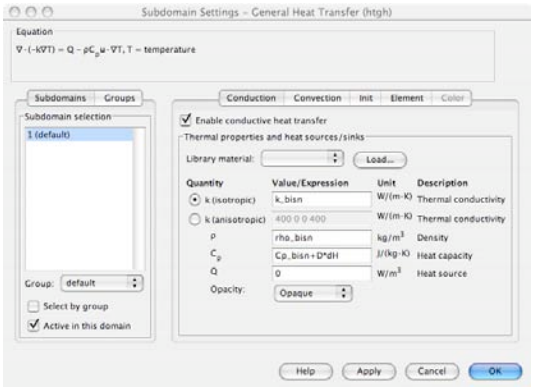

Figure 8 General Heat Transfer Physics Subdomain Conduction

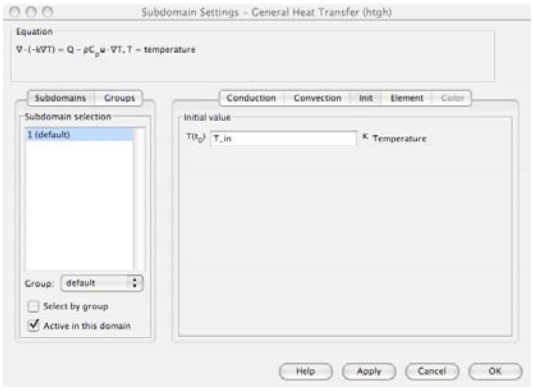

Figure 9 General Heat Transfer Physics Subdomain Init

2.5 Setting Up the Physics Boundary Settings

In the **Multiphysics > Model Navigator** select **Non-Isothermal Flow**. Move to the **Physics** menu and select **Boundary Settings.**

Boundary	Setting
1	Laminar inflow
2	Slip/Symmetry
3	Slip/Symmetry
4	Pressure (0)

Table 10 Non-Isothermal Flow Physics Boundary

On the **Coefficients** page, enter the values shown in **Table 10** above. On the **Laminar Inflow/Outflow settings** page, enter the values shown in **Table 11** below.

Parameter	Expression
U_0	u_cast
L_{ini}	1e-3

Table 11 Non-Isothermal Flow Physics Boundary Laminar Inflow/Outflow Settings

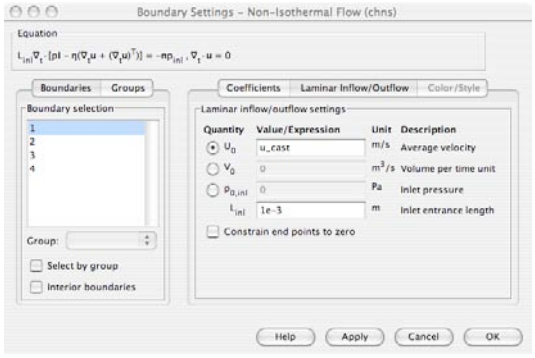

Figure 10 Non-Isothermal Flow Physics Boundary Laminar inflow/Outflow Settings

In the **Multiphysics > Model Navigator** select **General Heat Transfer.** Move to the **Physics** menu and select **Boundary Settings.** Insert the conditions and expressions as shown in **Table 12** below.

Boundary	Setting	Expression
1	Temperature	T_in
2	Thermal Insulation	
3	Thermal Insulation	
4	Temperature	T_out

Table 12 General Heat Transfer Physics Boundary Settings

3. Mesh Generation

Click on the **Initialize Mesh** button once. Click on the **Refine Mesh** button twice. This should yield 2816 elements.

4. Solver Parameters

From the **Solve** menu, select **Solver Parameters.**

Parameter	Setting
Analysis	Stationary
Solver	Parametric
Name of Parameter	dT
List of Parameter Values	65 21 11 5 2 1
Linear Solver System	Direct(UMFPACK)

Table 13 General Solver Settings

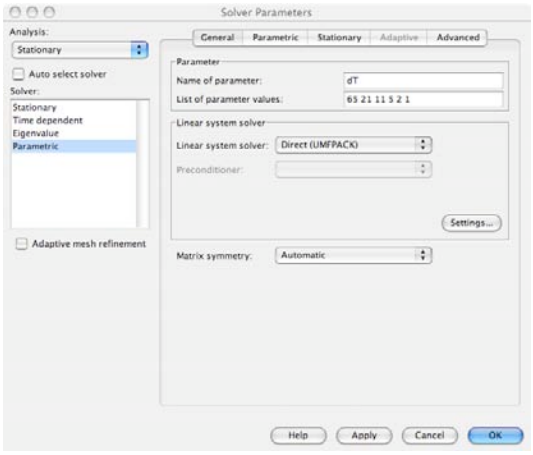

Figure 11 General Solver Settings

5. Solutions

Click the **Solve** button and the results should arrive in a several seconds. A separate model is required for each different material. Run each of the five models to arrive at the results shown in **Table 14** below.

6. Results Analysis

Solder	T_trans	Radial Location
BiPb(E)	124	0.0692
BiSn(E)	138	0.0549
In	157	0.0404
SnPb(E)	183	0.0283
SnZn(E)	199	0.0225

Table 14 Phase Transition Radial Location for Modeled Materials

Table 14 above shows the calculated location of the phase transition boundary for the four eutectic solder alloys and Indium that resulted from the collection of experimental physical property values that were inserted into this model for those metals.

A first principles test of these calculations can be made by comparing the thermal conductivity derived from the physical slope of the lines between the phase transition point and the two boundary points. **Figure 12** below shows an example of this using the Indium phase transition point.

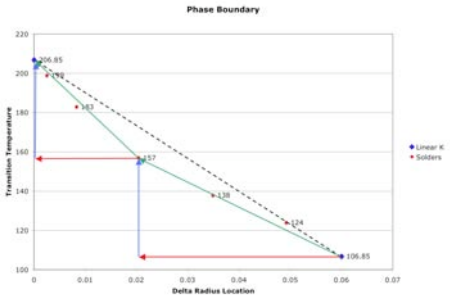

Figure 12 Comparison of Liquid-Solid Thermal Conductivity (k) as Modeled.

Reference experimental data sources differ (±20%) as to the absolute accuracy of the difference in the thermal conductivity across the phase transition boundary.

The herein modeled difference agrees well (± 15%) with reference values available for the thermal conductivity for Indium. Model results for the other four alloys appear to behave consistently with the basic physics involved and the Indium reference model.

7. Conclusions

A model has been presented that shows rapid convergence and yields calculated results that agree with the experimentally available thermal conductivity data for Indium to within ± 15%.

8. References

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