

Audio test:



# Termická analýza

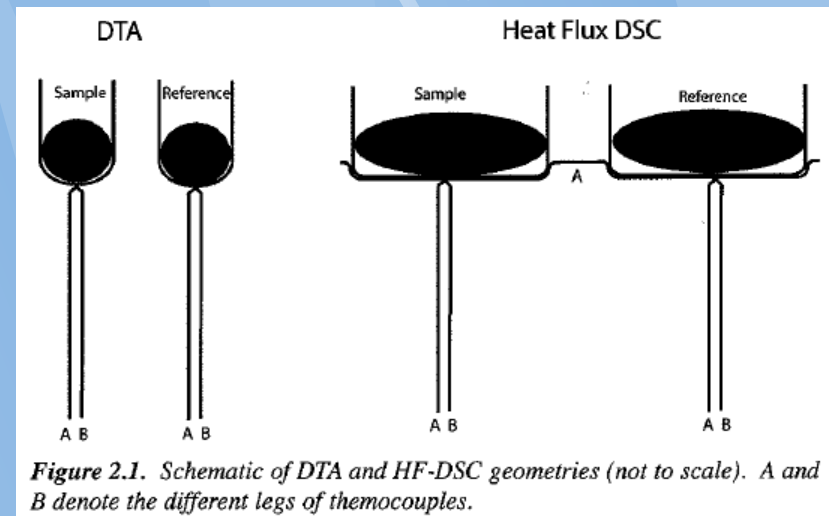


## Simulace DSC a DTA

Přednášející: Doc. Jiří Sopoušek

# Obsah

- Výpočty fázových diagramů metodou CALPHAD
- Výpočet entalpie vzorku a  $C_p$
- Simulace signálu DTA (pcDSC, hfDSC)
- Příklady použití



# Zdroje

[98Sau] N. Saunders, A. P. Miodovnik: '**CALPHAD** (Calculation of Phase Diagram) - A Comprehensive Guide', Pergamon Materials Series, Vol.1, Elsevier Science, Amsterdam (1998).

[02Sop] Sopoušek Jiří, Brno 2002, Fázové rovnováhy a difúzí řízené procesy ve vybraných soustavách kovů a jejich slitin (**komentář** k habilitační práci).

[06Boe] W. J. Boettinger - U. R. Kattner - K.-W. Moon - J. H. Perepezko, "**DTA and Heat-flux DSC Measurements of Alloy Melting and Freezing**", 2006, Washington, National Institute of Standards and Technology.

[07Kro] Kroupa, A.; Dinsdale, A. T.; Watson, A.; Vrestal, J.; Vizdal, J.; Zemanova, A.: The development of the **COST 531** lead-free solders thermodynamic database, JOM, 2007, 59, 20-25.

# CALPHAD (viz kurs Dr. Kroupa)

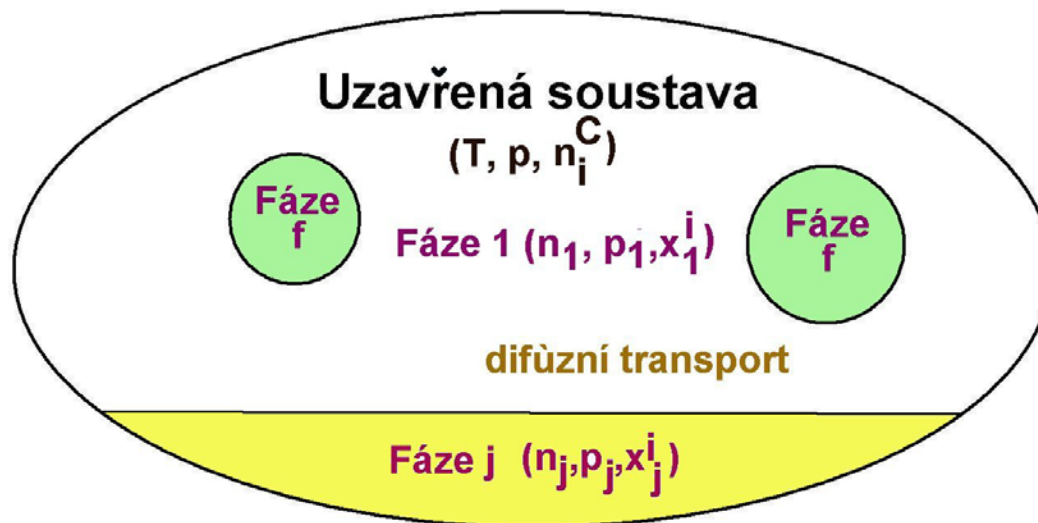
- semiempirická metoda, řešení fázové rovnováhy pro uzavřený systém

$$T_{\text{ex}}=T$$
$$P_{\text{ex}}=P$$
$$dn_i=0$$

$j=1,\dots,f$  (fáze)

Okolí

$i=1,\dots,s$  (složky)

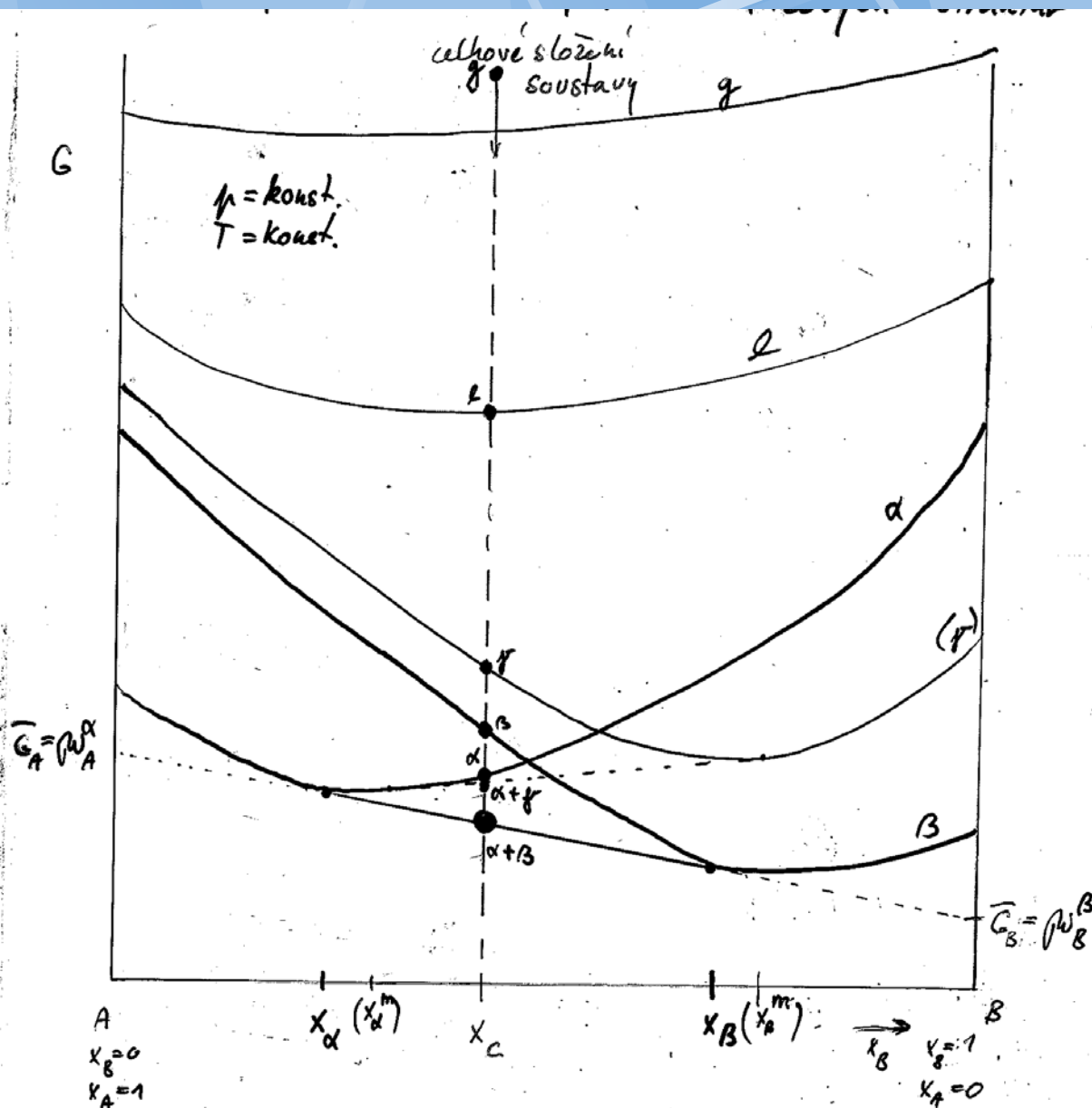


Nutný  
termodynamický  
popis fází:  
 $G_j=f(T,p,x_j^i)$

SW a  
termodyna  
-mická  
databáze

Nerovnovážný stav  $\rightarrow$  rovnovážný stav (řešení FR)

# Proč vzniká fázová rovnováha?



**K získání řešení používáme:**

- integrální podmínku FR (min. Gcelk)
- Diferenciální podmínku FR (rovnost chem pot.)

**Při hledání řešení dodržujeme:**

- zákon zachování hmoty
- Stechiometrii fází
- zachování náboje

# Řešení fázové rovnováhy

Output from POLY-3, equilibrium = 1, label A0 , database: SOLDER

Conditions:

T=473, P=100000, N=1, W(PB)=1E-1

DEGREES OF FREEDOM 0

Temperature 473.00, Pressure 1.000000E+05

Number of moles of components 1.00000E+00, Mass 1.24006E+02

Total Gibbs energy -2.59971E+04, Enthalpy 7.62867E+03, Volume 0.00000E+00

Component	Moles	W-Fraction	Activity	Potential	Ref.stat
PB	5.9848E-02	1.0000E-01	1.7267E-04	-3.4074E+04	SER
SN	9.4015E-01	9.0000E-01	1.5344E-03	-2.5483E+04	SER

BCT\_A5 Status ENTERED Driving force 0.0000E+00

Number of moles 6.7295E-01, Mass 8.0858E+01 Mass fractions:

PB 2.81641E-02 SN 9.71836E-01

Constitution:

PB 1.63324E-02 SN 9.83668E-01

LIQUID Status ENTERED Driving force 0.0000E+00

Number of moles 3.2705E-01, Mass 4.3148E+01 Mass fractions:

PB 2.34618E-01 SN 7.65382E-01

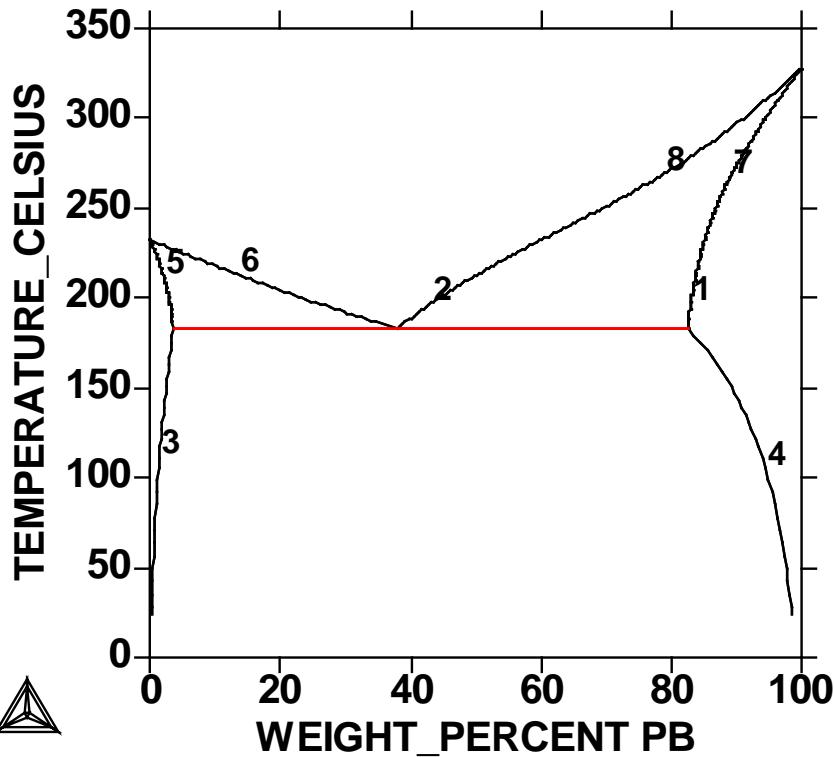
Constitution:

PB 1.49387E-01 SN 8.50613E-01

Entalpie  
pro DTA  
(DSC)

# Sn-Pb

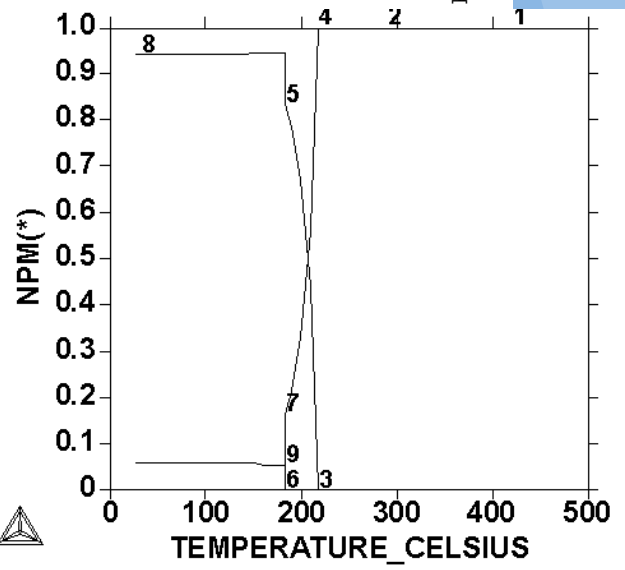
THERMO-CALC (2012.05.31:13.03) :Phase diagram PbSn  
 DATABASE: SOLDER  
 P=100000, N=1;



```

1.:*FCC_A1 LIQUID
2.:*FCC_A1 LIQUID
3.:*BCC_A5 FCC_A1
4.:*BCC_A5 FCC_A1
5.:*BCC_A5 LIQUID
6.:*BCC_A5 LIQUID
7.:*FCC_A1 LIQUID
8.:*FCC_A1 LIQUID
    
```

**Sn10wt%Pb**



by u  
 oušek from SOPOUSEK

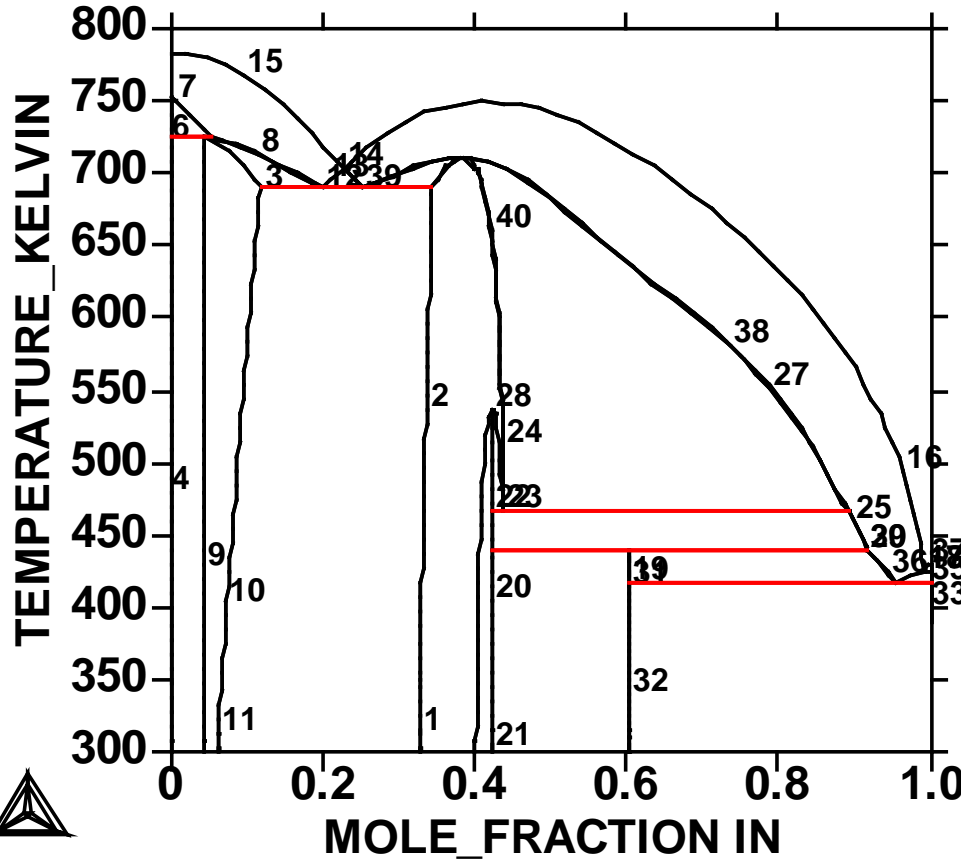


# Příklady výstupů metody CALPHAD

2004-06-09 13:46:21  
 ...strator from HERA

DATABASE:SOLDER  
 N=1, P=100000, X(AG)-X(SB)=-5.55111512E-17;

Databaze  
 SOLDER  
 ThermoCalc



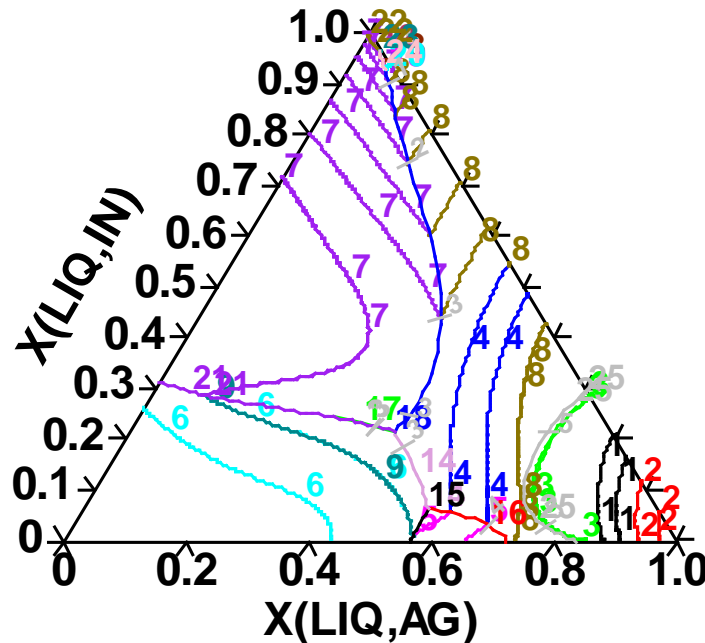
- 1:\*RHOMBOHEDRAL\_A7\_HCP\_A3\_ZINCBLLENDE\_B3
- 2:\*RHOMBOHEDRAL\_A7\_LIQUID\_ZINCBLLENDE\_B3
- 3:\*LIQUID\_HCP\_A3
- 4:\*HCP\_A3\_AGSB\_ORTHORHOMBIC
- 6:\*LIQUID\_AGSB\_ORTHORHOMBIC
- 7:\*AGSB\_ORTHORHOMBIC
- 8:\*HCP\_A3\_LIQUID\_ZINCBLLENDE\_B3
- 9:\*AGSB\_ORTHORHOMBIC
- 10:\*ZINCBLLENDE\_B3\_LIQUID
- 11:\*ZINCBLLENDE\_B3\_LIQUID\_TETRAGONAL\_A6
- 12:\*HCP\_A3\_LIQUID\_ZINCBLLENDE\_B3
- 13:\*ZINCBLLENDE\_B3\_LIQUID\_RHOMBOHEDRAL\_A7
- 14:\*RHOMBOHEDRAL\_A7\_LIQUID\_ZINCBLLENDE\_B3
- 15:\*RHOMBOHEDRAL\_A7\_LIQUID
- 16:\*ZINCBLLENDE\_B3\_LIQUID
- 17:\*ZINCBLLENDE\_B3\_LIQUID\_TETRAGONAL\_A6
- 18:\*TETRAGONAL\_A6\_LIQUID\_ZINCBLLENDE\_B3
- 19:\*LIQUID\_AGIN2\_ZINCBLLENDE\_B3
- 20:\*AGIN2\_AGIN2\_ZINCBLLENDE\_B3
- 21:\*AGIN2\_AGIN2\_ZINCBLLENDE\_B3
- 22:\*LIQUID\_AGIN2\_ZINCBLLENDE\_B3
- 23:\*AGIN2\_HCP\_A3\_ZINCBLLENDE\_B3
- 24:\*LIQUID\_HCP\_A3\_ZINCBLLENDE\_B3
- 25:\*AGIN2\_LIQUID\_ZINCBLLENDE\_B3
- 27:\*HCP\_A3\_LIQUID\_ZINCBLLENDE\_B3
- 28:\*HCP\_A3\_AGIN2\_ZINCBLLENDE\_B3
- 29:\*AGIN2\_LIQUID\_ZINCBLLENDE\_B3
- 30:\*AGIN2\_LIQUID\_ZINCBLLENDE\_B3
- 31:\*AGIN2\_AGIN2\_ZINCBLLENDE\_B3
- 32:\*TETRAGONAL\_A6\_AGIN2\_ZINCBLLENDE\_B3
- 33:\*AGIN2\_TETRAGONAL\_A6\_ZINCBLLENDE\_B3
- 35:\*LIQUID\_TETRAGONAL\_A6\_ZINCBLLENDE\_B3
- 36:\*AGIN2\_LIQUID\_ZINCBLLENDE\_B3
- 37:\*TETRAGONAL\_A6\_LIQUID
- 38:\*HCP\_A3\_LIQUID\_ZINCBLLENDE\_B3
- 39:\*RHOMBOHEDRAL\_A7\_LIQUID\_ZINCBLLENDE\_B3



# Plocha liquidu

## Bod tání dle termické analýzy

THERMO-CALC (2004.06.16:10.35) :  
DATABASE: SOLDER  
Z-AXIS = 400.0 + 100.0 \* Z

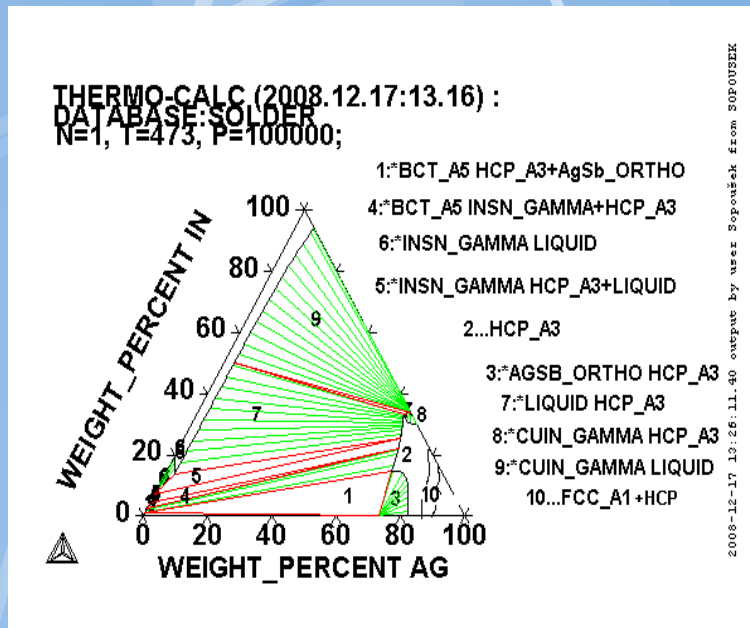


- 1:\* LIQUID FCC\_A1
- 2:\* FCC\_A1 LIQUID
- 3:\* FCC\_A1 HCP\_A3
- 4:\* LIQUID HCP\_A3
- 5:\* AGSB\_ORTHO LIQUID
- 6:\* RHOMBOHEDRAL\_A7 LIQUID
- 7:\* ZINCBLLENDE\_B3 LIQUID
- 8:\* HCP\_A3 LIQUID
- 9:\* LIQUID RHOMBOHEDRAL\_A7
- 10:\* AGZIN ZINCBLLENDE\_B3
- 11:\* AG2IN TETRAGONAL\_A6
- 12:\* ZINCBLLENDE\_B3 TETRAGONAL
- 13:\* AG2IN LIQUID
- 14:\* LIQUID HCP\_A3 F0 RHOMBOHEDRAL\_A7
- 15:\* AGSB\_ORTHO F0 LIQUID RHOMBOHEDRAL\_A7
- 16:\* AGSB\_ORTHO HCP\_A3 F0 LIQUID
- 17:\* LIQUID F0 RHOMBOHEDRAL\_A7
- 18:\* LIQUID HCP\_A3 F0 ZINCBLLENDE\_B3
- 19:\* AGZIN F0 LIQUID ZINCBLLENDE\_B3
- 20:\* AG2IN HCP\_A3 F0 LIQUID
- 21:\* RHOMBOHEDRAL\_A7 LIQUID F0
- 22:\* TETRAGONAL\_A6 LIQUID F0
- 23:\* AG2IN LIQUID F0 TETRAGONAL
- 24:\* AGZIN LIQUID F0 ZINCBLLENDE\_B3
- 25:\* HCP\_A3 FCC\_A1 F0 LIQUID

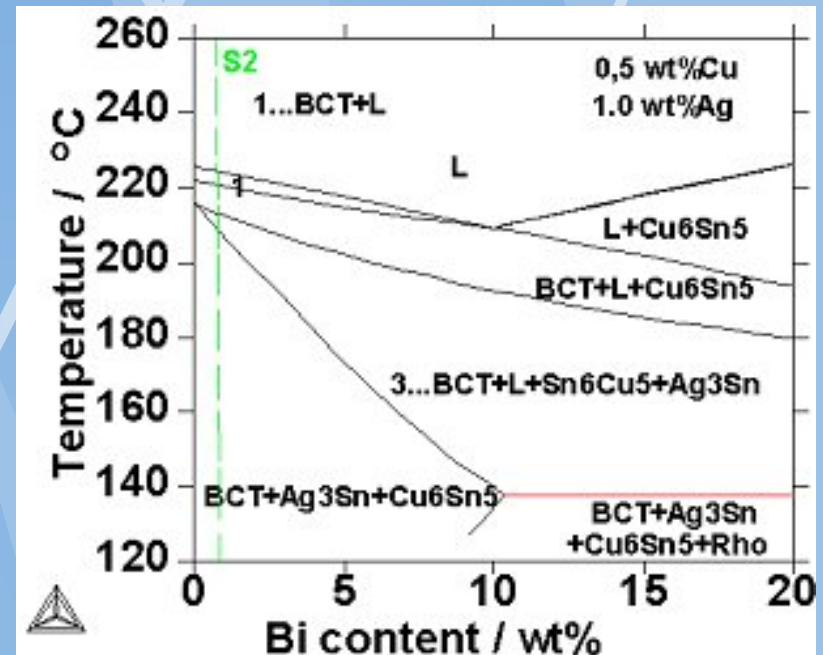
2004.06.16:10.35 output by user Sopoušek fr



# Aplikace metody – fázové diagramy

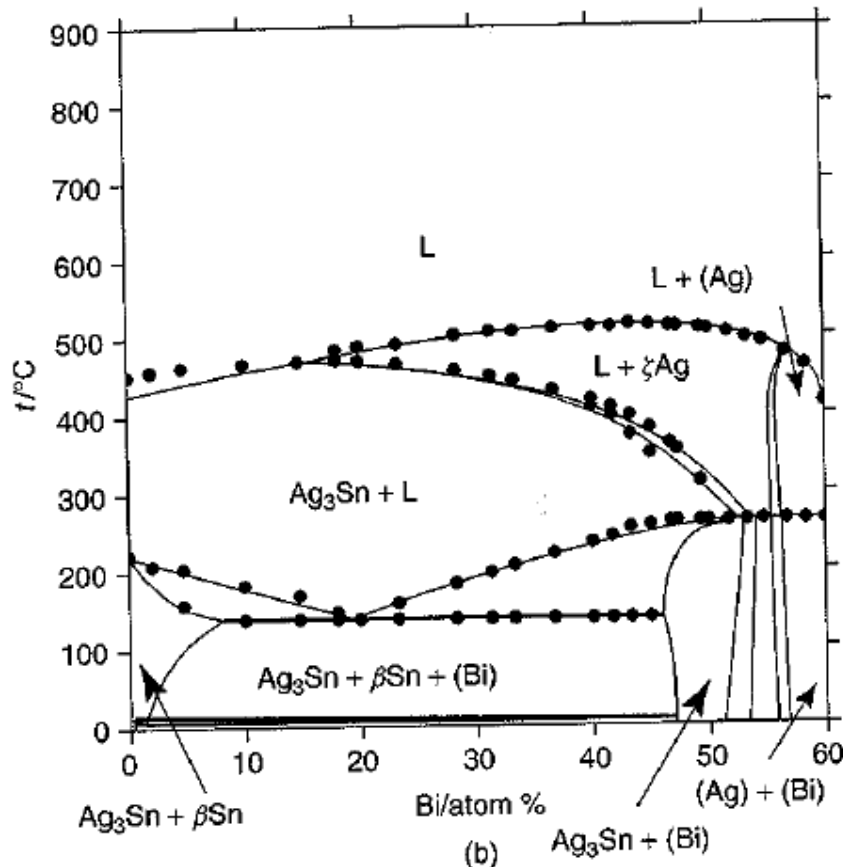


Predikovaný isotermní řez fázovým diagramem soustavy Sn-Ag-In pro 200°C.



Predikovaný isokoncentrační řez fázovým diagramem soustavy Sn-1%Ag-0,5%Cu-Bi. Zelená přerušovaná čára vyznačuje složení sledované slitiny Sn-3,5%Ag-0,7%Cu-1%Bi.

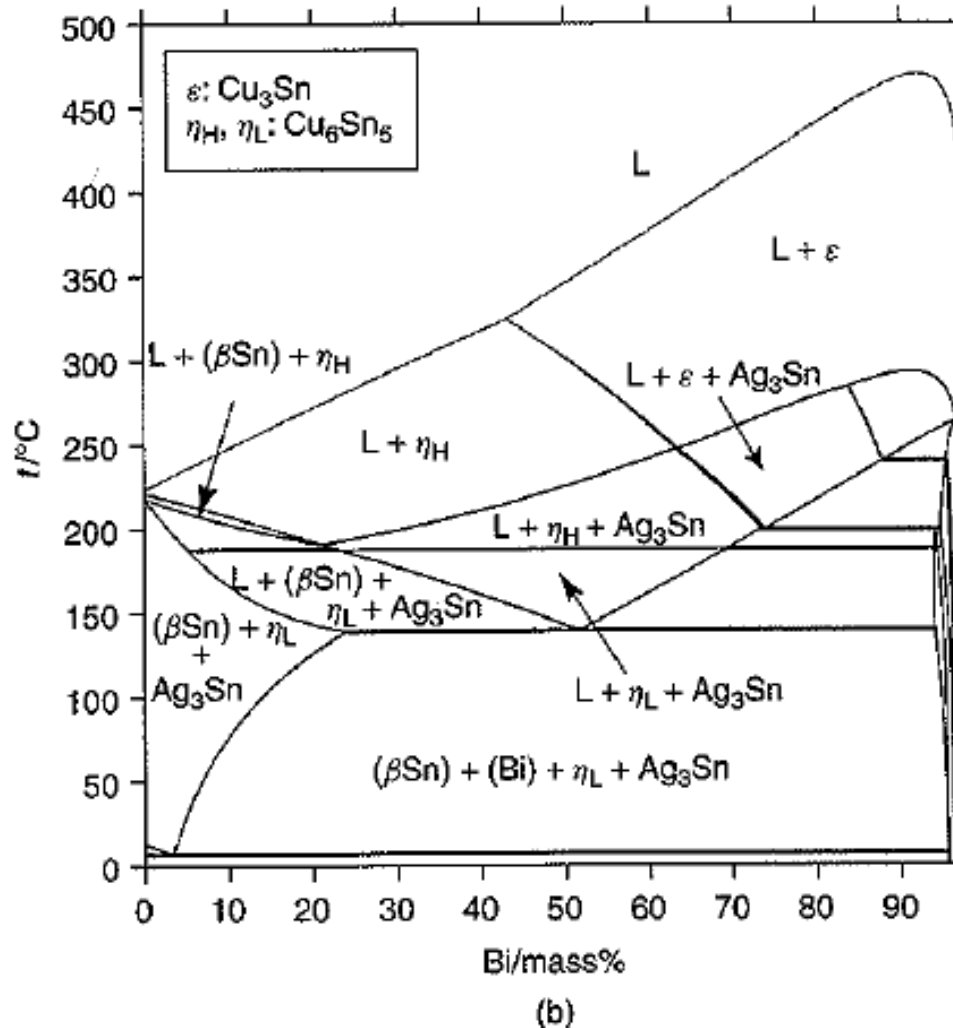
# CALPHAD – výpočet FD



**Figure 1** Comparison of the calculated vertical section diagrams of the Sn-Ag-Bi system with the DSC data at: (a) 10 mol% Bi; and (b) 40 mol% Ag

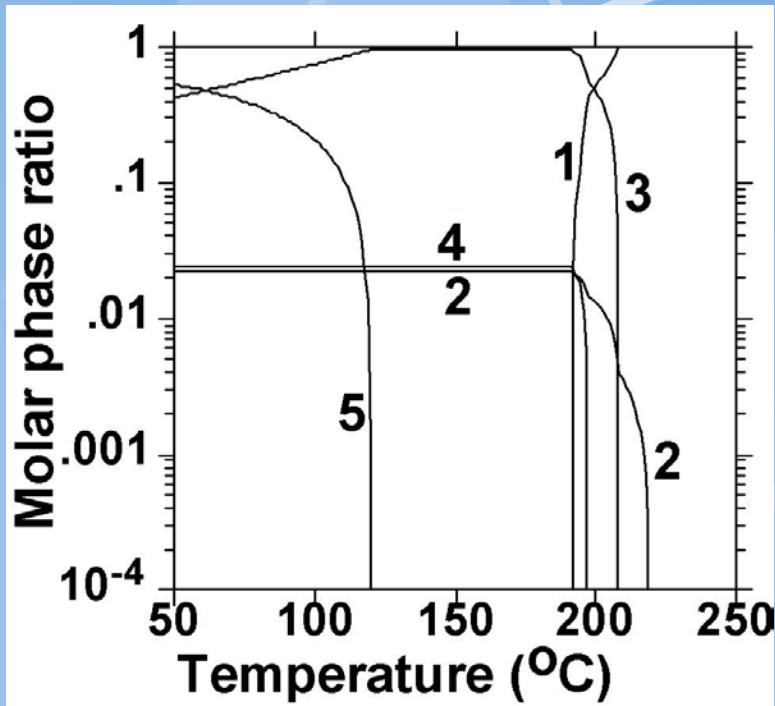
Včetně exp.  
Měření DSC

# FD Sn-Bi-Ag pájek

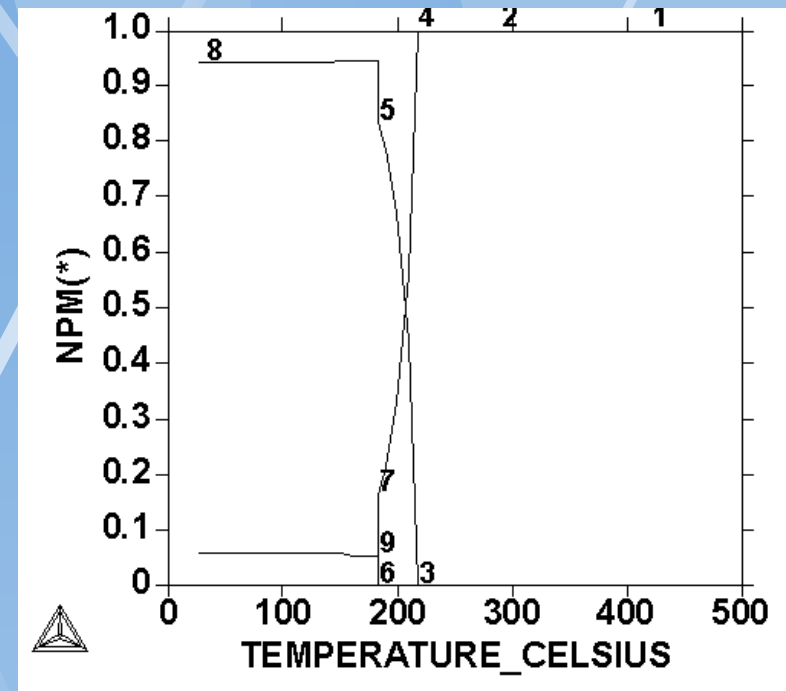


**Figure 2** Comparison of the vertical section diagrams of: (a) Sn-Bi-2mass%Ag; and (b) Sn-Bi-2mass% Ag-0.7 mass% Cu alloys

# Teplotní stabilita fází



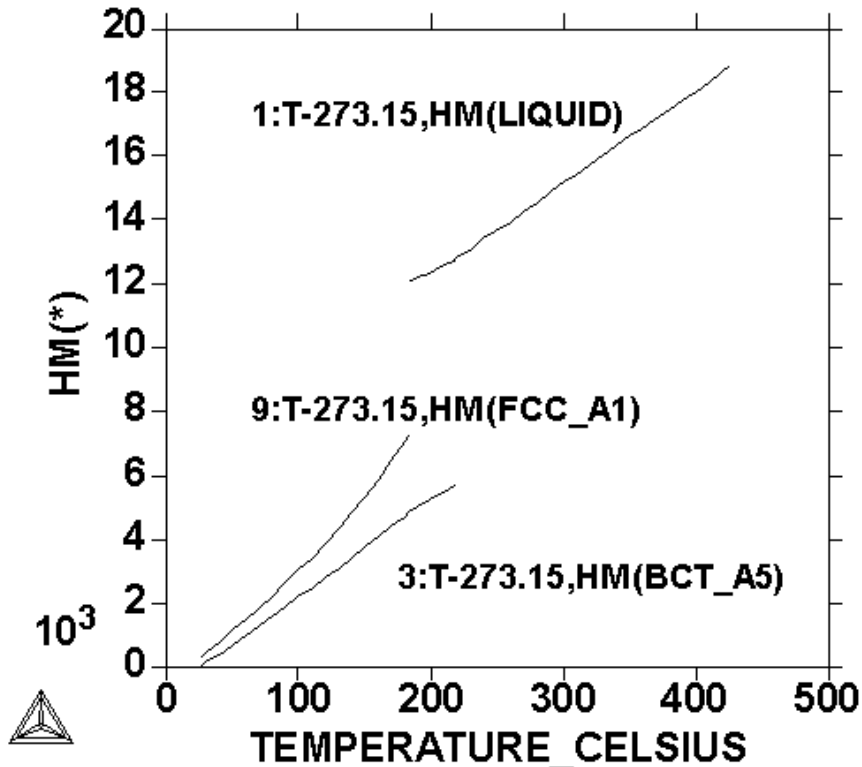
Závislost rovnovážného molárního podílu fází na teplotě pro soustavu Sn-3,5wt%Ag-0,7%Cu (1-liquid, 2-Cu<sub>3</sub>Sn<sub>6</sub>, 3-Ag<sub>3</sub>Sn). Bod tání 217°C.



Závislost rovnovážného molárního podílu fází na teplotě pro soustavu Sn-10wt%Pb (1-liquid, 5-BCT\_A5, 7-FCC\_A1). Bod liquidu 218°C, solisu 182 °C.

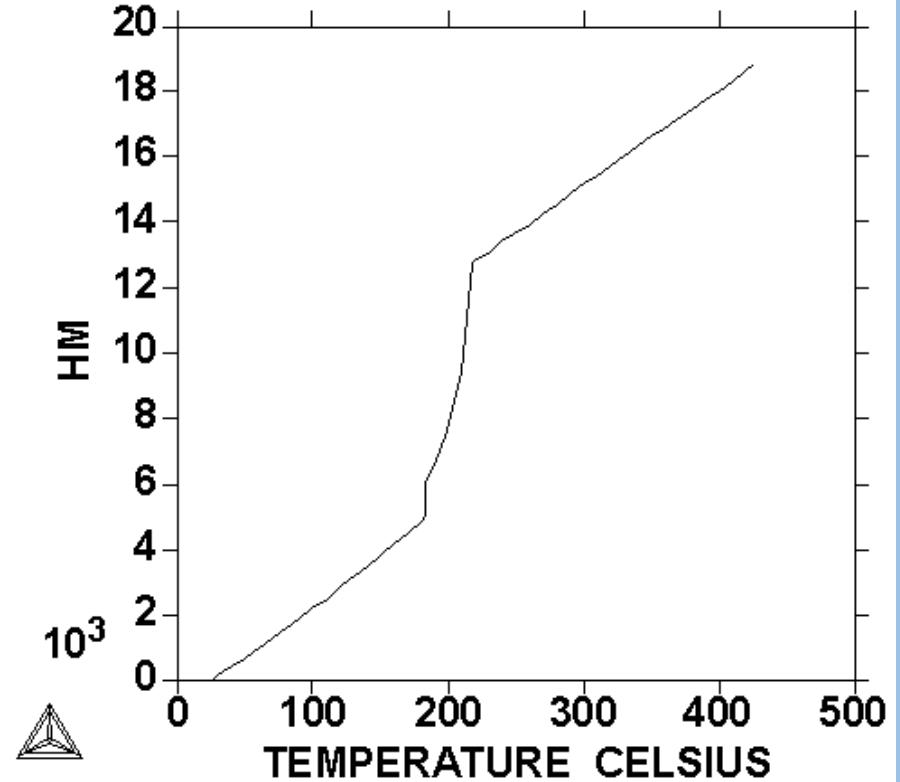
# Entalpie slitiny 10Wt%Pb-Sn

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DATABASE: SOLDER  
P=100000, N=1., W(PB)=1E-1;



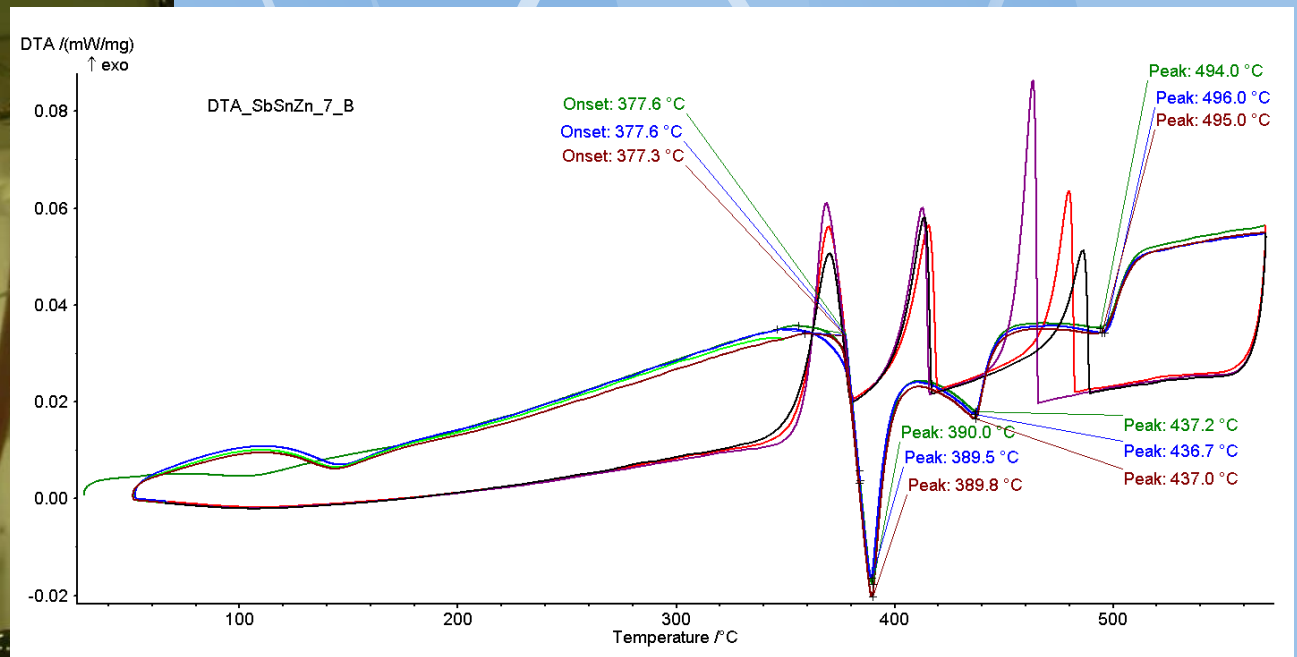
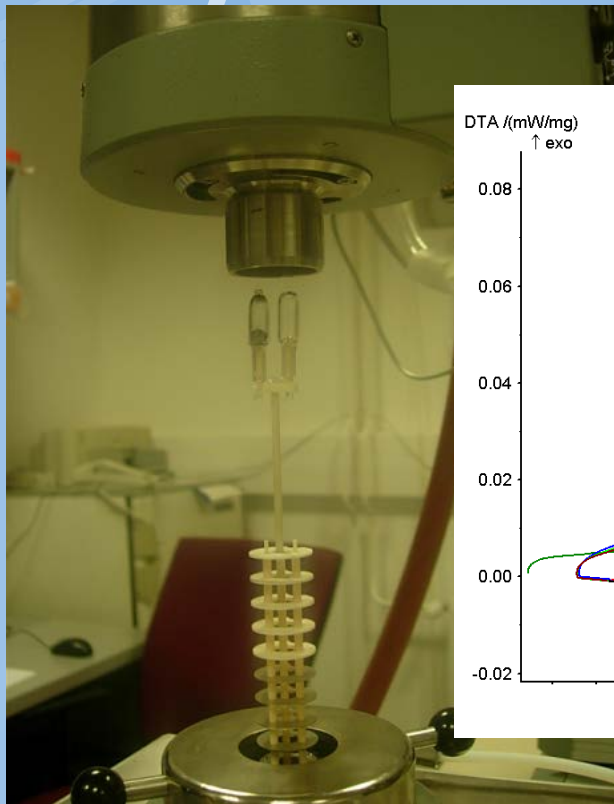
**Entalpie koexistujících fází.**

DATABASE: SOLDER  
P=100000, N=1., W(PB)=1E-1;



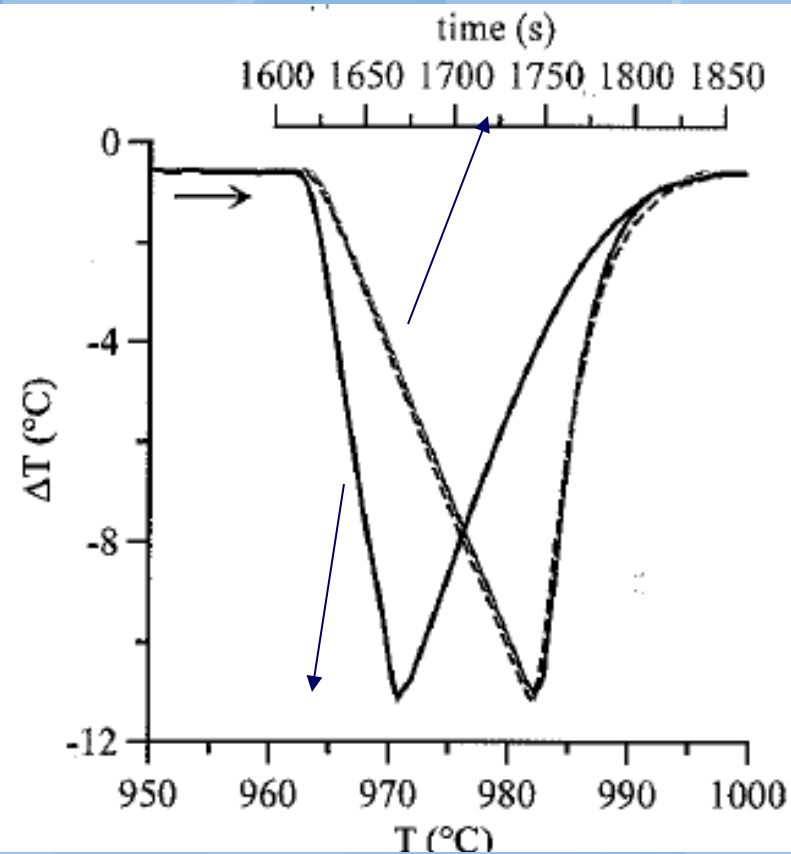
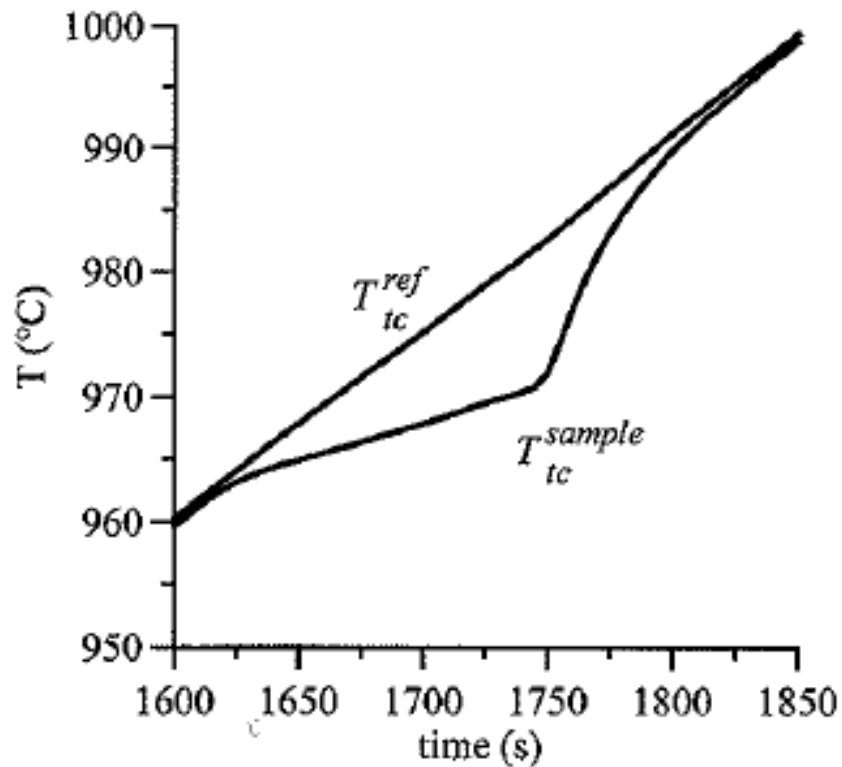
**Entalpie celková.**

# Simulace signálů DTA, pcDSC a hfDSC



**Dobře reprodukovatelné měření**

## Signál DTA (hfDSC)

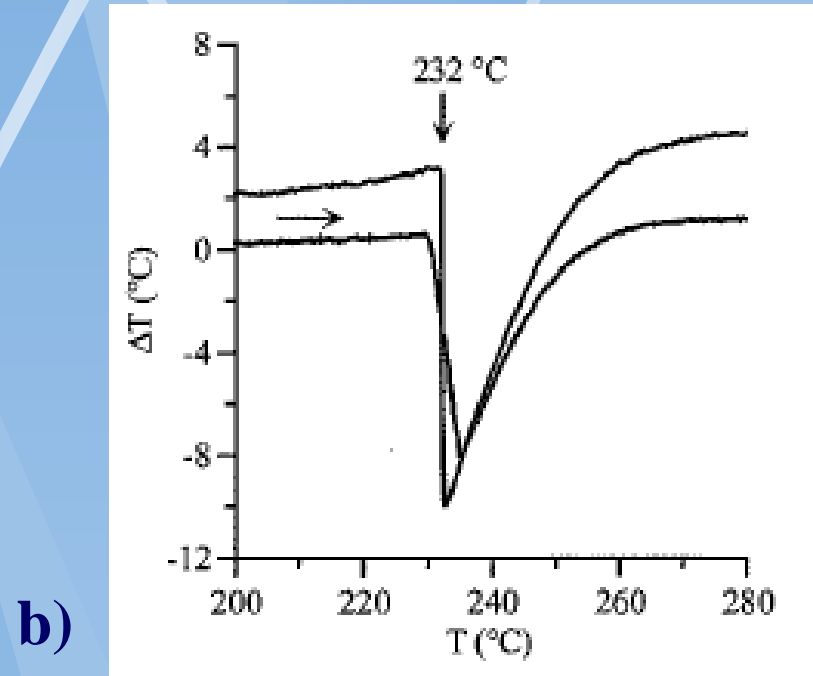
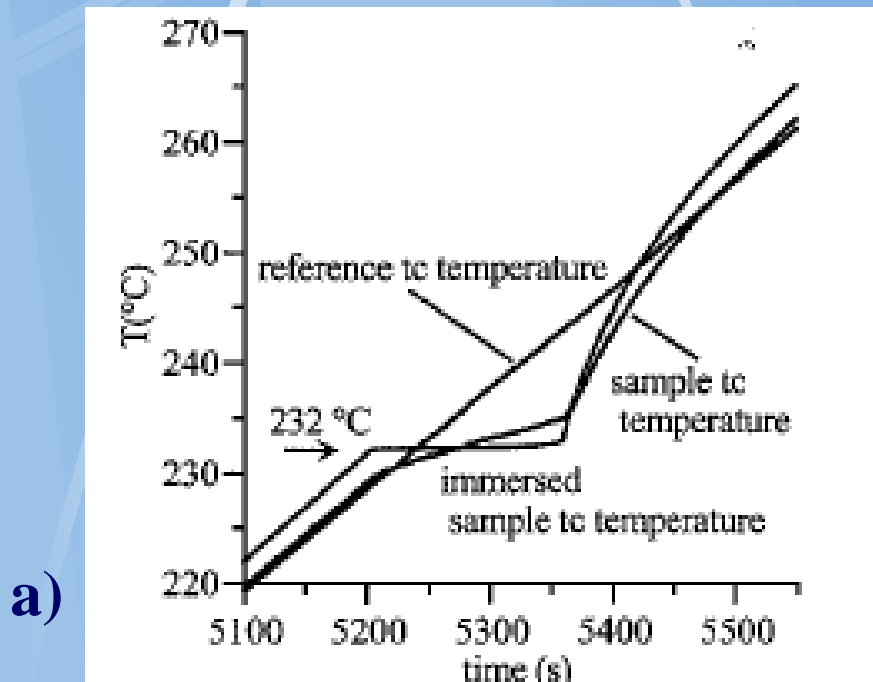


**Figure 2.2.** DTA melting of a 211.6 mg of pure Ag at 10 K/min. (a) Reference thermocouple temperature  $T_{tc}^{ref}$  and sample thermocouple temperature  $T_{tc}^{sample}$  vs. time. (b) Differential signal  $\Delta T = T_{tc}^{sample} - T_{tc}^{ref}$  vs. time (red), vs. sample temperature (solid black), and vs. reference temperature (dashed black). For this data, the reference temperature remains quite linear in time as the sample melts, so that a linear scaling of the time axis makes the plots with x-axes of time and reference temperature practically identical.



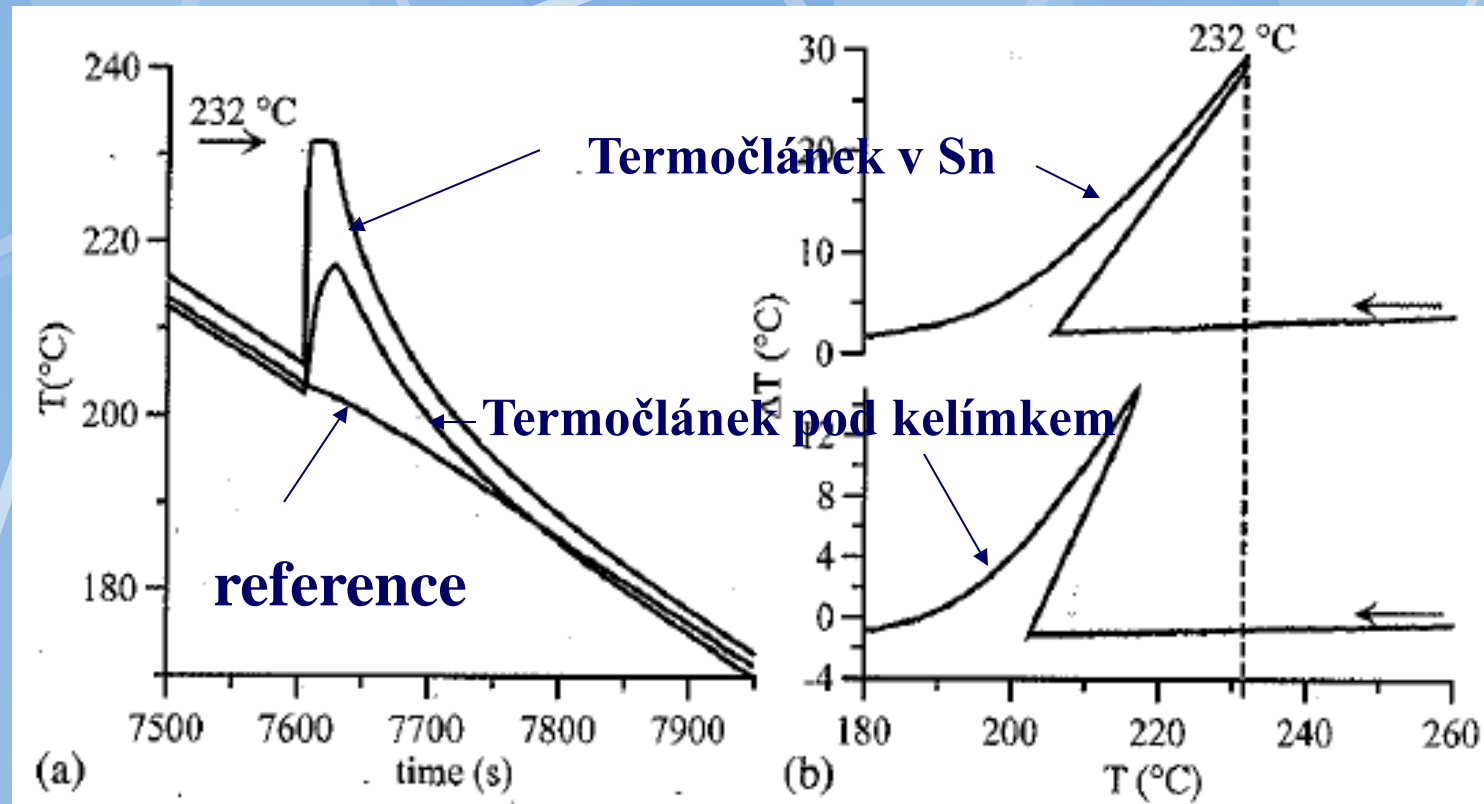
# Zpoždění reálného signálu

Přestup tepla (šikmost) v.s. přímé vložení termočládku (kolmé)



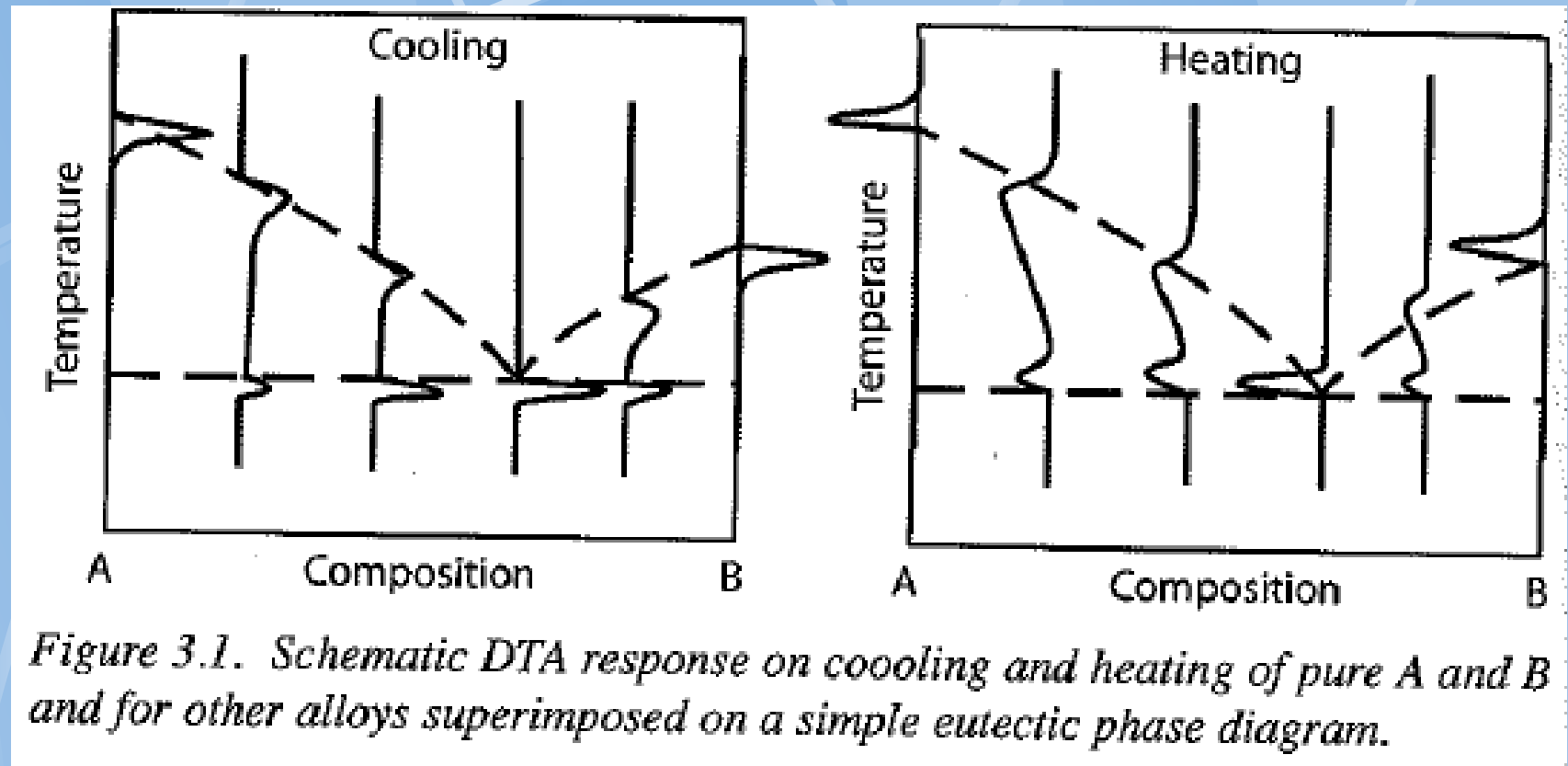
*Figure 2.6. Measured (a) temperature vs. time plots and (b) associated DTA plots for melting of pure Sn. The instrument thermocouple readings are black and the readings from a thermocouple immersed directly in the Sn in the sample cup is red. Mass = 163.2 mg; heating rate = 5 K/min.*

# Efekt podchlacení na křivce chladnutí čistého Sn



**Figure 3.15.** Measured (a) temperature vs. time plots and (b) associated DTA plots for the freezing of pure Sn. The instrument thermocouple readings (sample and reference) are black and the readings from a thermocouple immersed directly into the Sn in the sample cup are red. Significant supercooling has occurred prior to freezing inducing the rapid temperature rise upon solidification in (a) and the associated positive slope in (b); mass = 163.2 mg; heating rate = 5 K/min.

# DTA binárních slitin Klasické výhodnocení



**Aplikovatelné jen pro  
jednoduché případy**

# Princip simulace DTA (DSC)

**Figure 2.5.** Schematic a) enthalpy vs. temperature for a pure metal; b) corresponding derivative  $dH_S(T_S)/dT_S$  curve; c) DTA signal for melting (bottom) and freezing (top). The small difference in heat capacity of liquid and solid leads to a small offset of the baseline before and after melting. The onsets in the DTA curves are shown with a small deviation from the melting point,  $T_M$ , due to heat flow limitation in the DTA. This difference on melting is adjusted to zero by the calibration procedure, at least for one heating rate.

$$dH^m/dt = C_p^m$$

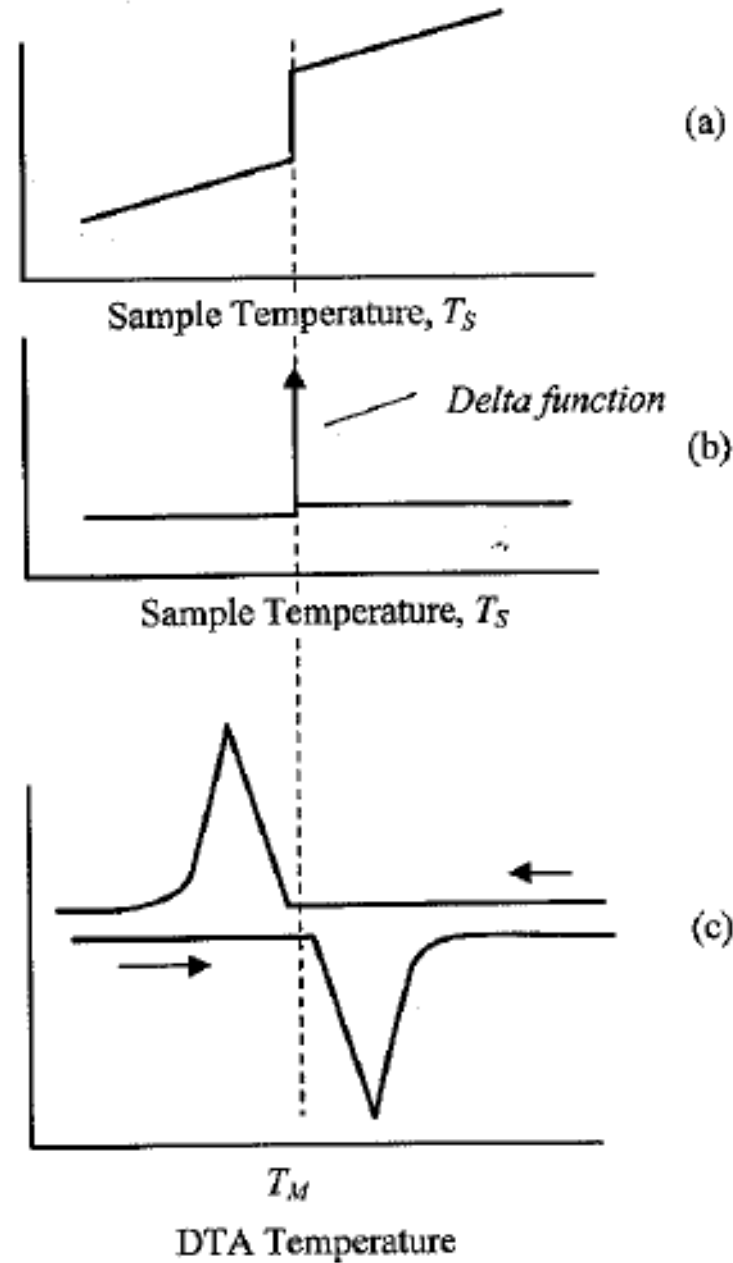
Pro fázovou přeměnu 1.ř:

$dH^m/dt = \text{neko}$   
nečno. (delta funkce)

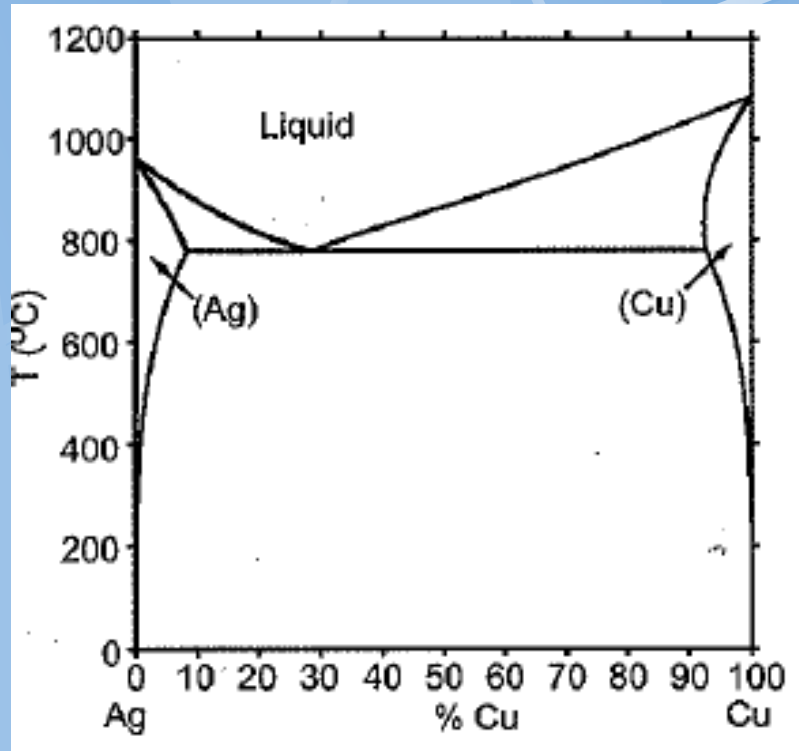
Zpoždění,  
podchlazení,  
posuv

Sample Enthalpy,  $H_S$

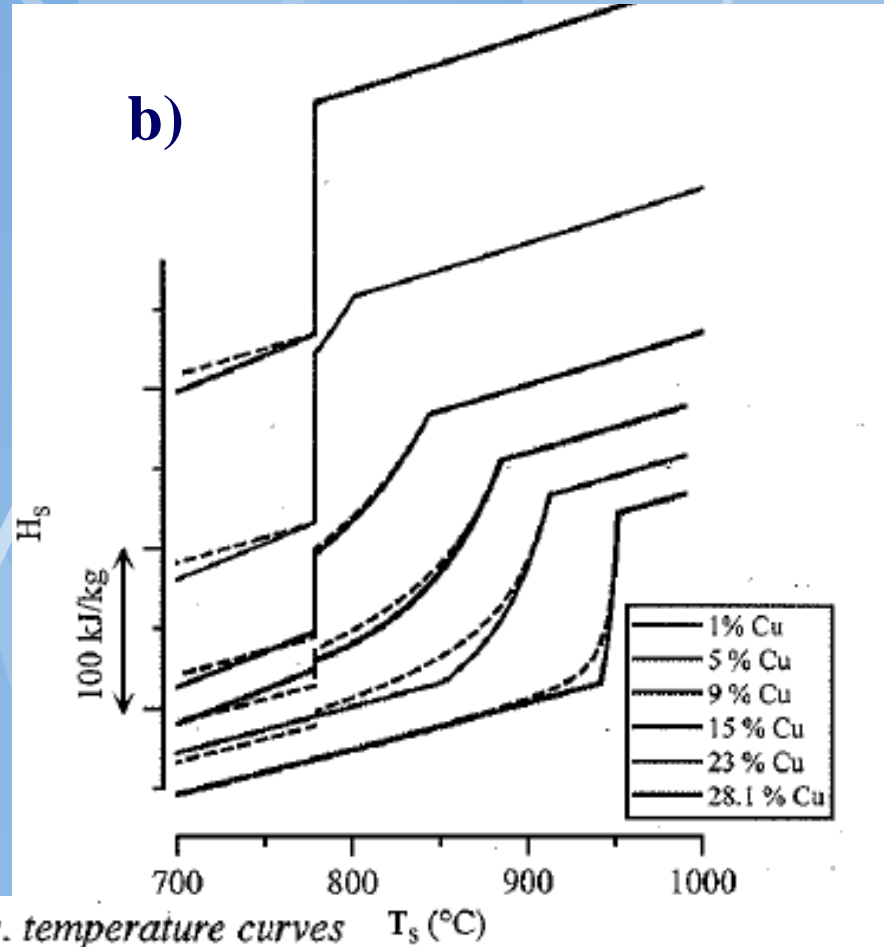
$dH_S/dT_S$



# CALPHAD přínos – výpočet entalpie

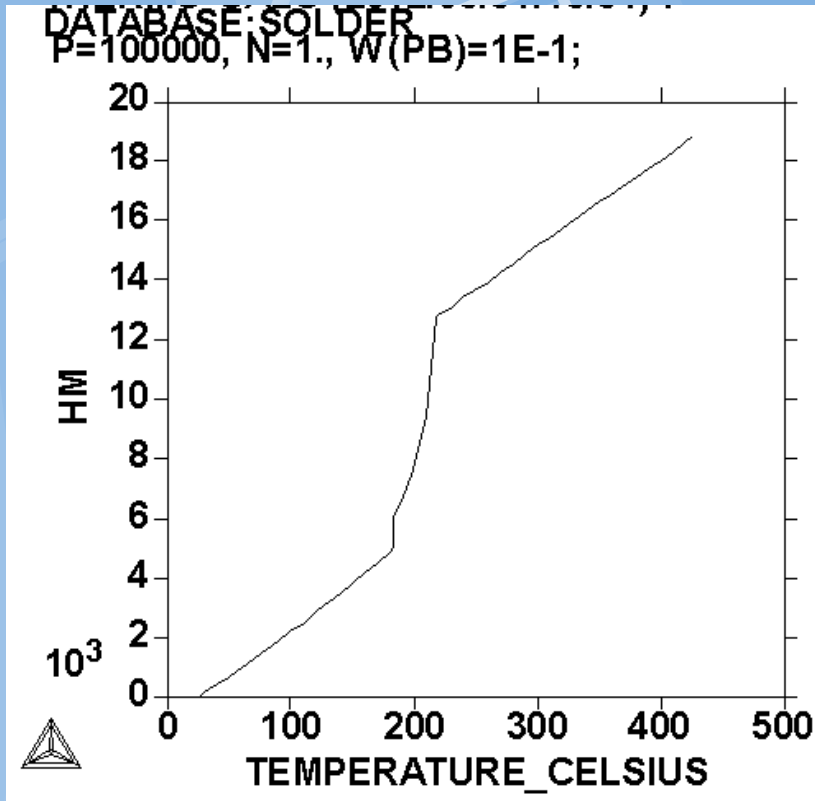


a)

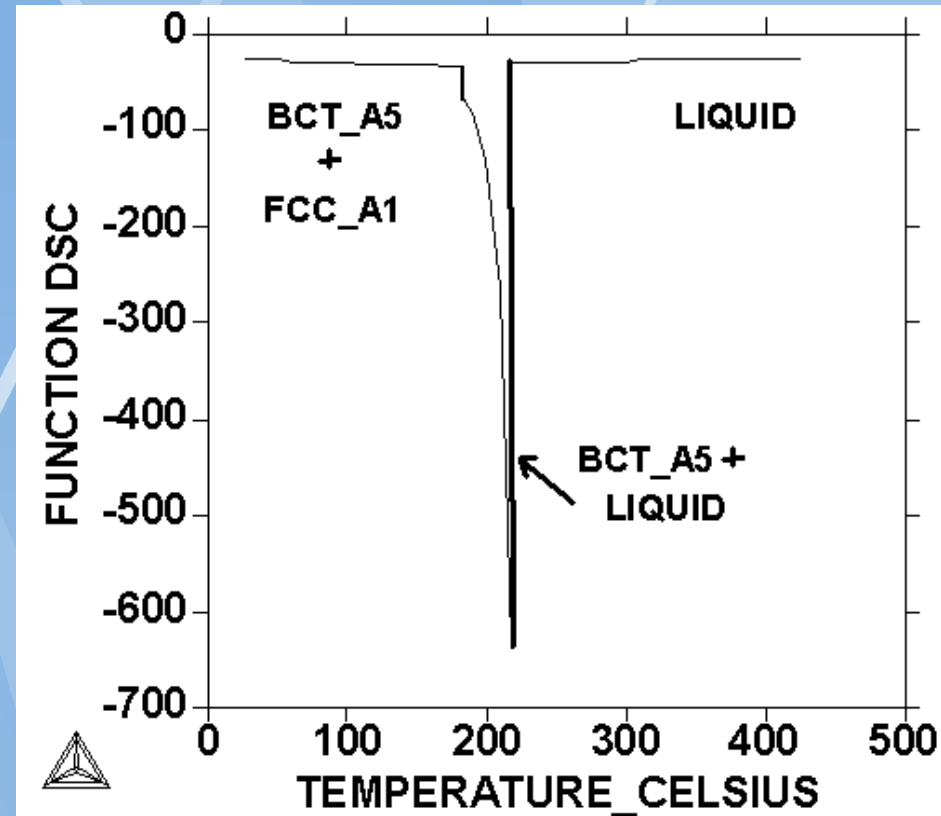


**Figure 3.2.** (a) Ag-Cu phase diagram; (b) Enthalpy vs. temperature curves for five Ag-Cu alloys (solid, equilibrium; dashed, Scheil); the curves have been shifted vertically for clarity, only differences of enthalpy are relevant; (c)  $dH_S / dT_S$  vs.  $T_S$  curves for equilibrium conditions for various Ag-Cu alloys derived from the equilibrium enthalpy curves (overleaf). The vertical arrows at the eutectic temperature (779°C) represent delta functions of the indicated strength in kJ/kg.

# Sn-10wt%Pb

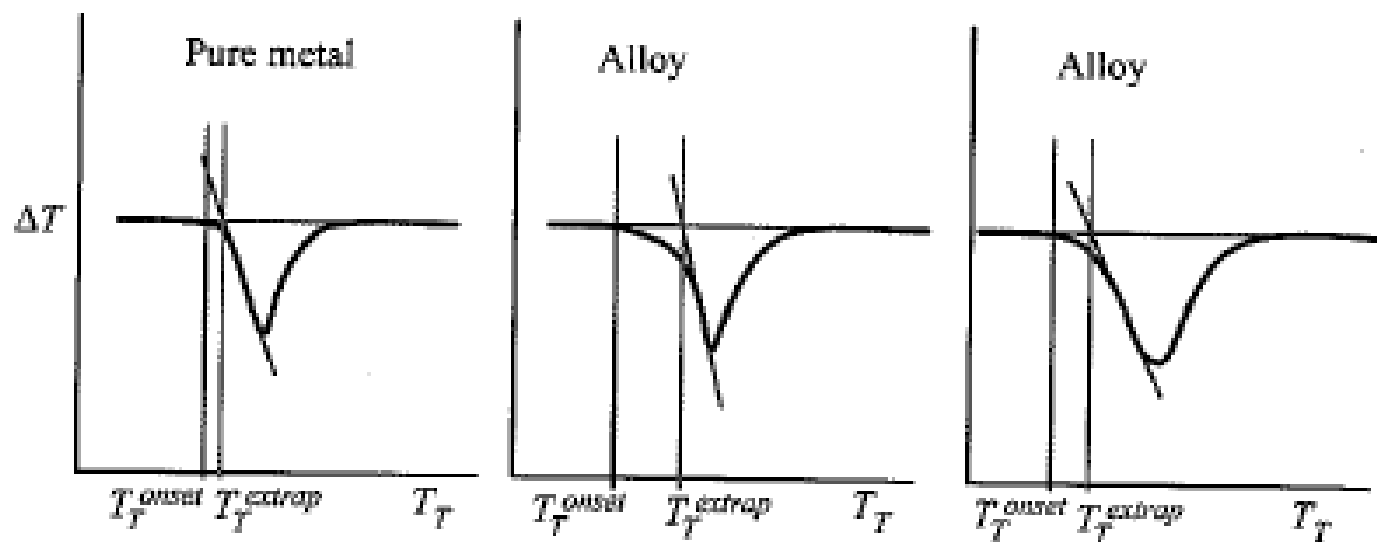


Entalpie celková.



Funkce DSC =  $dH^m/dt = C_p^m$

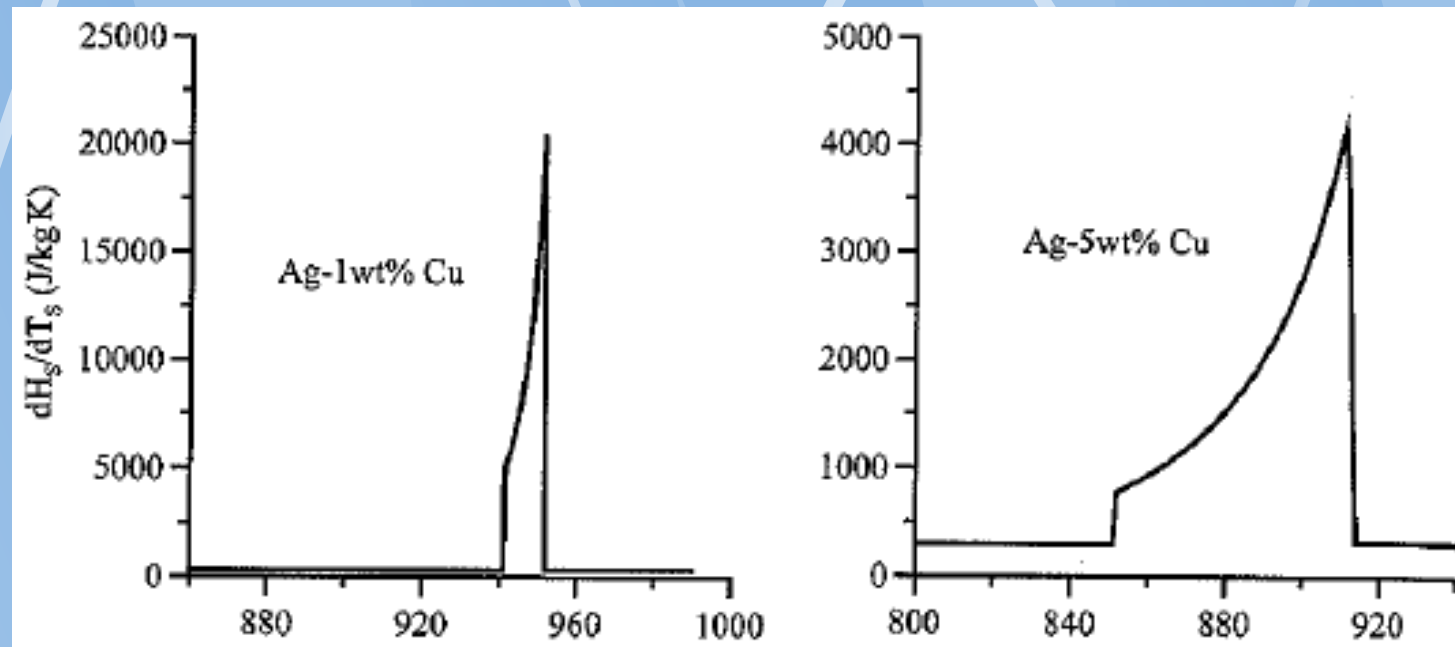
# DSC čisté látky a binární nízkoalegované slitiny



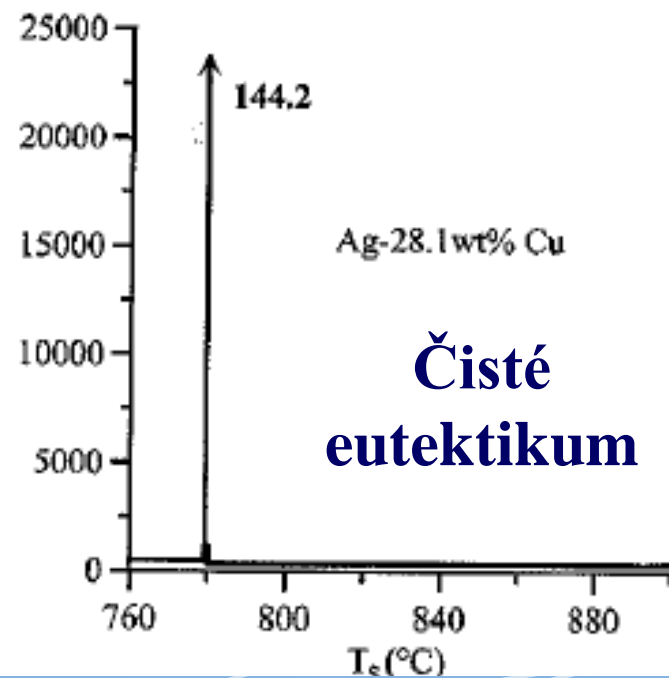
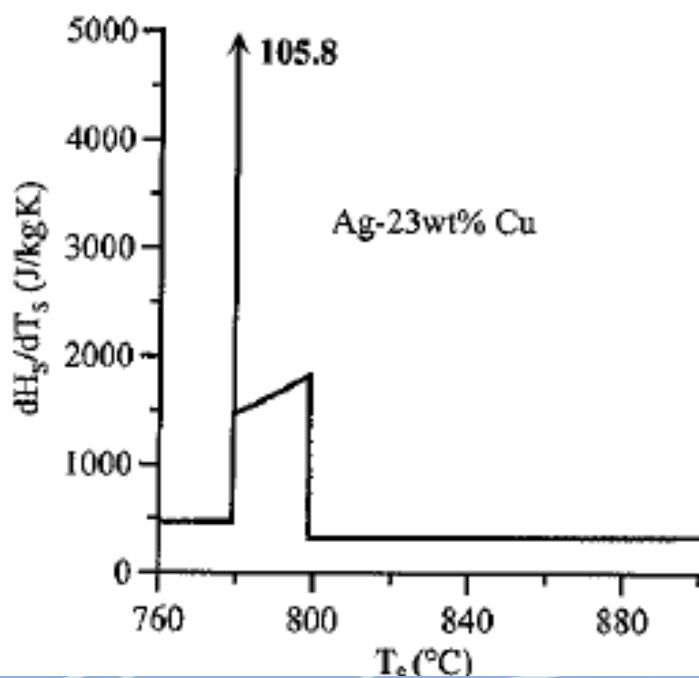
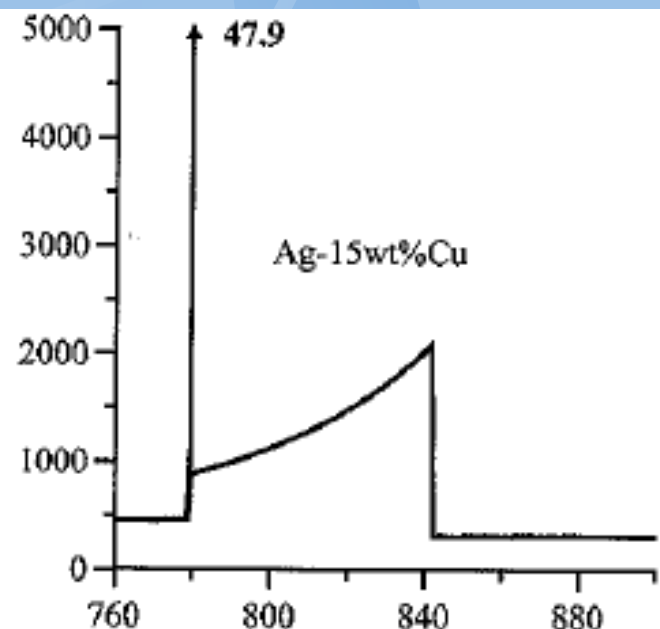
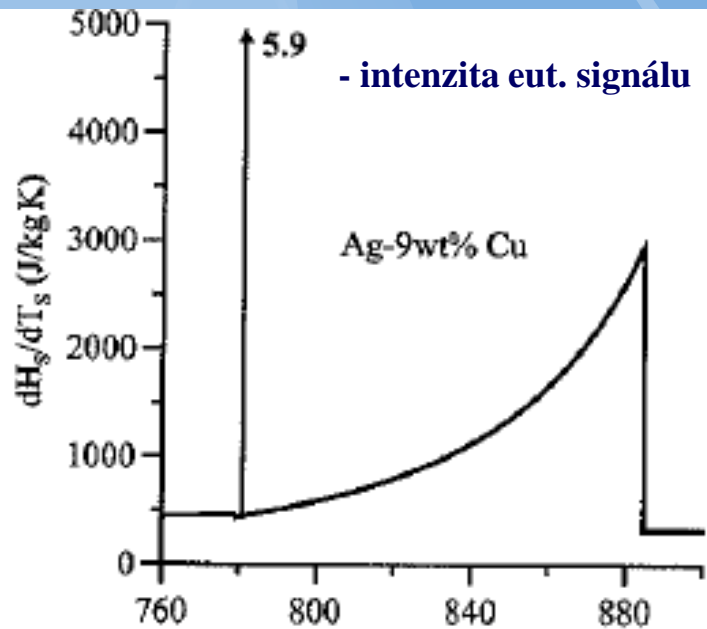
*Figure 3.8. Schematic DTA plots showing error introduced by using the extrapolation method for onset determination rather than the first detectable departure from baseline.*

**Použití i pro testy čistoty  
látek.**

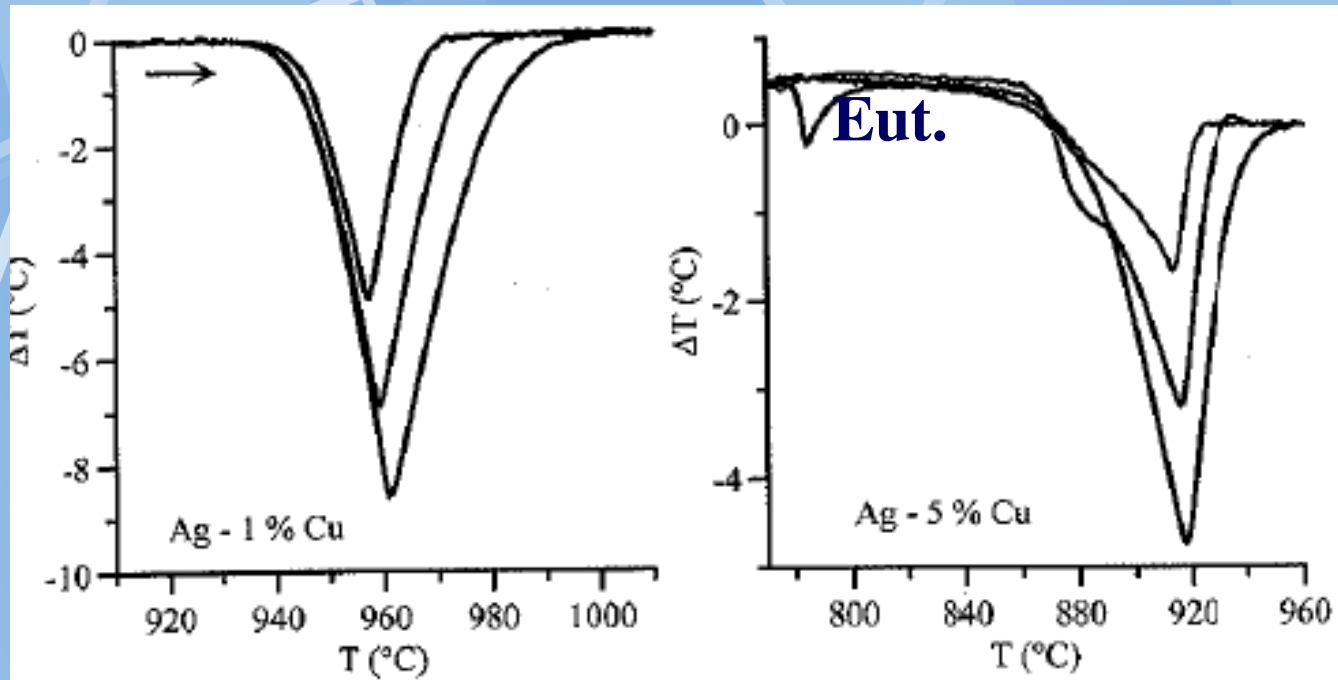
# Derivace entalpie bináru SnAg





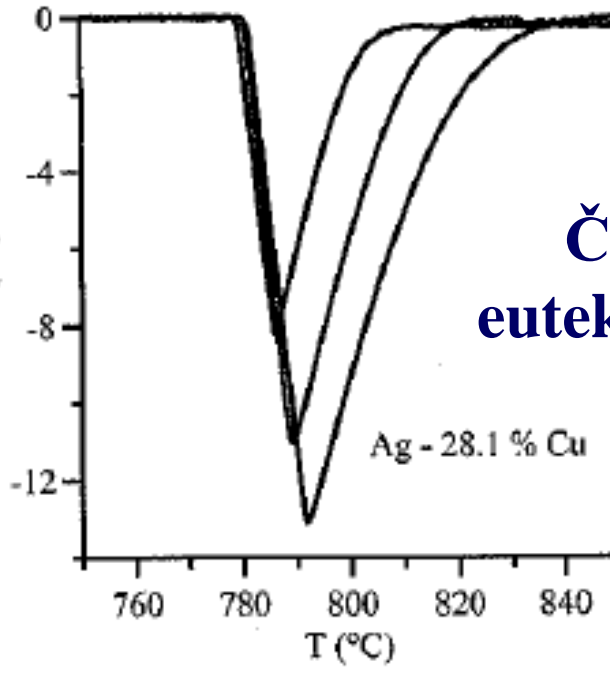
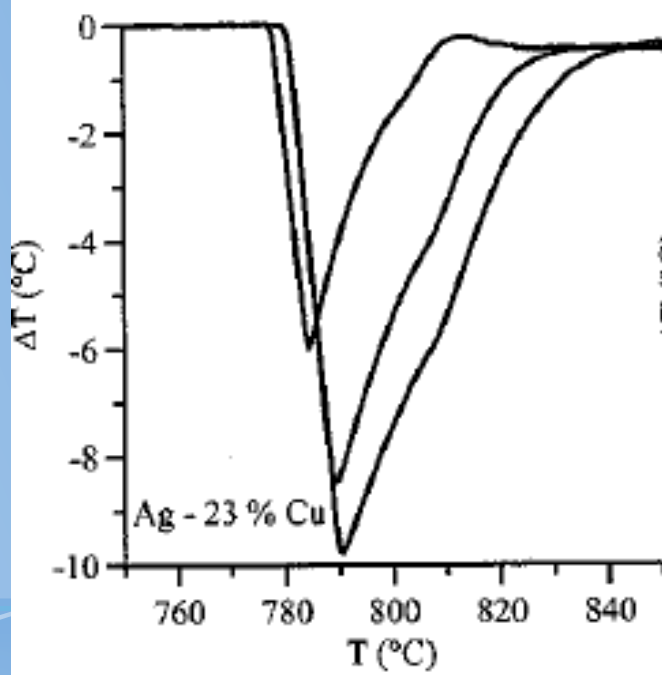
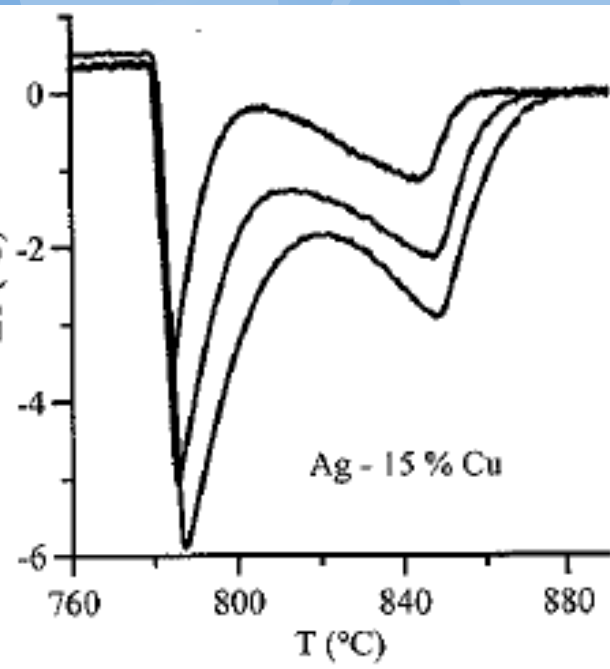
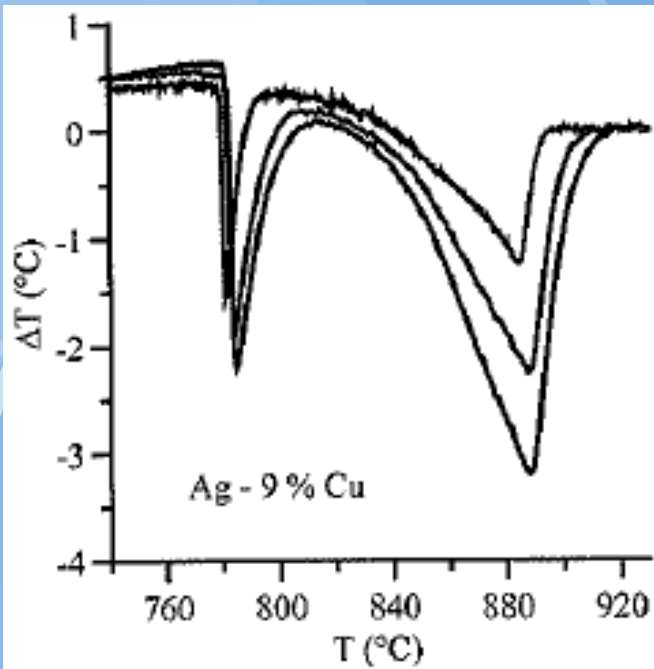


# Reálný DTA (DSC) signál bináru SnAg



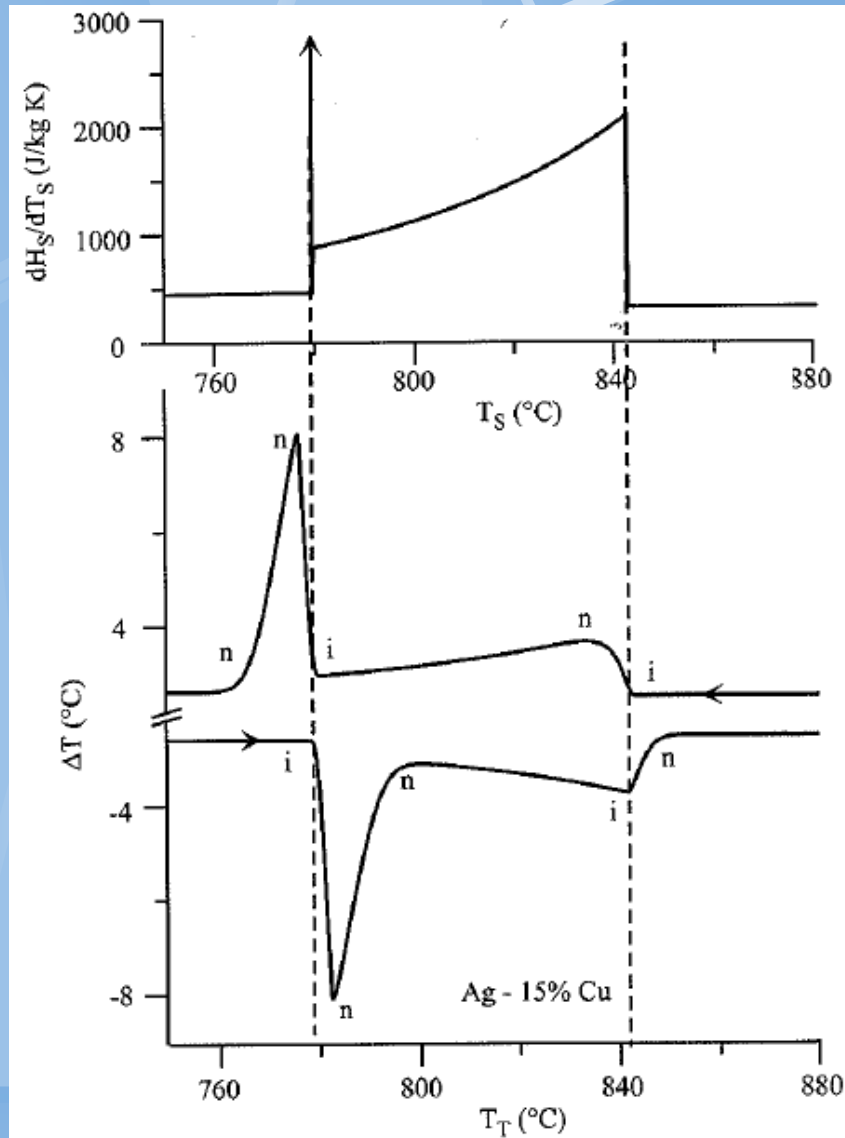
*Figure 3.3. Experimental DTA melting scans for a series of Ag-Cu alloys at three different heating rates, 5 K/min (blue), 10 K/min (red) and 15 K/min (black). Note that the small signal for the eutectic melting is absent in the Ag-5 % Cu alloy at the slower heating rates. Note also the absence of a distinct second peak in Ag-23 % Cu. Percentage is by mass.*

**Snižování rychlosti vede k separaci peaků.**



**Čisté  
eutektikum**

# Obecná analýza DTA (DSC) signálu



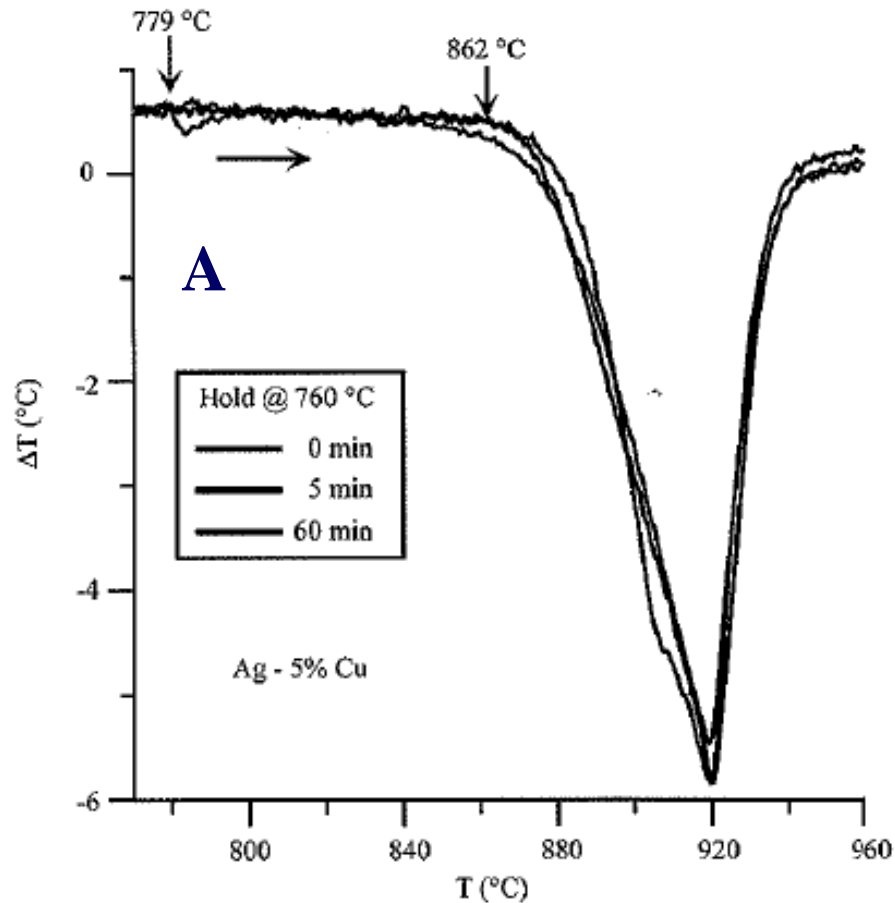
**Simulace signálu  
metodou  
CALPHAD**

**Teplotní  
posuv a  
„rozmytí“**

**Reálný signál  
odpovídající  
simulaci**

Figure 3.9.  $dH_S/dT_S$  vs.  $T_S$  (top) and computed DTA scans for melting and freezing at 5 K/min (bottom) for Ag-15% Cu using equilibrium enthalpy. Features on the DTA scans are labeled with: *i* = important or *n* = not important.

# Efekt isotermní prodlevy



**A...Delší prodleva  
na 760stC**

**Přesnější  
určení  
solidu**

*Figure 3.5. DTA signal for melting of Ag- 5 % Cu showing the effect of hold time at 760°C and subsequent heating at 15 K/min.*

# Vliv isotermní prodlevy na rozpuštění Lavesovy fáze

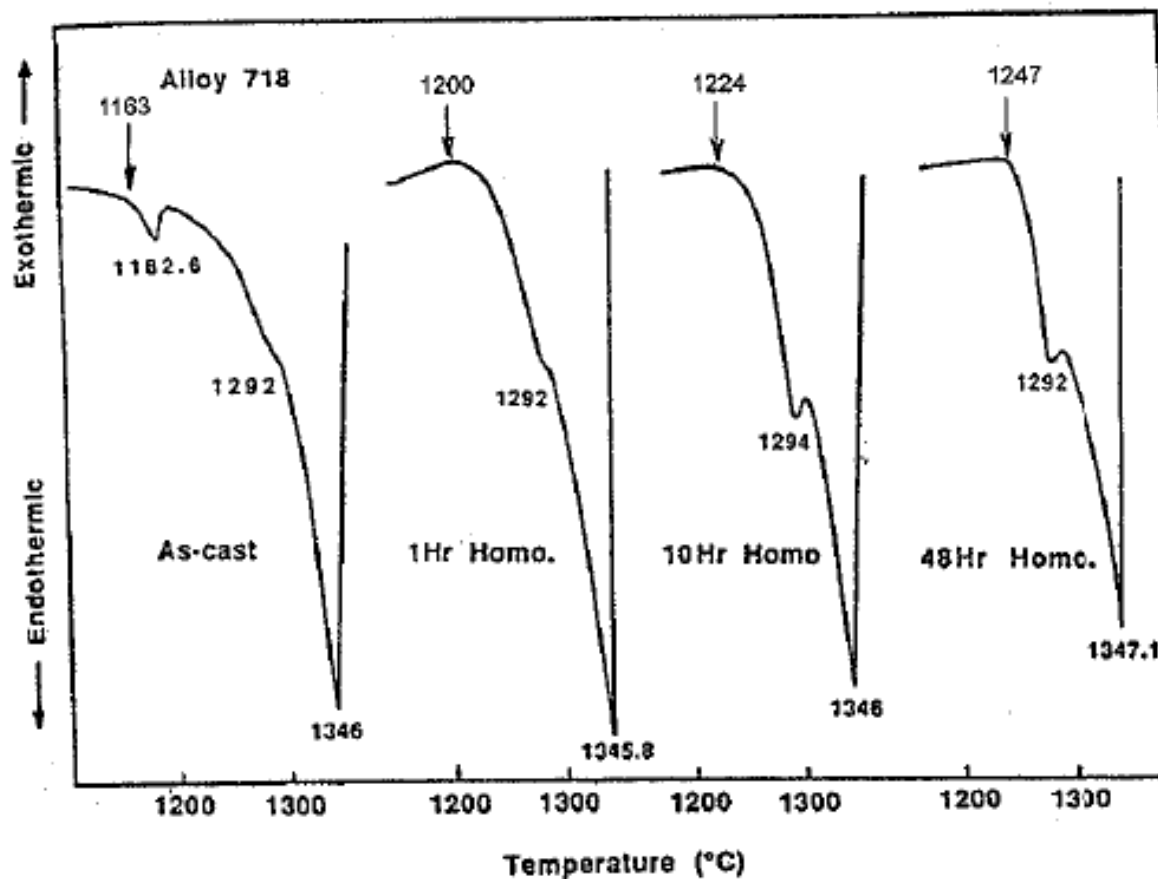
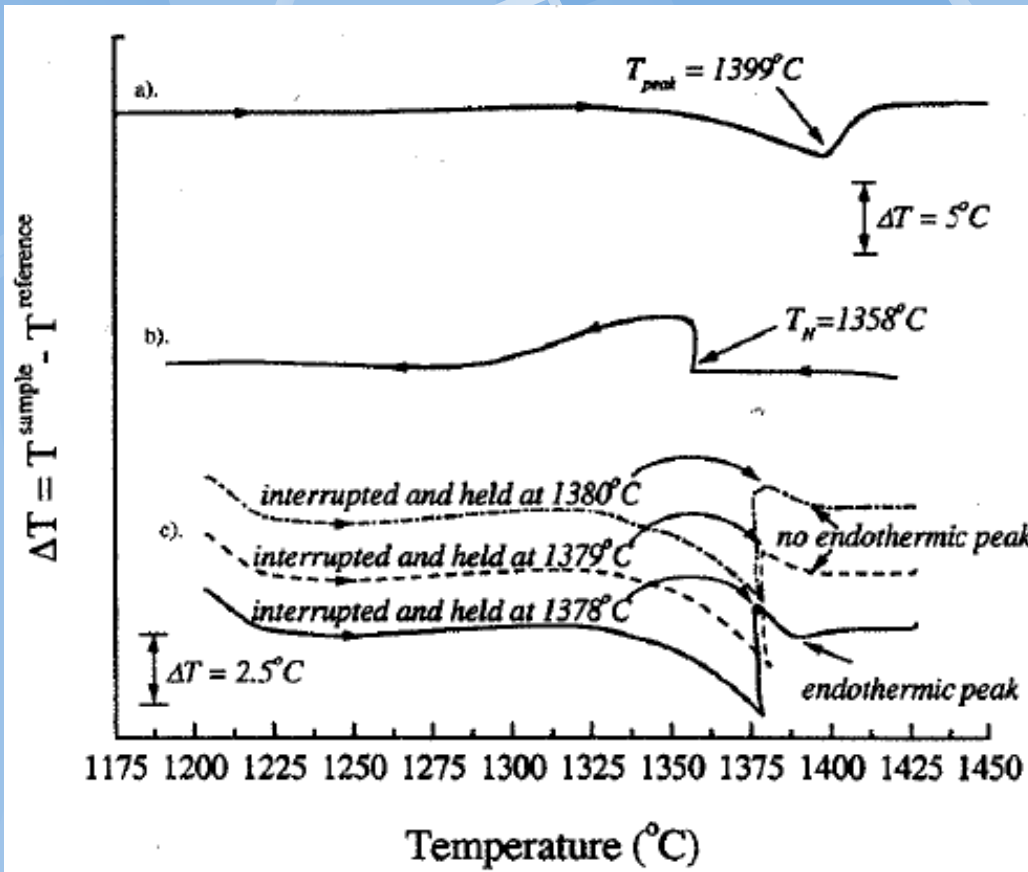


Figure 3.7. DTA signal for Inconel 718 showing the effect of annealing time [91Cao]. With annealing, the  $(Fe,Cr)_2Nb$  Laves phase dissolves and the onset of melting increases from 1163°C to 1247°C.

# Upřesnění teploty liquidu, solidu,..



Použitelné pro velmi úzké dvoufázové oblasti

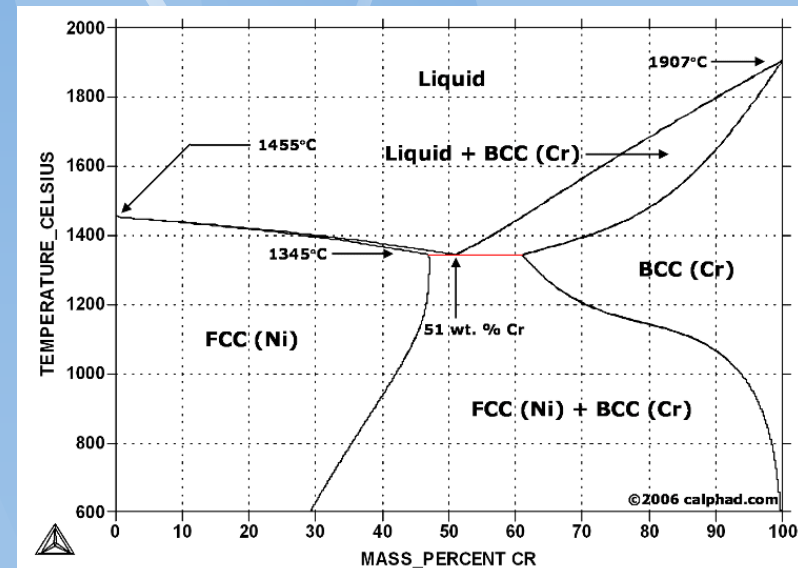


Figure 3.12. a) Normal DTA scan on heating for a small greezing range Ni-base superally; b) Normal DTA scan on cooling. Supercooling has occurred; c) Cycling DTA to determine the liquidus temperature [00Wu].

# Rovnovážený výpočet vs. Sheil-Gulliver aprox.

## Rovnovážený výpočet

Rovnováha v každém  
okamžiku (chladnutí i  
ohřevu).

Soulad s  
experimentem  
při nízkých  
rychlostech

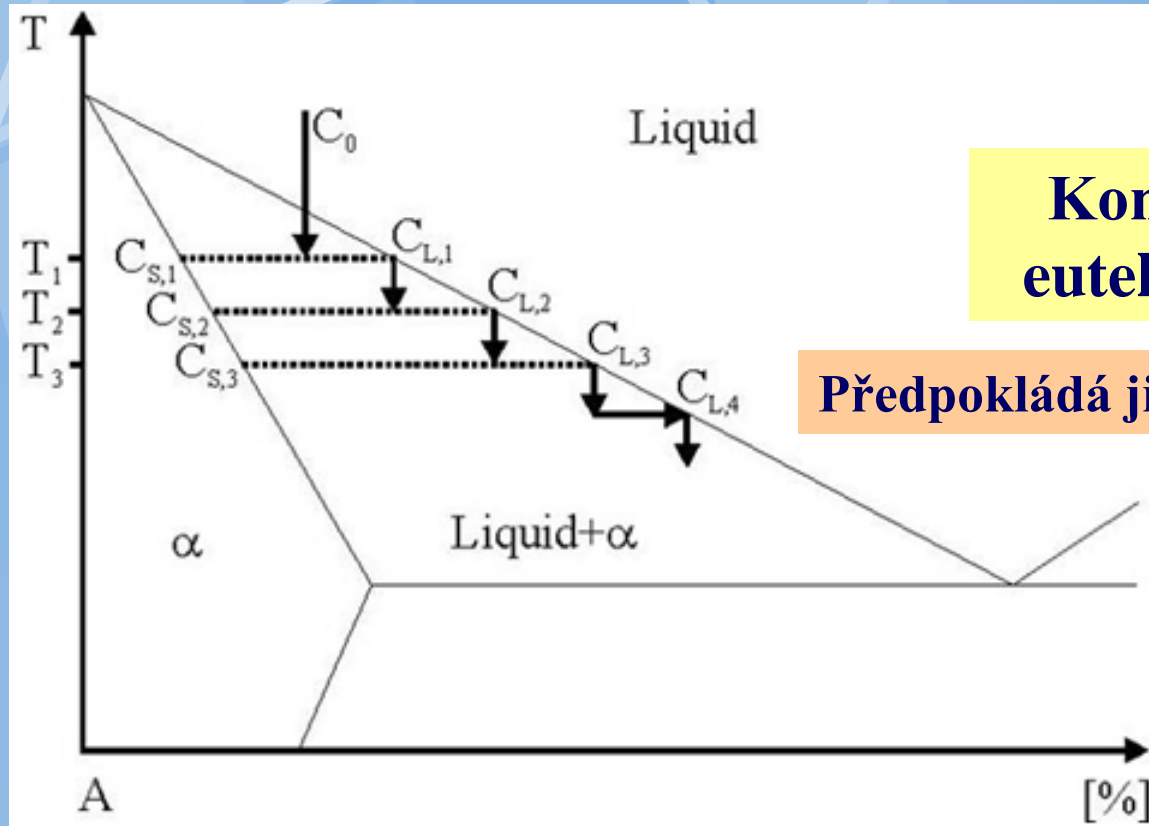
## Sheil aproximace

Vylučování tuhé fáze  
(bezdifúzní) z kapalně  
(nekonečná difúze) s  
definovaným podchlazením  
nebo množstvím odnímaného  
tepla

Soulad s  
experimentem  
při vyšších  
rychlostech  
změny teploty



# Scheil-Gulliver approx.

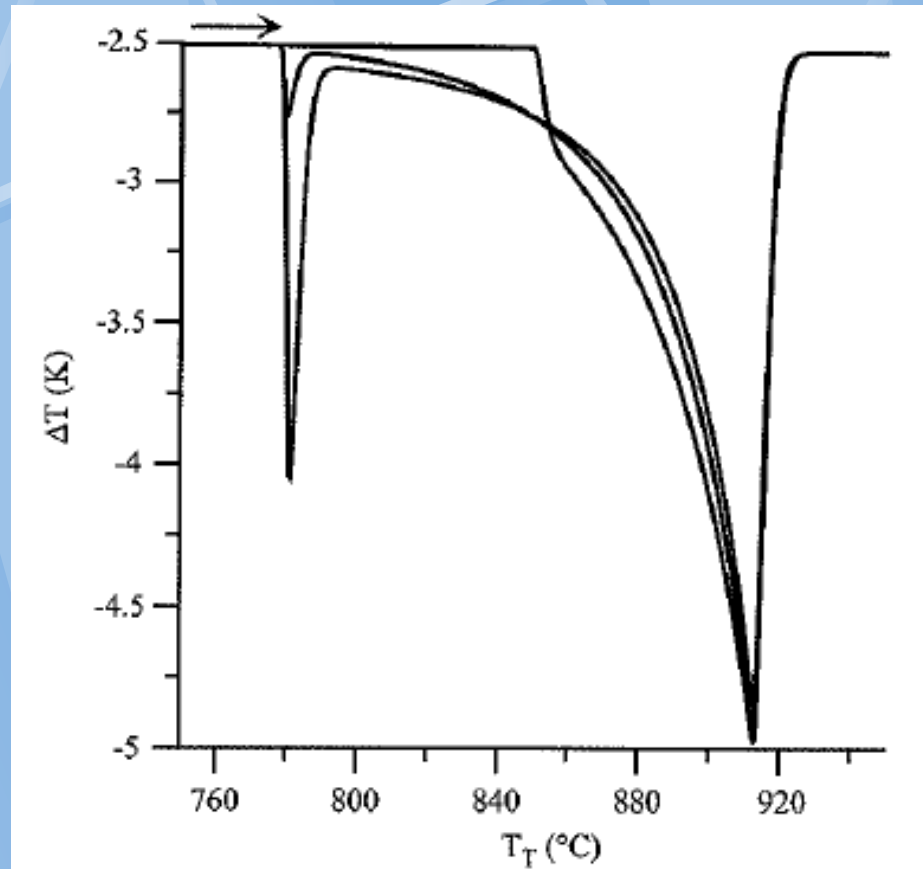


**Končí v  
eutektiku**

**Předpokládá jisté podchlazení**

Scheme of Scheil solidification of a hypothetical Fe-C alloy. During solidification the actual liquid phase, beginning with  $C_0$ , is undercooled and solidifies according to the lever rule enriching the liquid phase with solute atoms

# Scheil vs. equilibrium



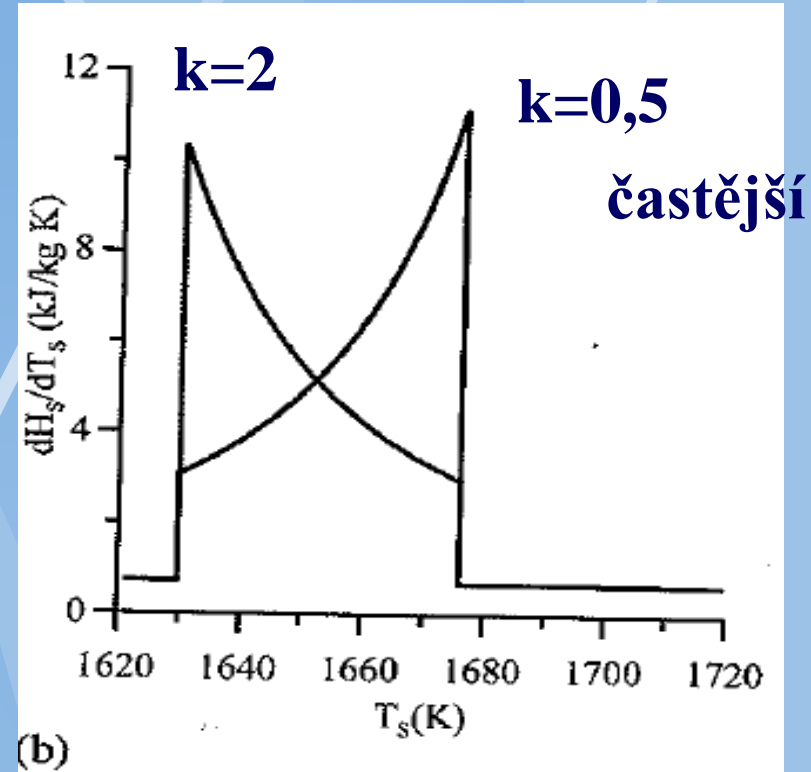
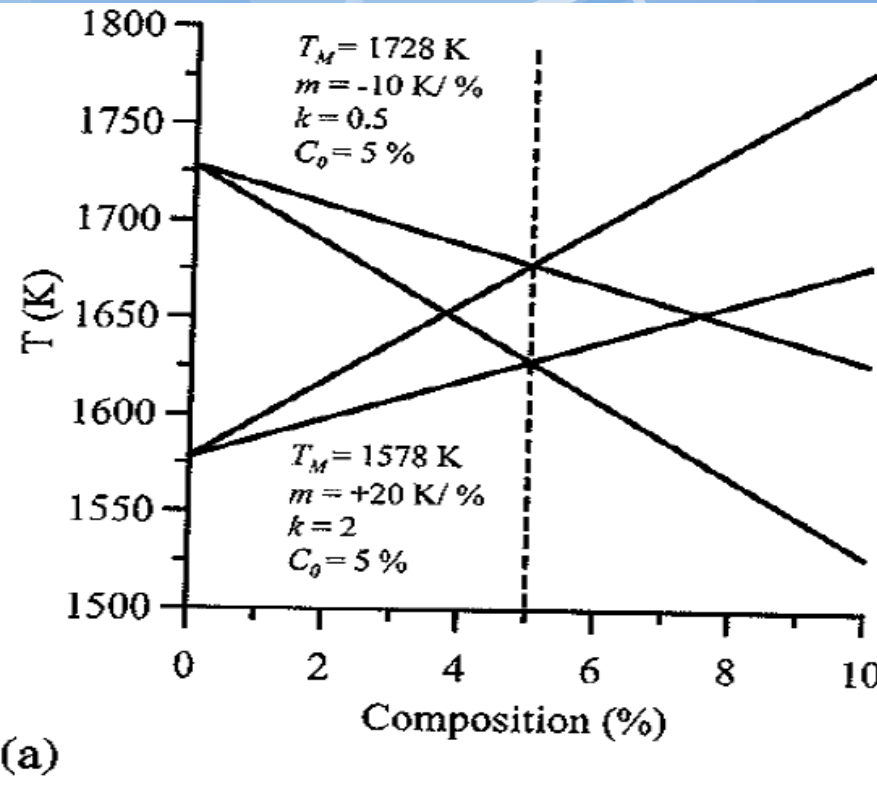
**Figure 3.6.** Computed DTA curve for an enthalpy vs. temperature relation derived from a back diffusion model of solidification at 5 K/min of Ag 5 % Cu is shown blue.  $D_S = 1 \times 10^{-14} \text{ m}^2 / \text{s}$ ,  $\lambda_2 = 3.8 \times 10^{-5} \text{ m}$ . The equilibrium curve is black and the Scheil is red. The peak eutectic signal at approx. 780°C is intermediate between that for the Scheil and equilibrium cases but is not as small as the measured eutectic signal with no annealing in Figure 3.5.

k...rozdělovací koeficient

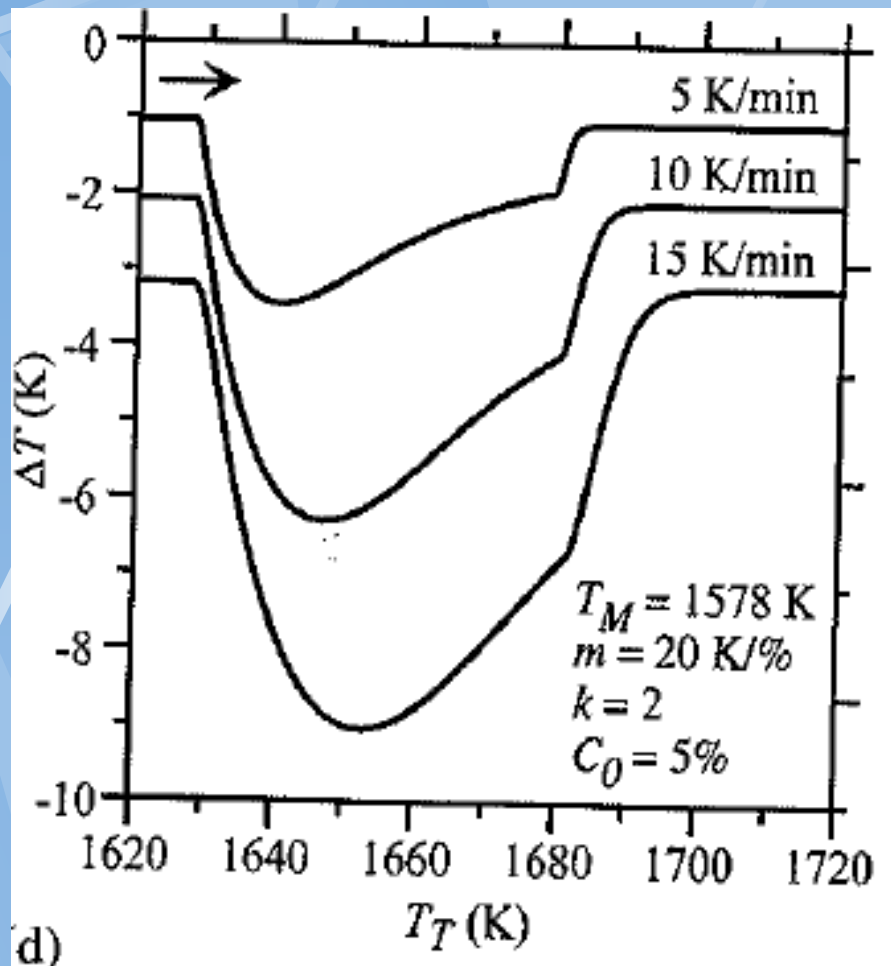
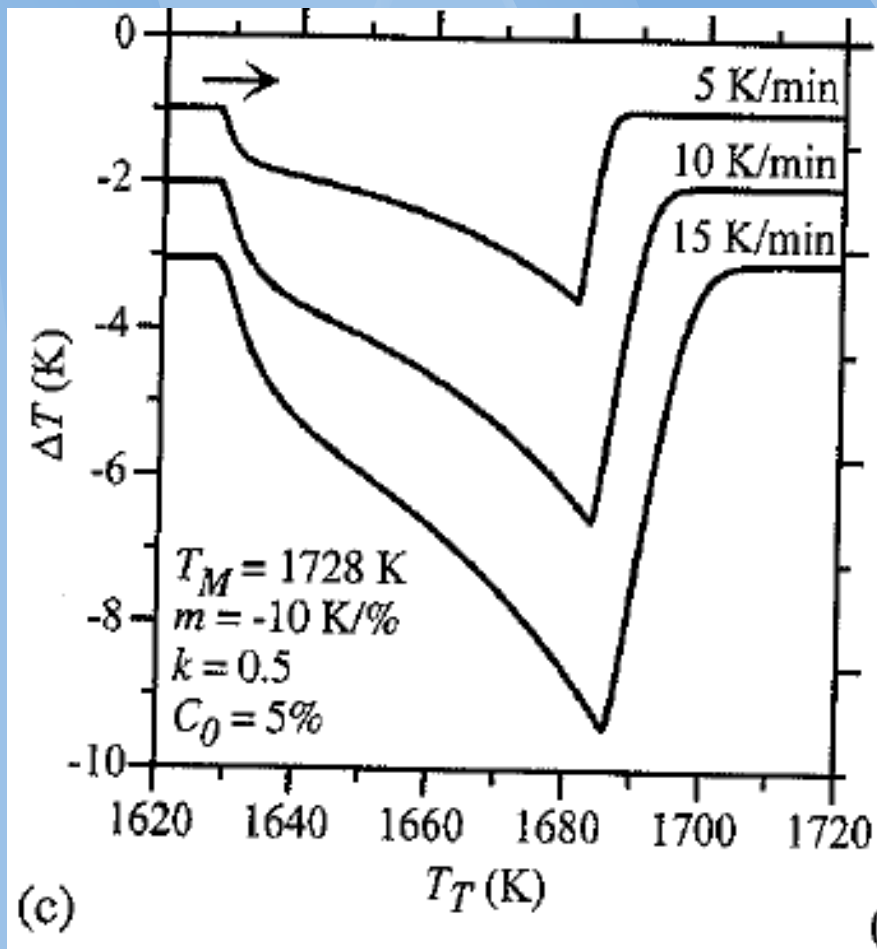
$$k = x_1^s / x_1^l$$

Přerozdělovaná složka

# Tvar signálu DTA (DSC) I-s binární rovnováhy



**Figure 3.13.** Comparison of two hypothetical alloys with identical heat of fusion, liquidus and solidus temperatures but differing having  $k < 1$  and  $k > 1$ . a) Phase diagram, b)  $dH_S / dT_S$  for  $k < 1$  (black) and  $k > 1$  (red), c) DTA for  $k < 1$  and d) DTA for  $k > 1$ . For  $k < 1$ , the latent heat is released higher in the



Častější případ (eutektika)

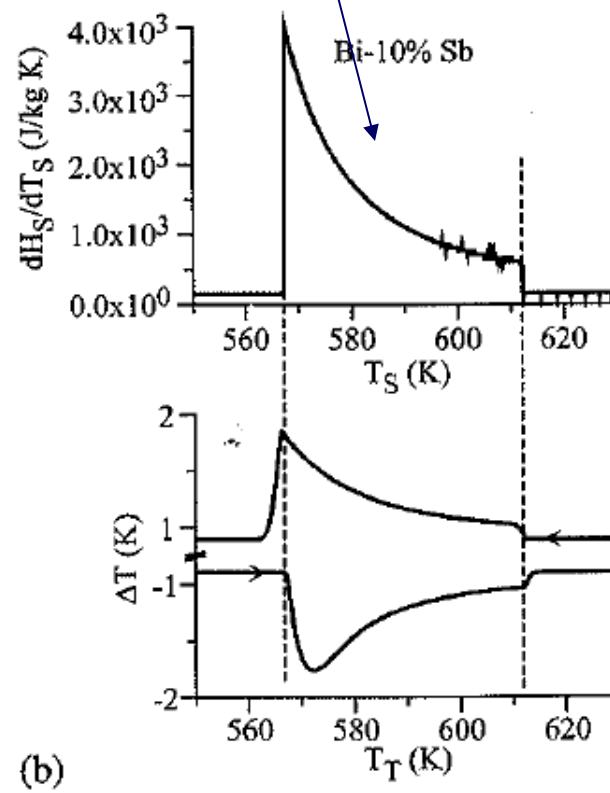
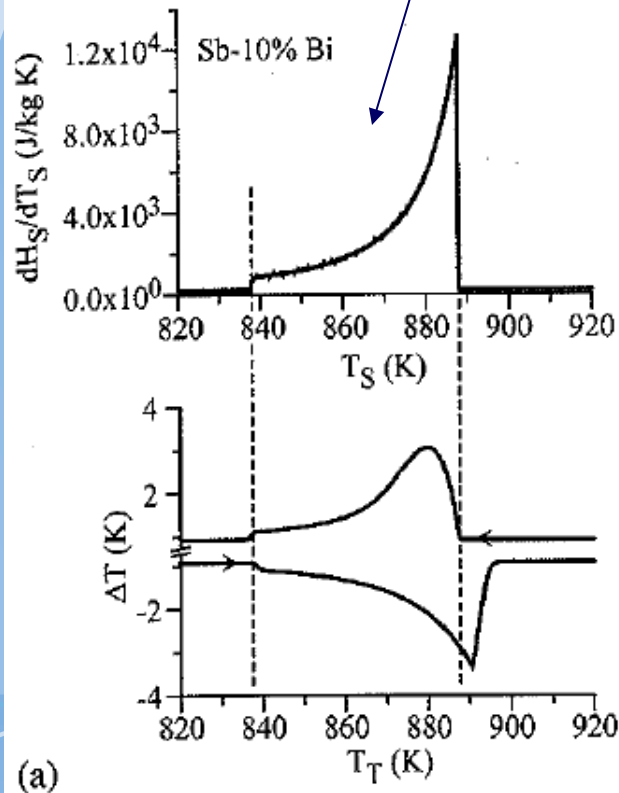
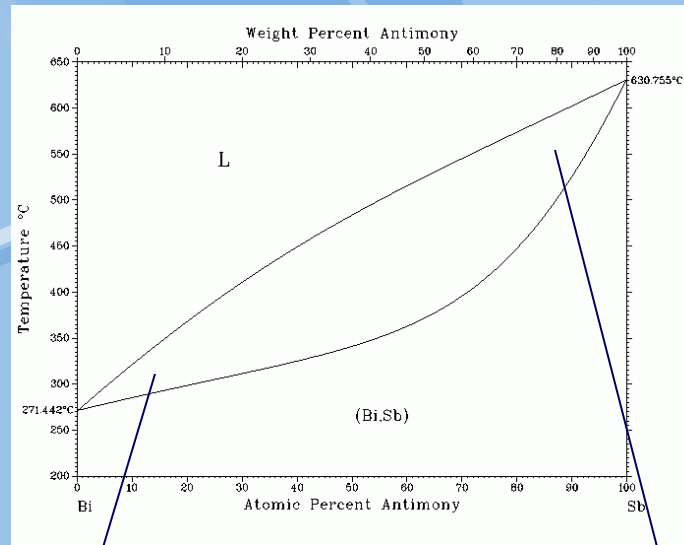
Méně časté (peritektika)

# Sn-Bi

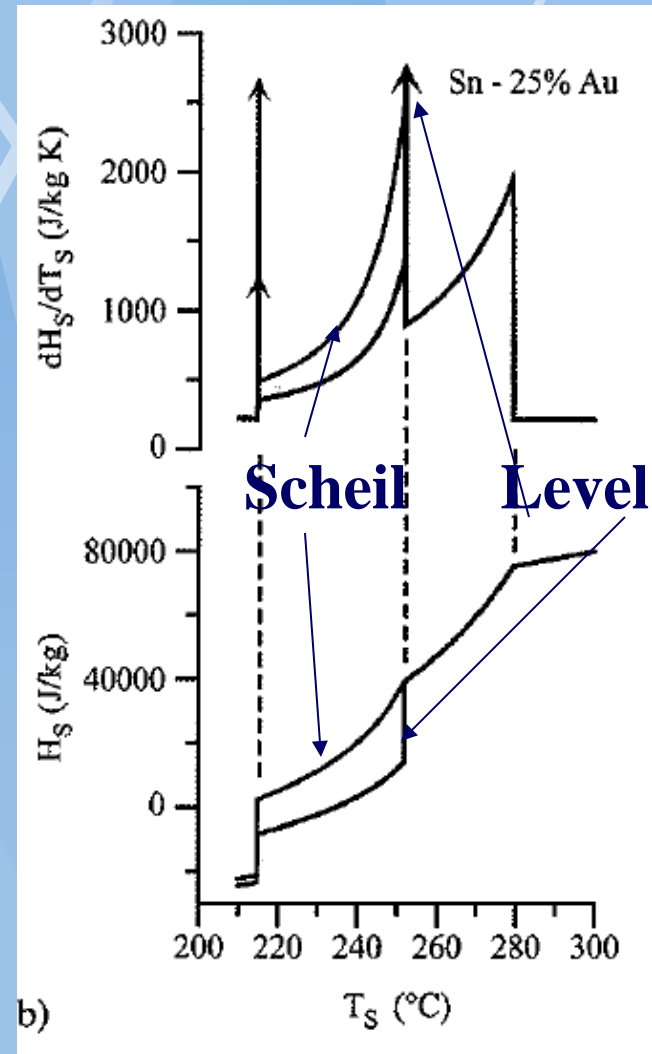
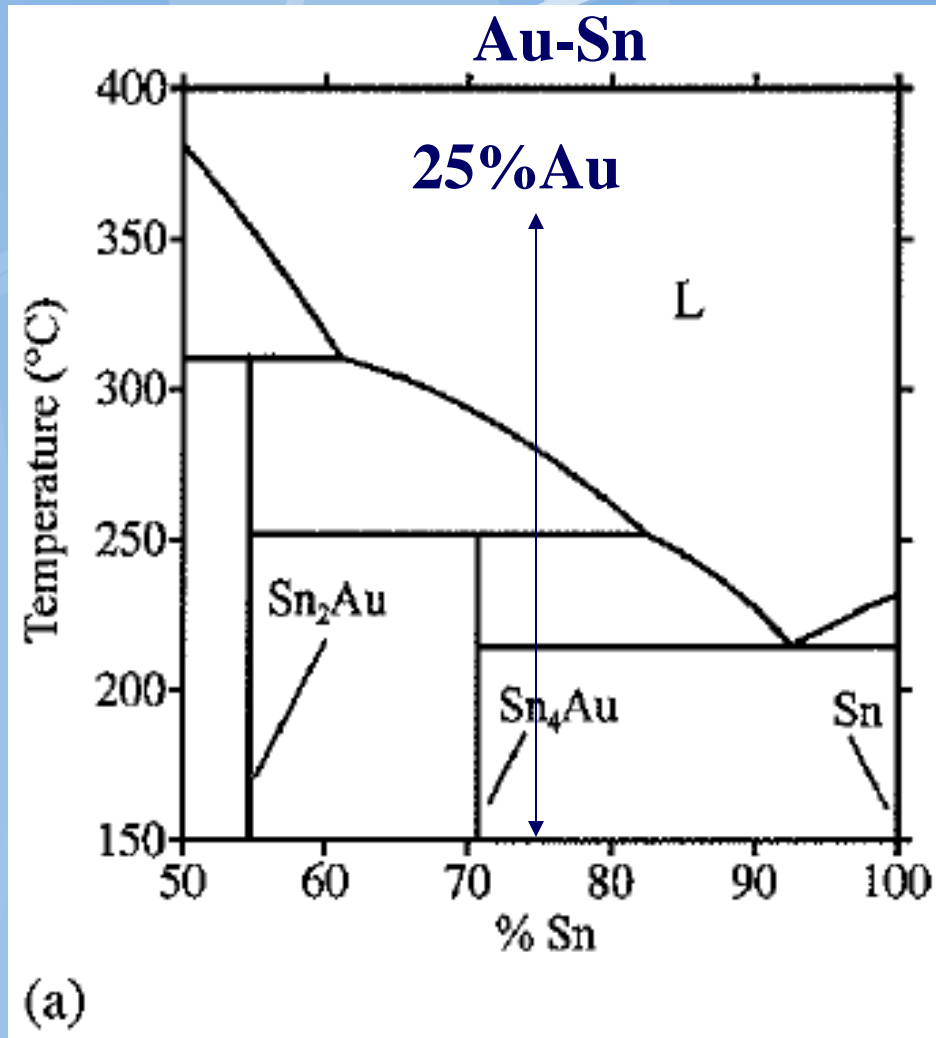
# CALPHAD DATABASE

Sb

Bi

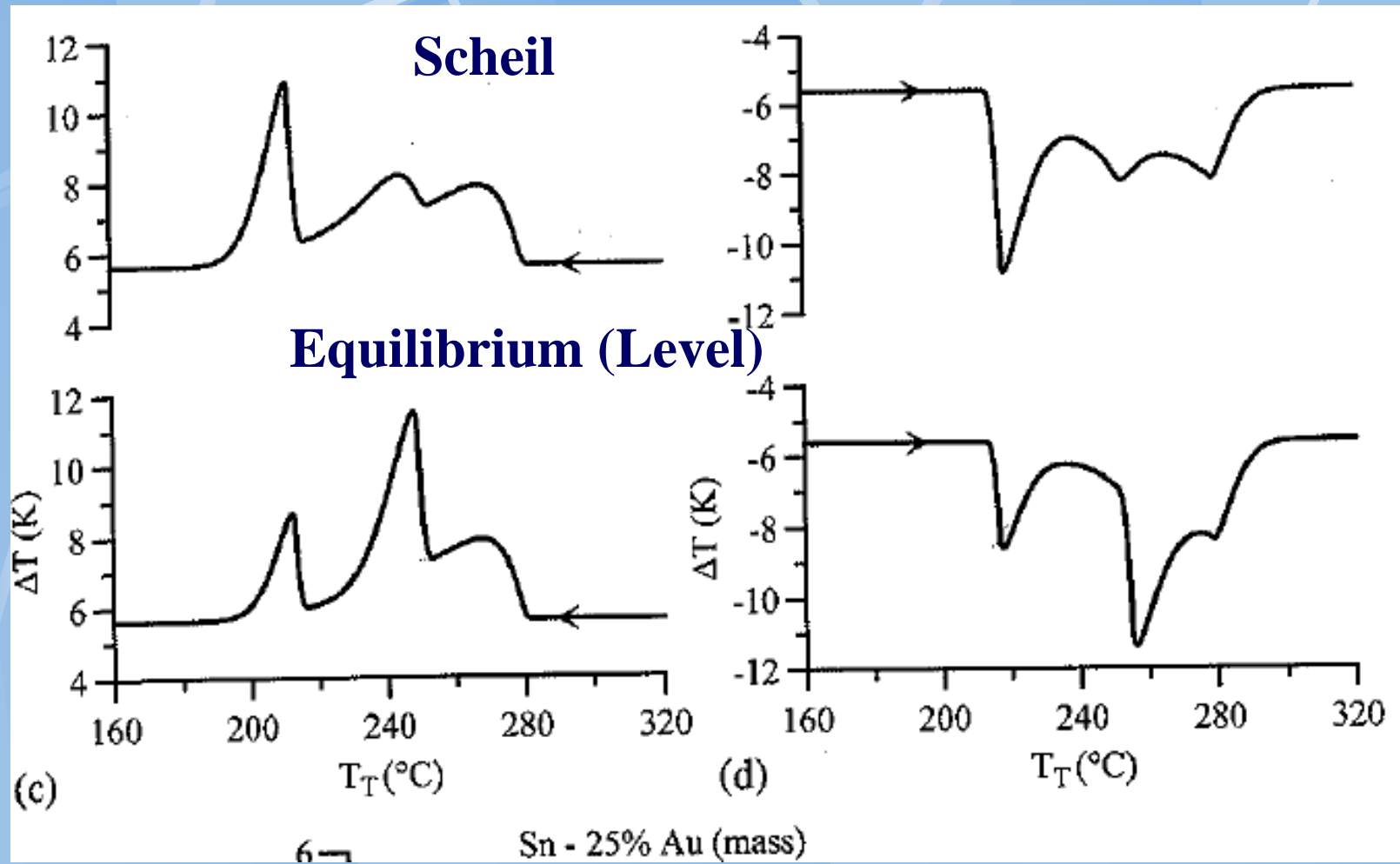


# Eutektické a peritektické reakce



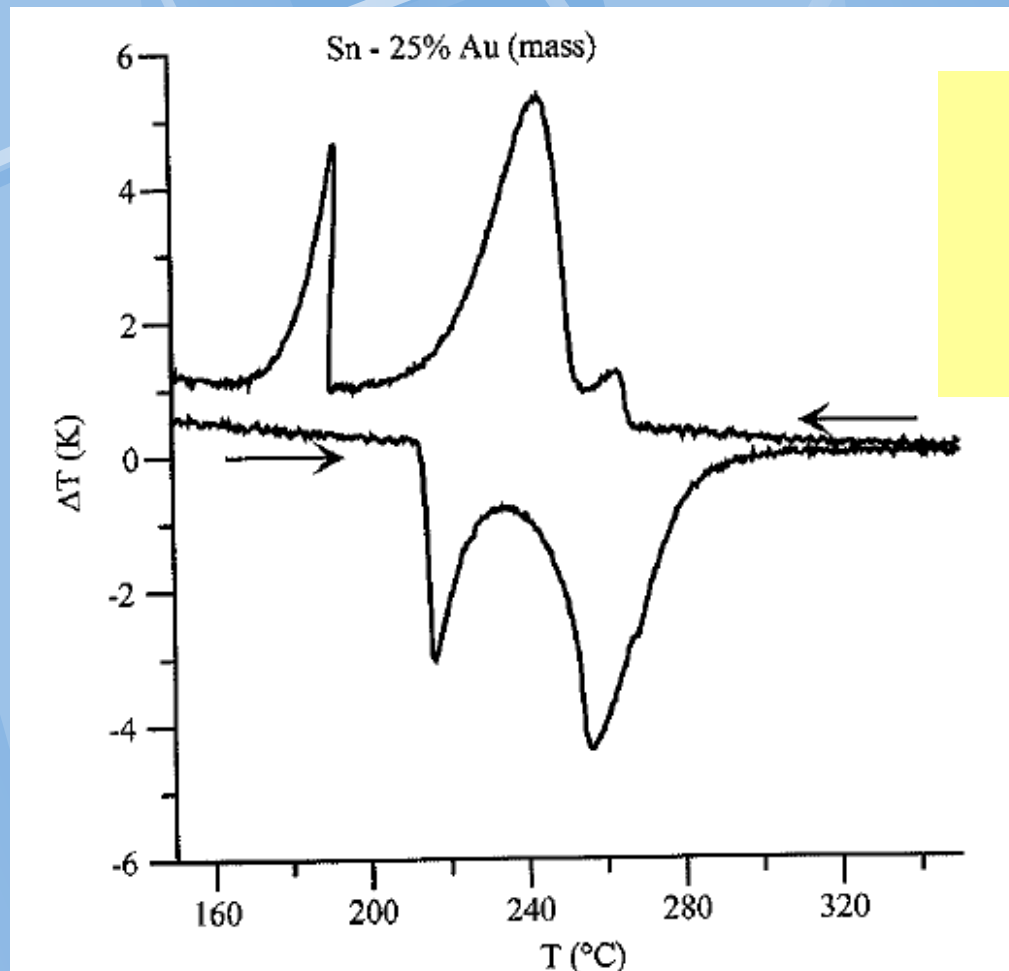
**Pozn.: Equilibrium výpočet = Level**

# Vypočtený signal Au-Sn s uplatněním přístrojových konstant



S přístrojovými parametry pro přenos tepla a jeho  
zpoždění v přístroji

# Reálný signál Sn-25Au



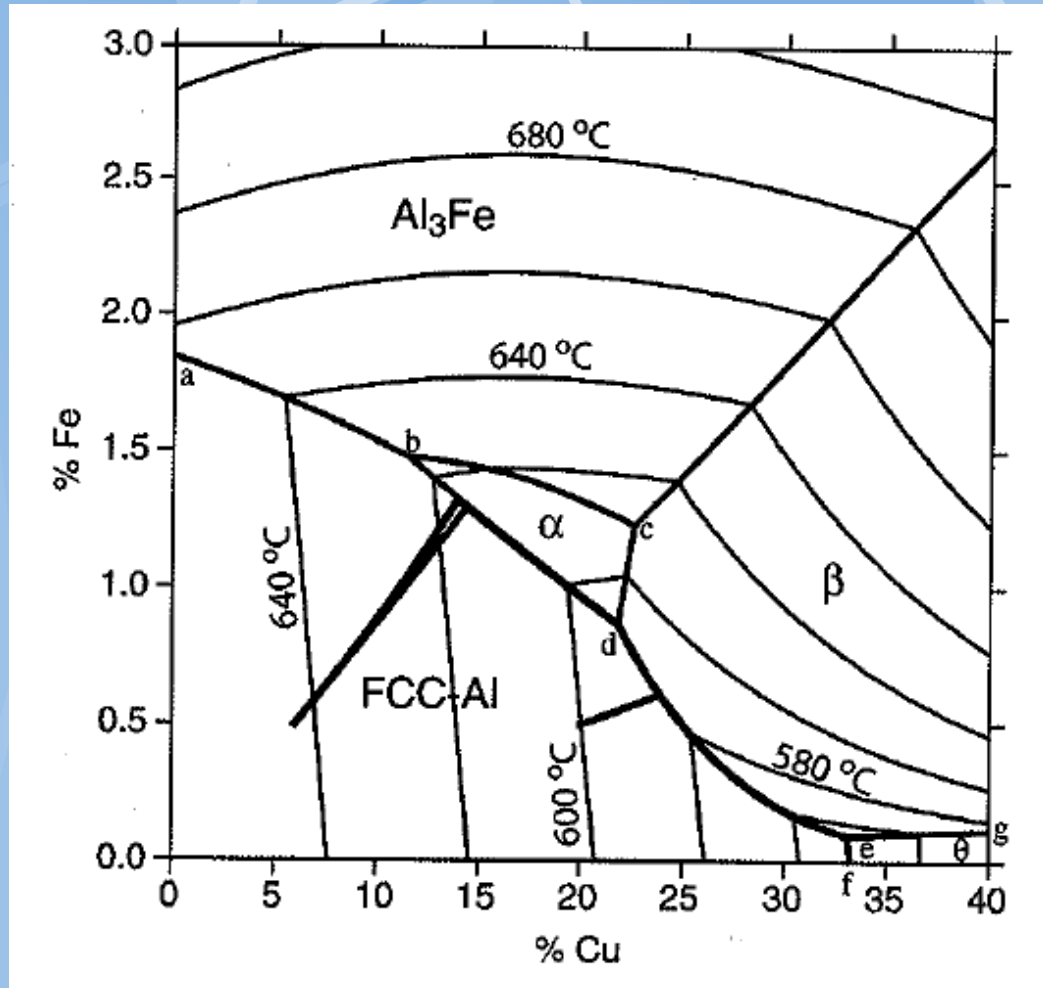
**Signál  
odpovídá  
spíše  
rovnováze**

*e) Experimental melting and freezing curves at 5 K/min.*



# Ternární slitiny

*Liquidus surface of Al-rich corner of Al-Cu-Fe alloy*



*Al - 6% Cu - 0.5% Fe*

*Al-20 wt% Cu- 0.5% Fe*

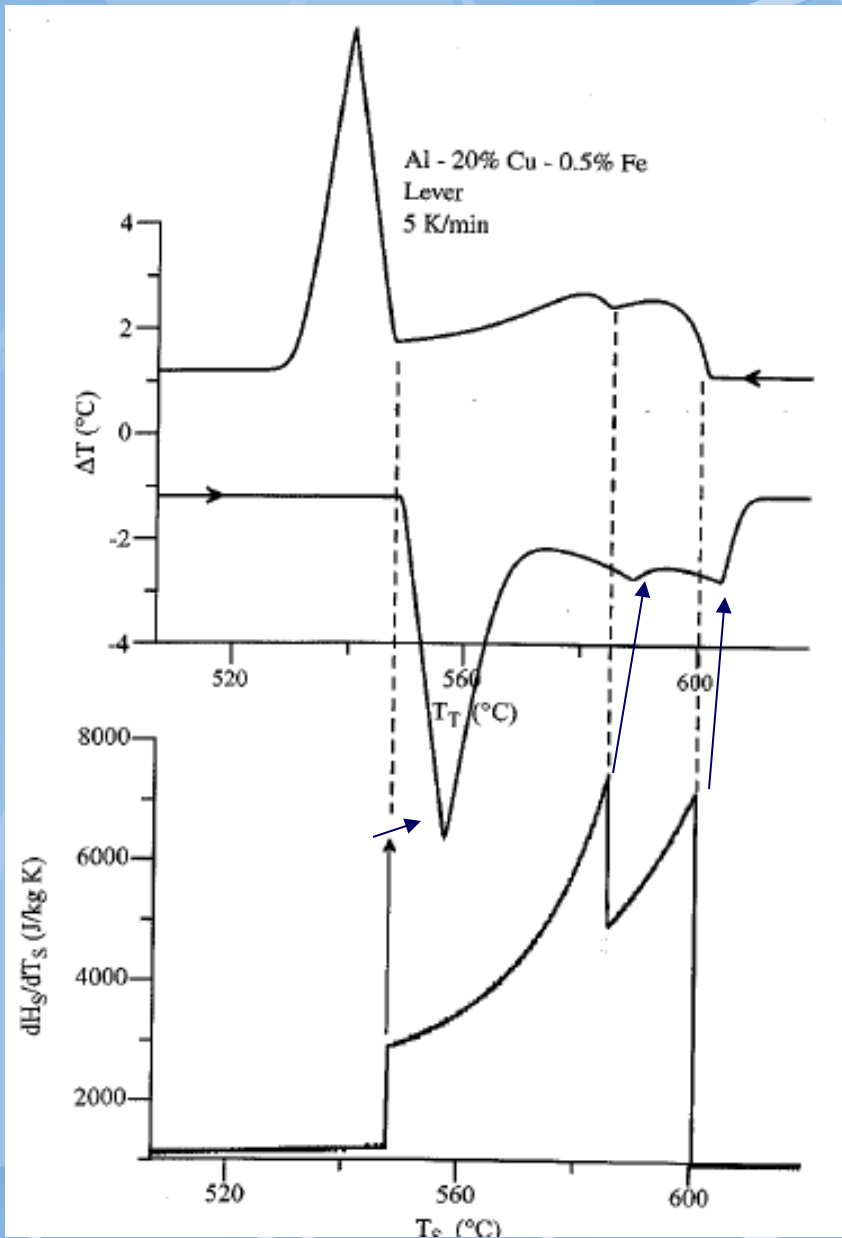
**Scheil a Lever  
aproximace**

# Al-20Cu-0,5Fe

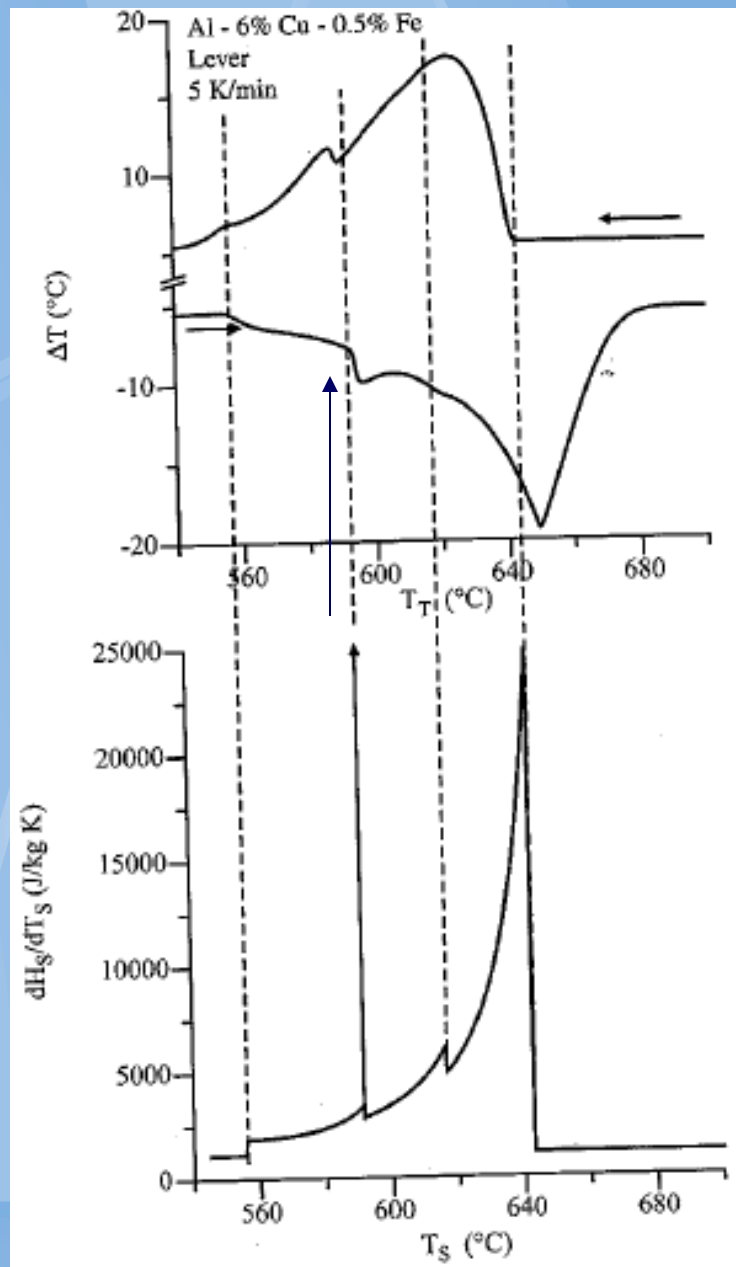
**Reálný  
signál**

$L \rightarrow \text{FCC}$ ,  
 $L \rightarrow \text{FCC} + \text{Al}_7\text{Cu}_2\text{Fe}$ ,  
 $L \rightarrow \text{FCC} + \text{Al}_7\text{Cu}_2\text{Fe} + \text{Al}_2\text{Cu}$ .

**Lever  
(rovnovážný  
výpočet**



# Al-6Cu-0,5Fe – rovnovážná simulace



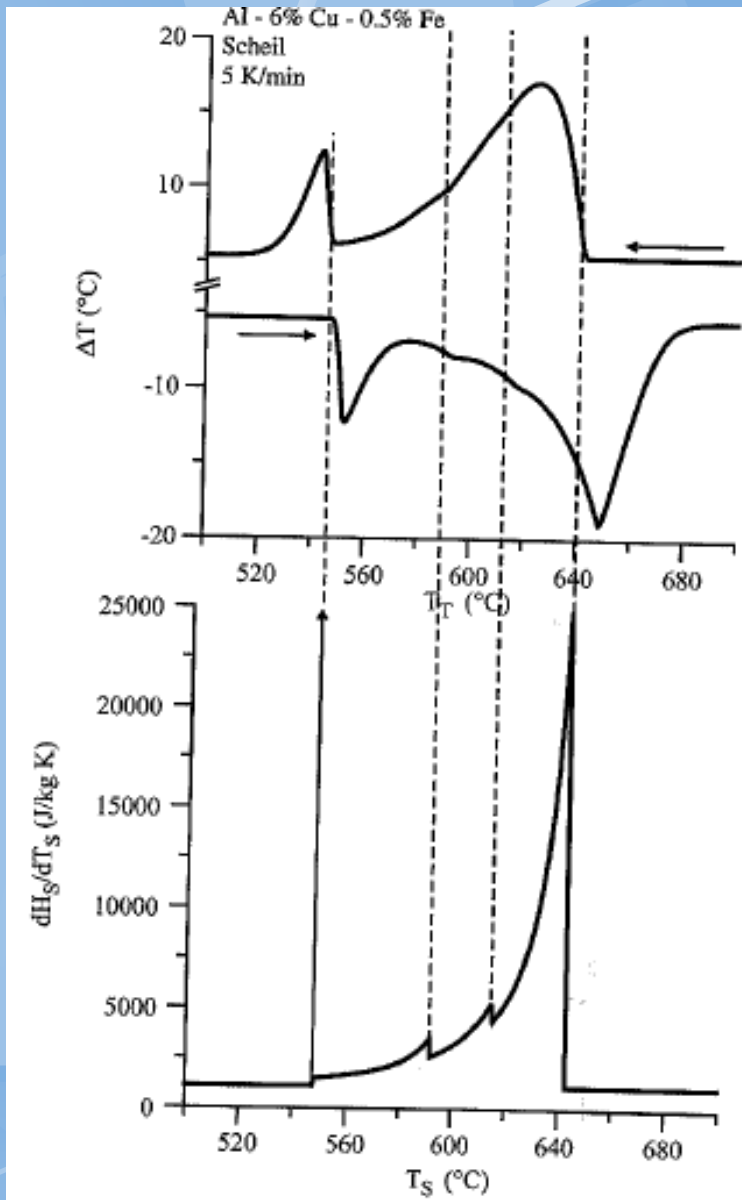
**Reálný  
signál  
5K/min**

L $\rightarrow$ FCC,  
L $\rightarrow$ FCC+Al<sub>6</sub>(Fe,Cu),  
L+Al<sub>6</sub>(Fe,Cu) $\rightarrow$ Al<sub>7</sub>Cu<sub>2</sub>Fe+FCC (invariant); Lever path only.

**Lever  
(rovnovážný  
výpočet**

**Vyhovuje**

# Al-6Cu-0,5Fe – nerovnovážná simulace



**Reálný  
signál  
15K/min**

**Scheil (nerovnovážný  
výpočet)**

**Vyhovuje**

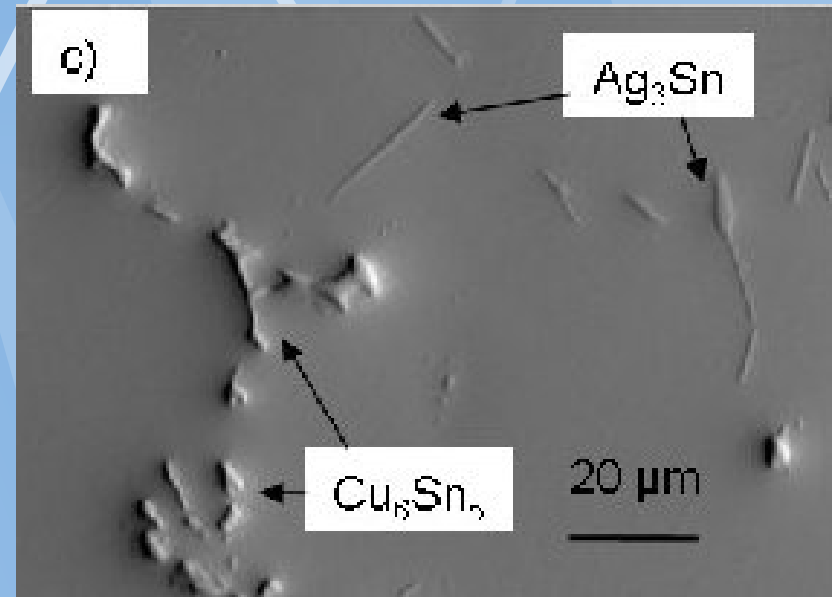
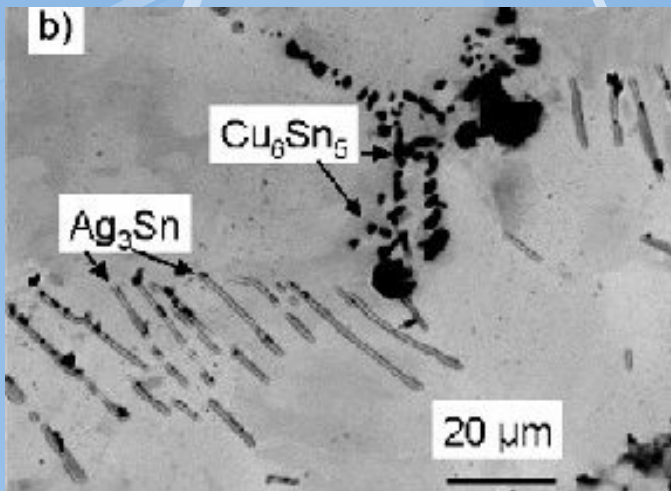
# Přístrojové parametry

## Příklad konstant tepelného zpoždění

	Sn (232°C)			Ag (961°C)			Ni (1453°C)		
Mass (g)	0.163			0.237			0.180		
Heating rate (K/min)	5	10	15	5	10	15	5	10	15
$t_{S,C}$ (s)	13.5	15.3	15.9	6.2	6.7	6.7	6.5	6.0	5.5
$t_{W,C}$ (s)	34.5	29.2	26.3	13.0	12.7	13.1	5.1	5.0	4.7
$t_{T,C}$ (s)	27.6	18.9	17.0	14.5	12.4	11.7	7.4	6.5	6.7
$t_{W,C} / t_{S,C}$	2.56	1.91	1.65	2.10	1.90	1.96	0.78	0.83	0.85

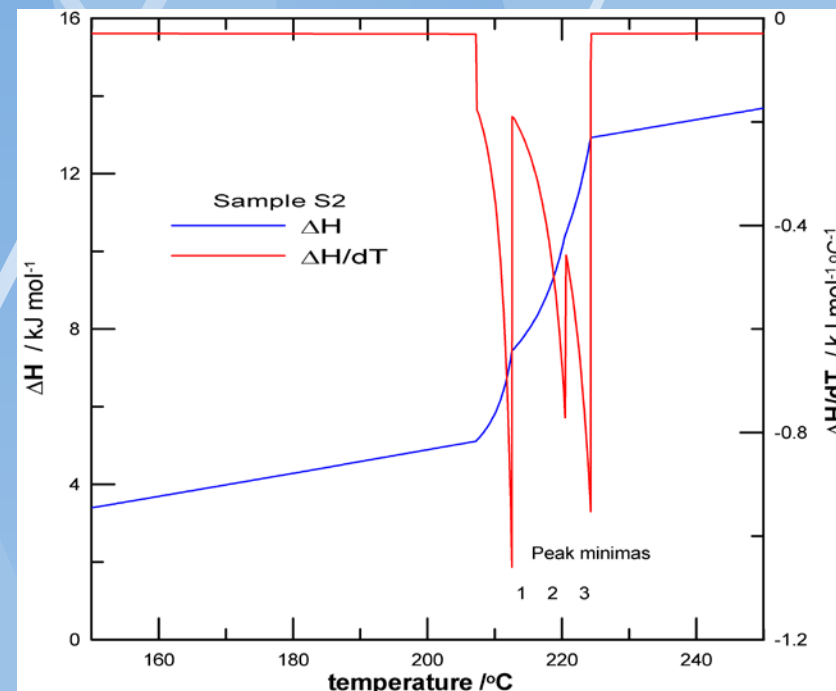
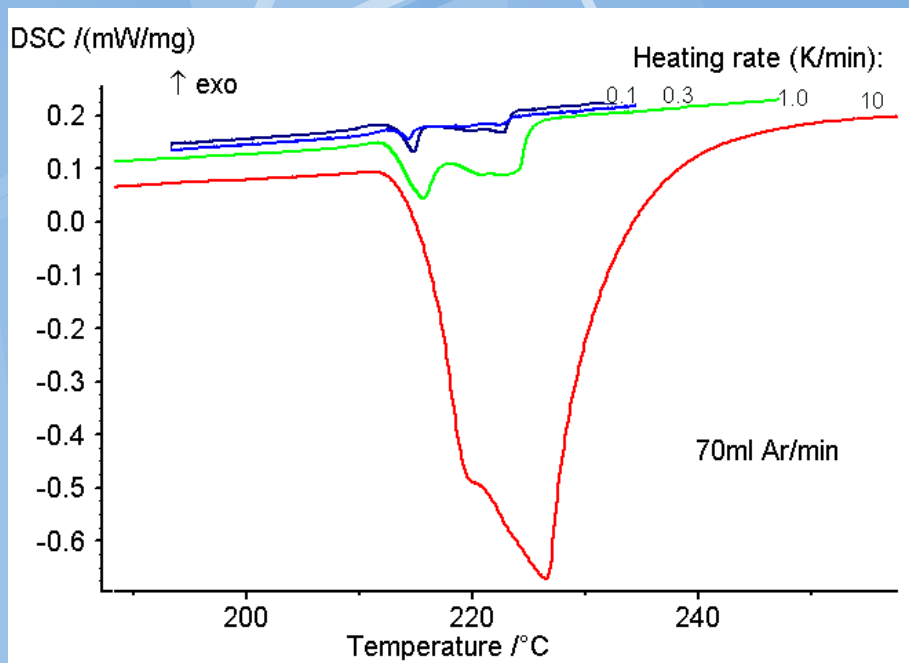
# Vícesložkové slitiny

Slitiny na bázi Sn  
bez olova



Microstructura slitiny Sn-  
3.5%Ag-0,7%Cu-1%Bi.  
Světelná mikroskopie (b), SEM  
(c).

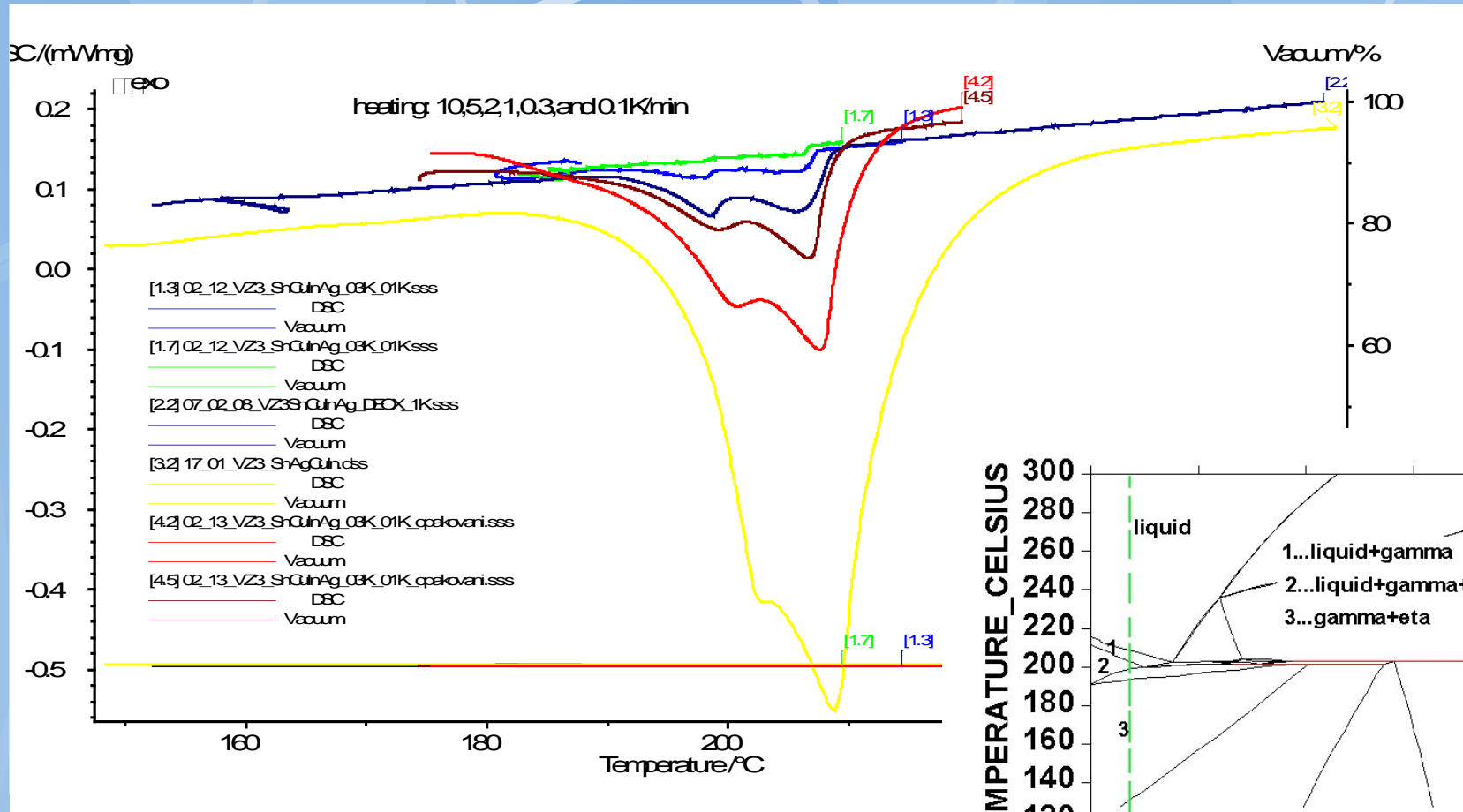
# Simulace DSC křivek



Experimentálně naměřený DSC signál pro různé rychlosti ohřevu slitiny Sn-3.5%Ag-0,7%Cu-1%Bi.

Vypočtená závislost entalpie a tepelné negativní kapacity sledované slitiny.

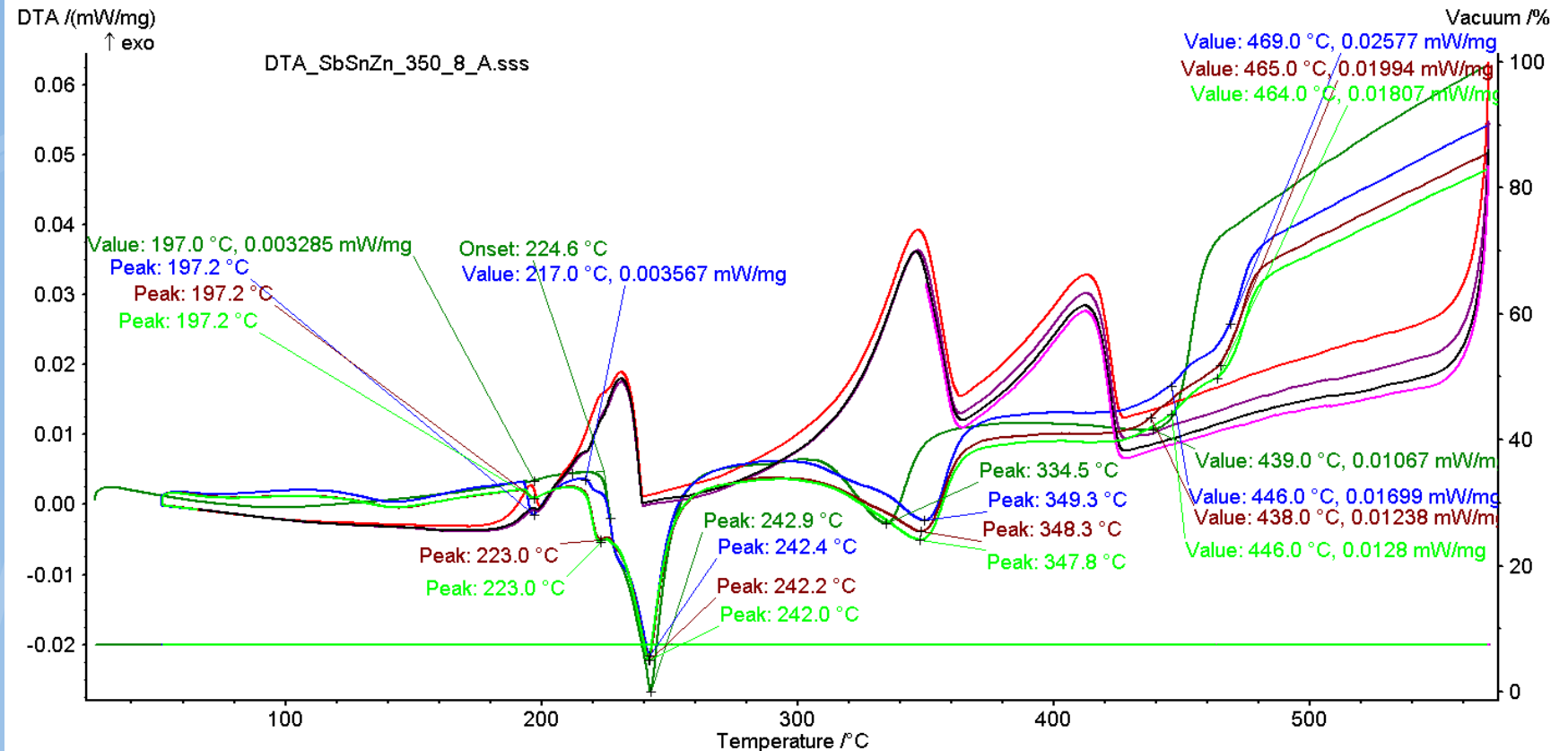
# Termická analýza a temod. rovnováha



**DSC signál slitiny Sn-0,7wt%Cu-1,5%Ag-9,5%In při různých rychlostech ohřevu v korelaci s fázovým diagramem.**



# Diskuze



signál DTA slitiny SbSnZn

# The Calphad Approach

## Phase Equilibria & Thermodynamics

**Experiments**  
DTA, Metallography,  
X-ray Diffraction,  
Calorimetry, EMF,  
Vapor Pressure

Physics-based  
**Model Functions**  
with *Adjustable*  
*Parameters*

**Theory**  
Quantum Mechanics  
Statistical Thermodynamics

Parameter  
**Optimization**  
for *Thermodynamic*  
*Description*

**Thermodynamic**  
**Database**

## Diffusion

**Experiments**  
Tracer, Intrinsic,  
Chemical (Interdiffusion)

**Theory**  
Atomistic  
Calculations

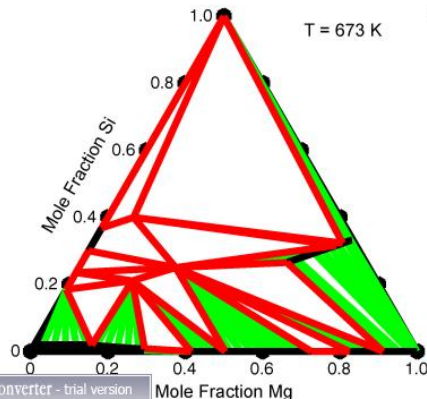
Parameter  
**Optimization**  
for *Diffusion Mobility*  
*Description*

**Diffusion Mobility**  
**Database**

Thermodynamic  
Factor

Thermodynamic  
Factor

**Applications**  
Solidification,  
Phase Transformation Kinetics,  
...



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