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Al-B-C ternary compounds: synthesis, structure, composition and thermal stability

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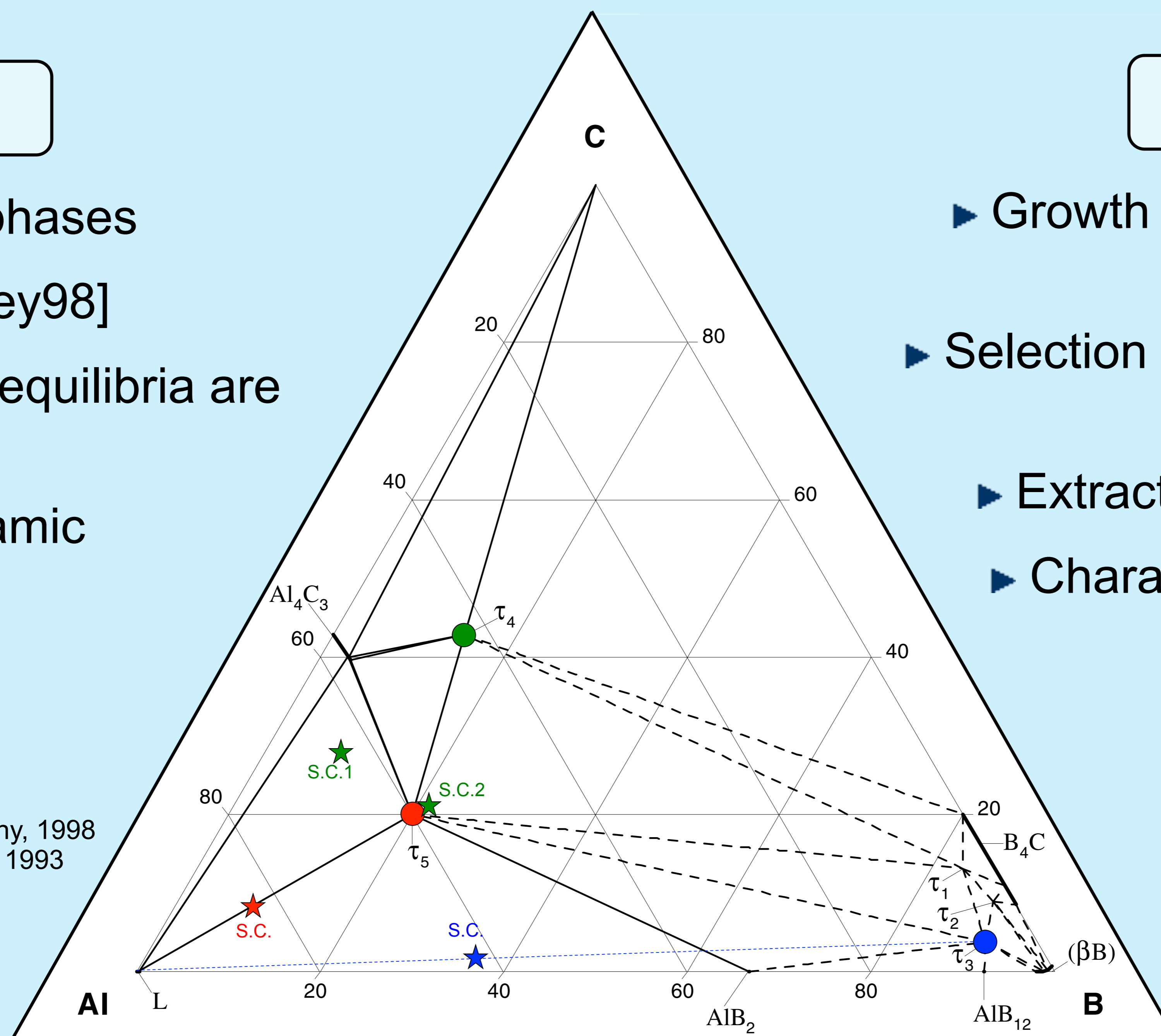
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The Al-B-C system

- ▶ 5 stoichiometric ternary phases
- ▶ Structures are known [Mey98]
- ▶ High temperature phase equilibria are mostly **unknown**
- ▶ **No** complete thermodynamic assessment [Wen93]

Synthesis of phases

- ▶ Growth in Al melt between 1273 and 1800 K
- ▶ Selection of compositions in dedicated triangles
- ▶ Extraction by selective acid etching
- ▶ Characterization of crystals : DRX, Raman, EDX, DTA, DSC-Cp



N.B. : each starting composition used is given with a star and the S.C. label (color code)

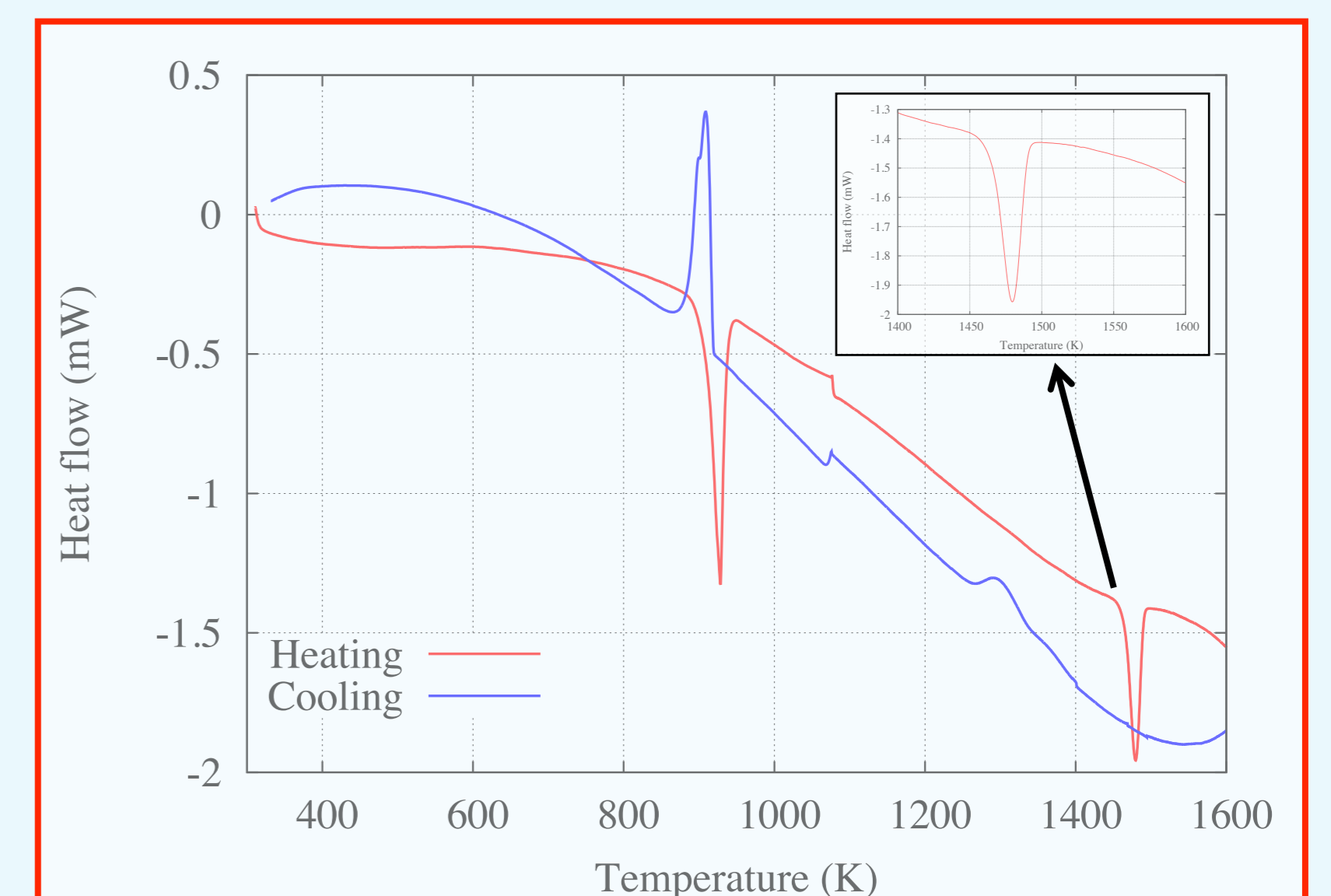
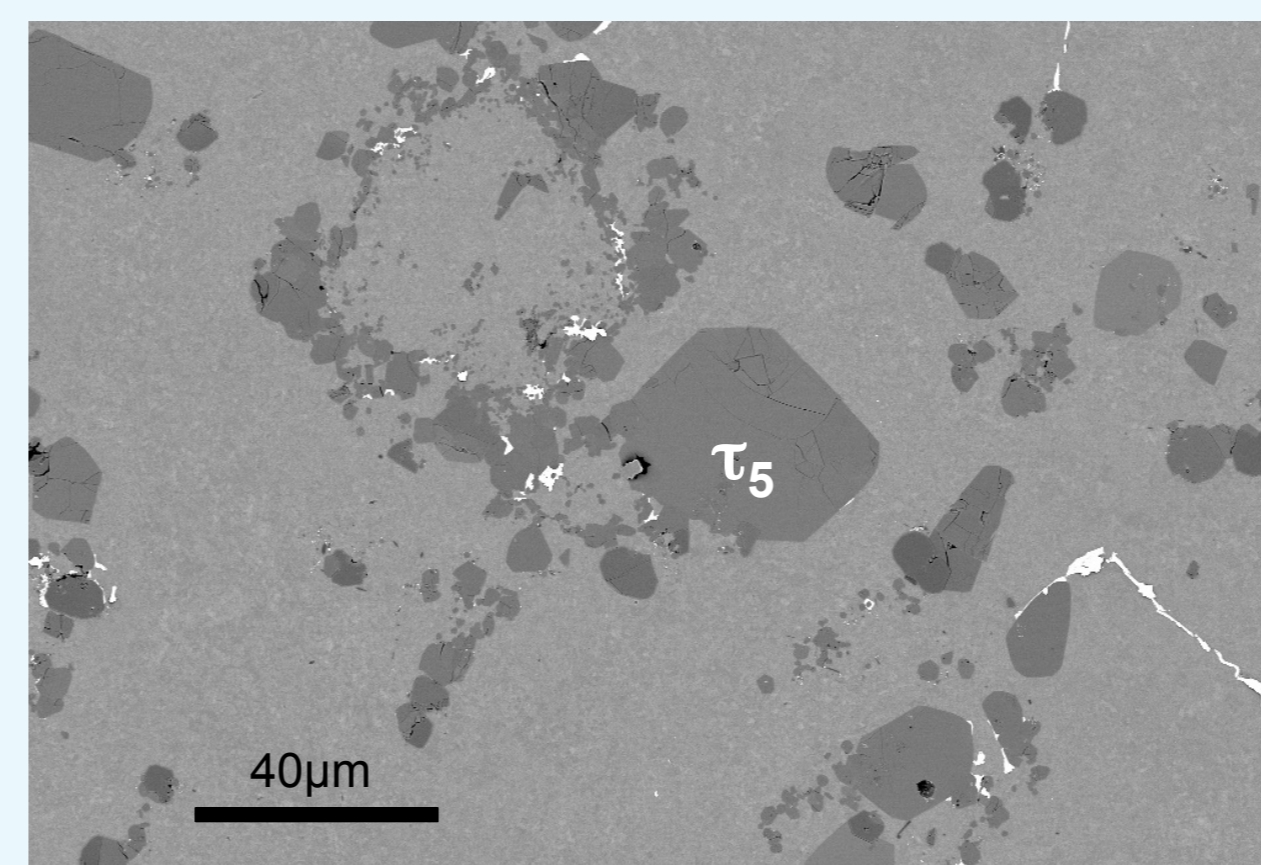
Isothermal section at 900 K according to [Gry04]

References

[Mey98] Meyer F.D., Thesis, Univ. Freiburg, Germany, 1998
 [Wen93] Wen, H., Thesis, Univ. Stuttgart, Germany, 1993
 [Gry04] A. Grytsiv and P. Rogl, G. Effenberg (ed.)
 MSI Eureka in SpringerMaterials (2004)
 [Gon93] J. Gonzalez-Reyes, Thesis INSA-Lyon,
 France (1993)

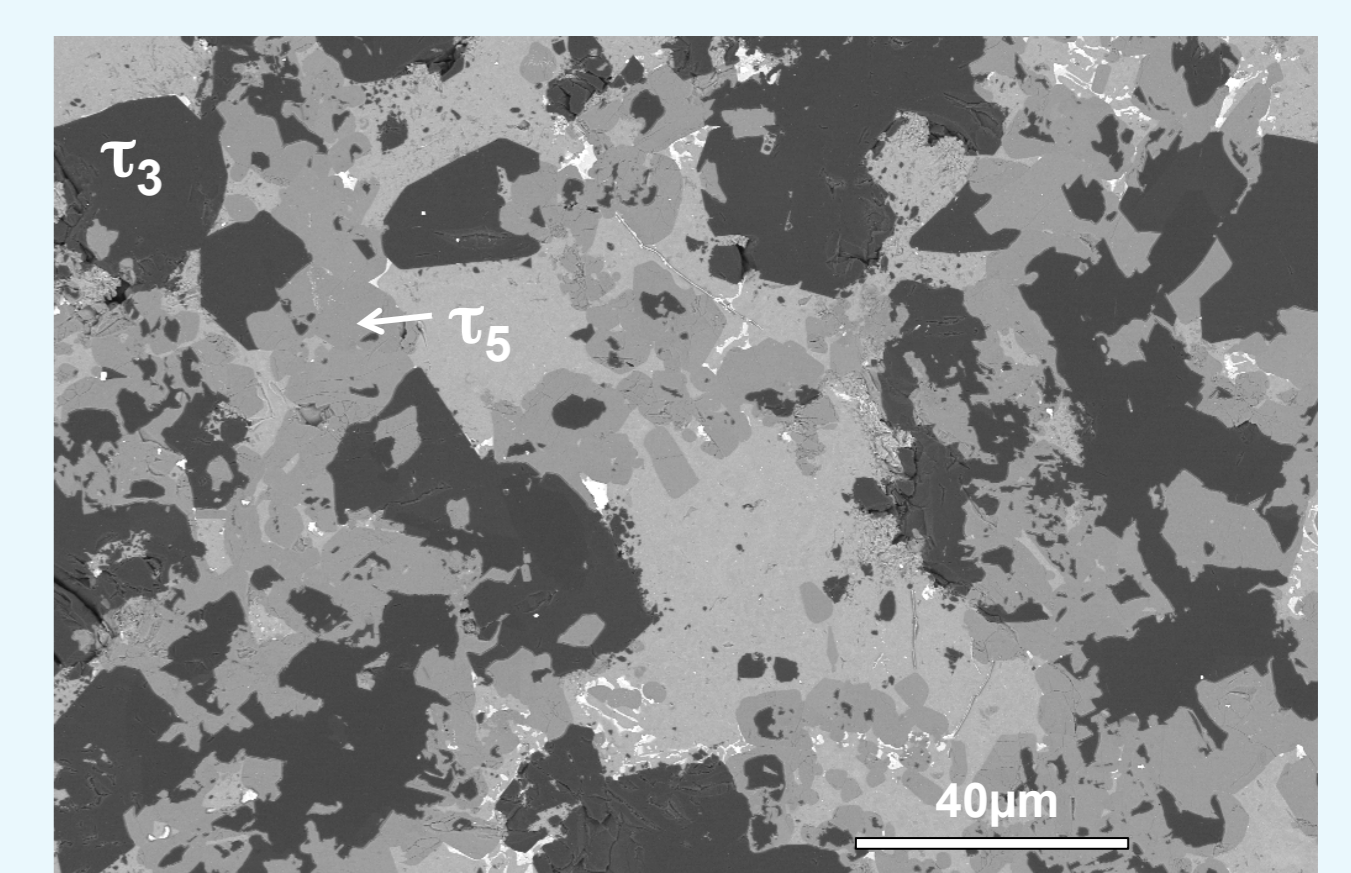
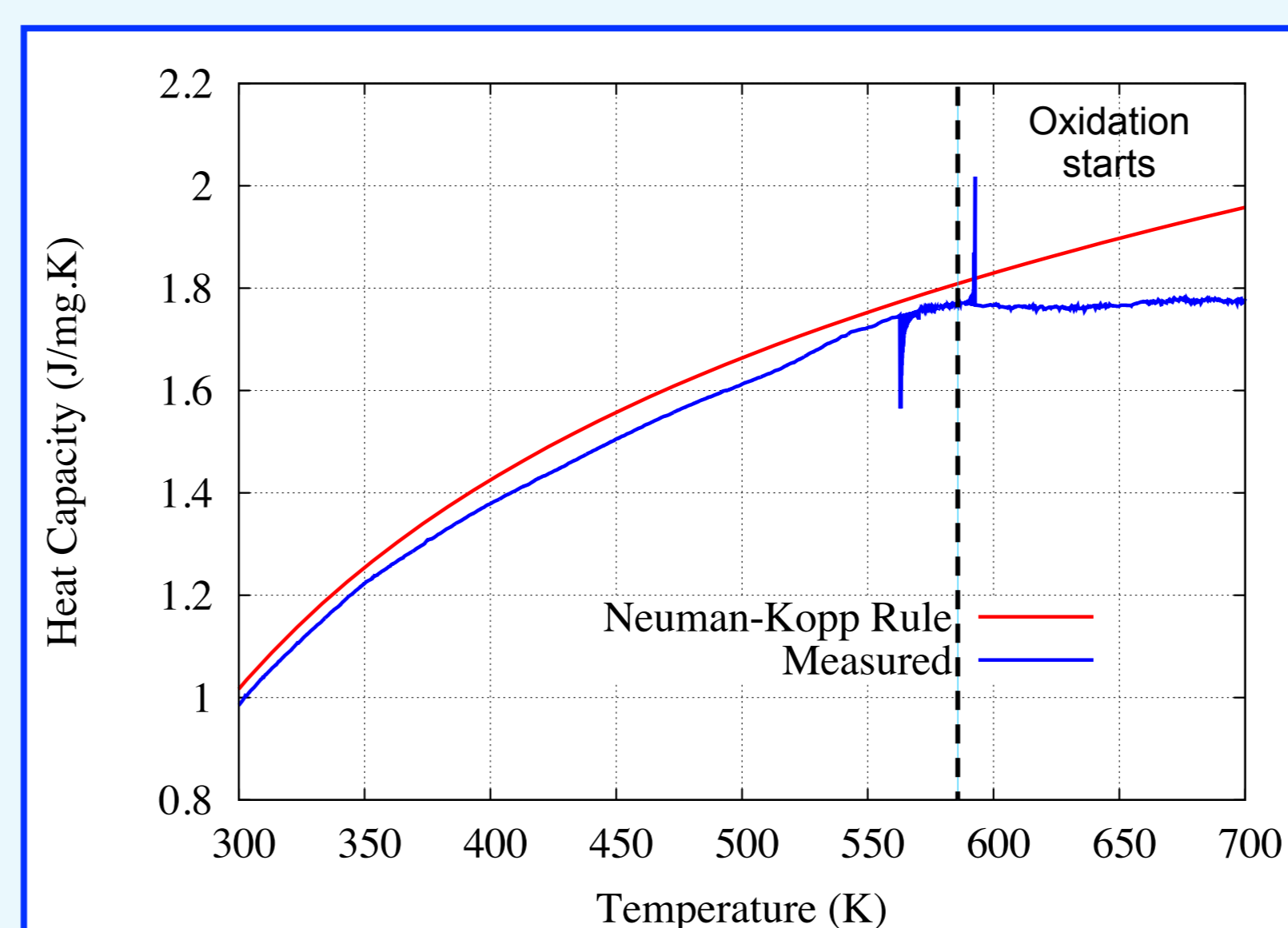
τ_5 - Al_3BC

- ▶ 340h at 1173 K - Al_2O_3 crucible
- ▶ TGA-DSC - 10 K.min⁻¹: decomposition at 1465 ± 10 K
- (reported as in between 1273-1800 K [Gon93])



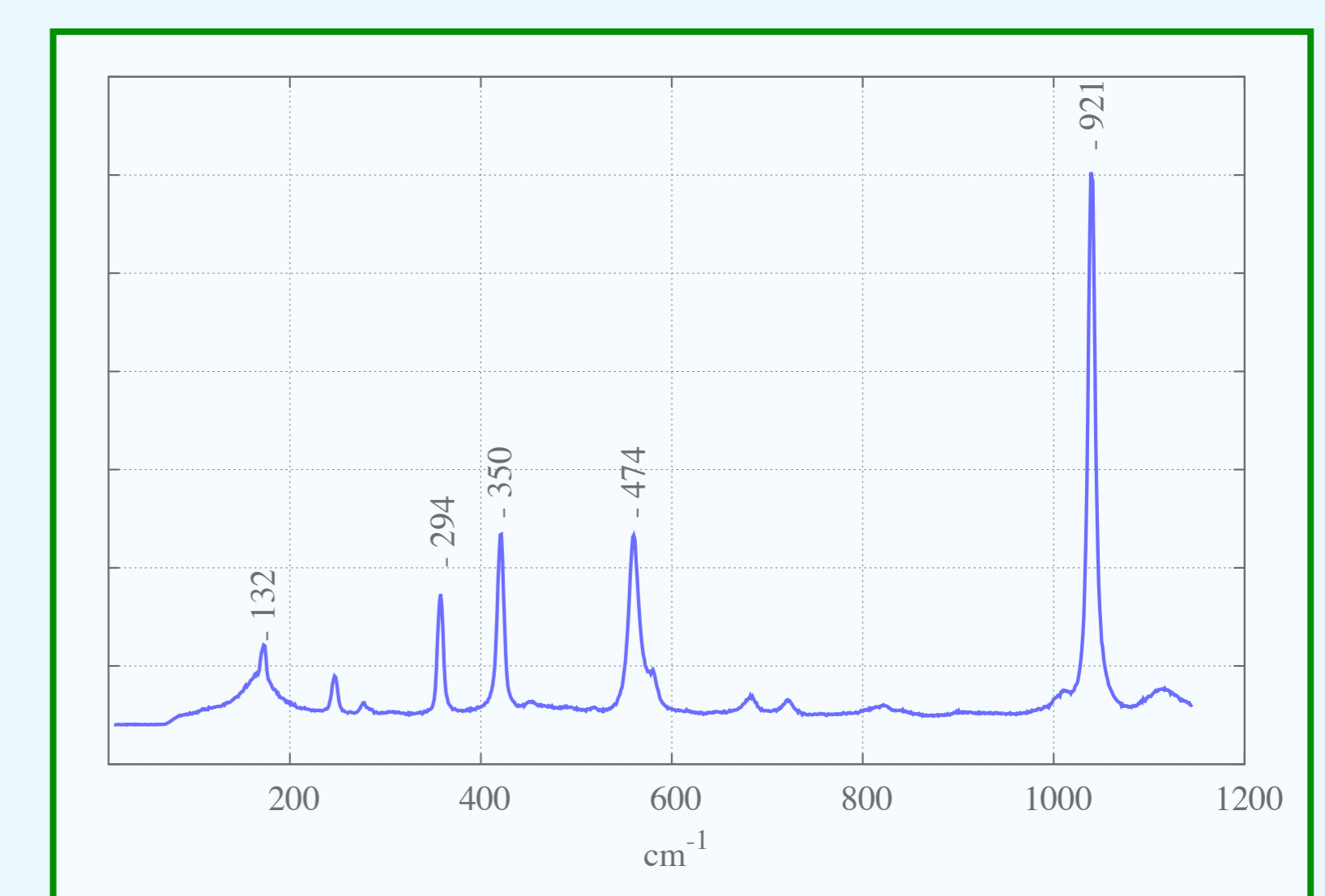
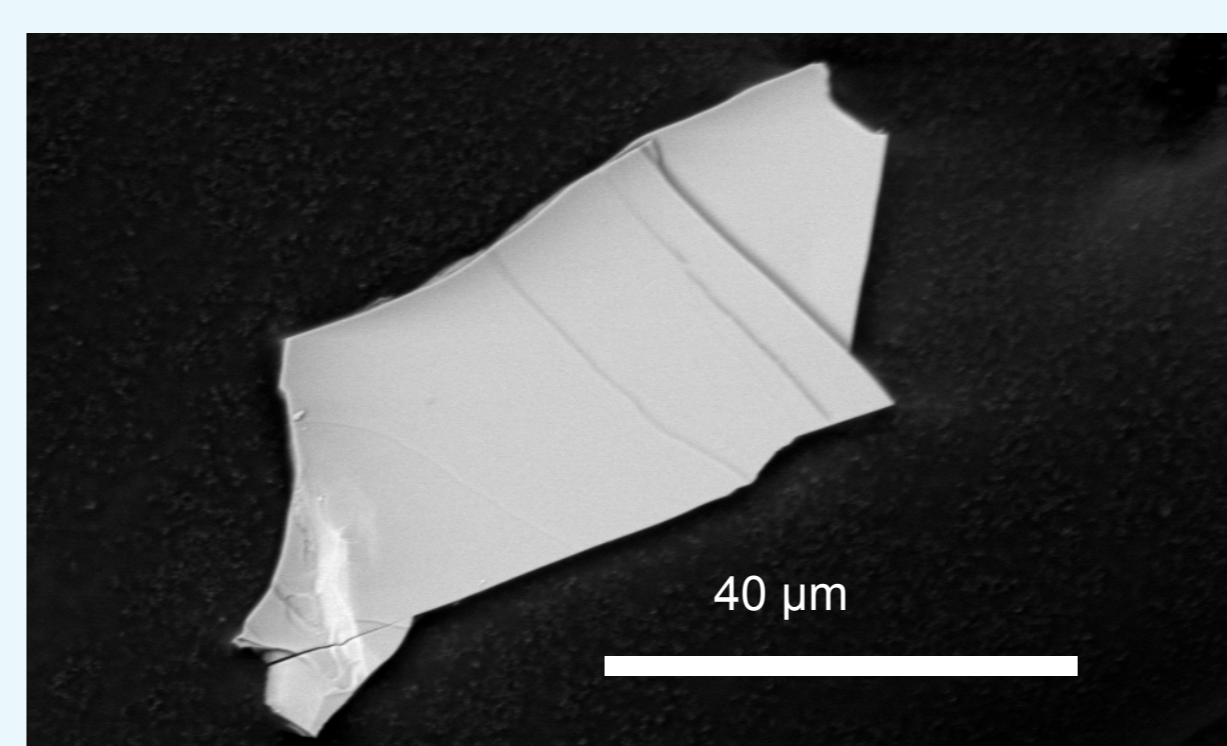
τ_3 - $Al_3B_{48}C_2$

- ▶ 1173 K - 360h - Al_2O_3 crucible
- ▶ Al - τ_3 - τ_5 at equilibrium, only τ_3 after HCl etching
- ▶ Heat capacity measured from 0 to 573 K by sapphire method



τ_4 - Al_3BC_3

- ▶ Arc melting + 1973 K - 30 min in Graphite
- ▶ Same composition in equilibrium with Al_4C_3 and with τ_1 : stoichiometric compound
- ▶ XRD and Raman spectroscopy on single crystal : structure is confirmed [Mey98]



Under progress and Future Work

- ▶ DFT calculations of ΔH_{298K}
- ▶ Heat capacity measurement on τ_4
- ▶ Synthesis and characterization of τ_1 and τ_2
- ▶ Decomposition of phases by DTA (high temperature)
- ▶ Thermodynamic optimization of the Al-B-C system