



20th DISCUSSION MEETING ON THERMODYNAMICS OF ALLOYS
20 - 24 September 2026
BLED - SLOVENIA

EXPERIMENTAL INVESTIGATION OF PHASE EQUILIBRIA AND THERMODYNAMIC DESCRIPTION OF B-NB-TA SYSTEM

Viera Homolová, Lucia Čiripová, František Kromka

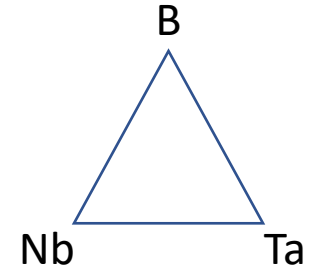


Institute of Materials Research, Slovak Academy of Sciences

Outlines

- Introduction to the System
- Binary subsystems
- Experimental Results and Modeling of the Ternary System
- Conclusions

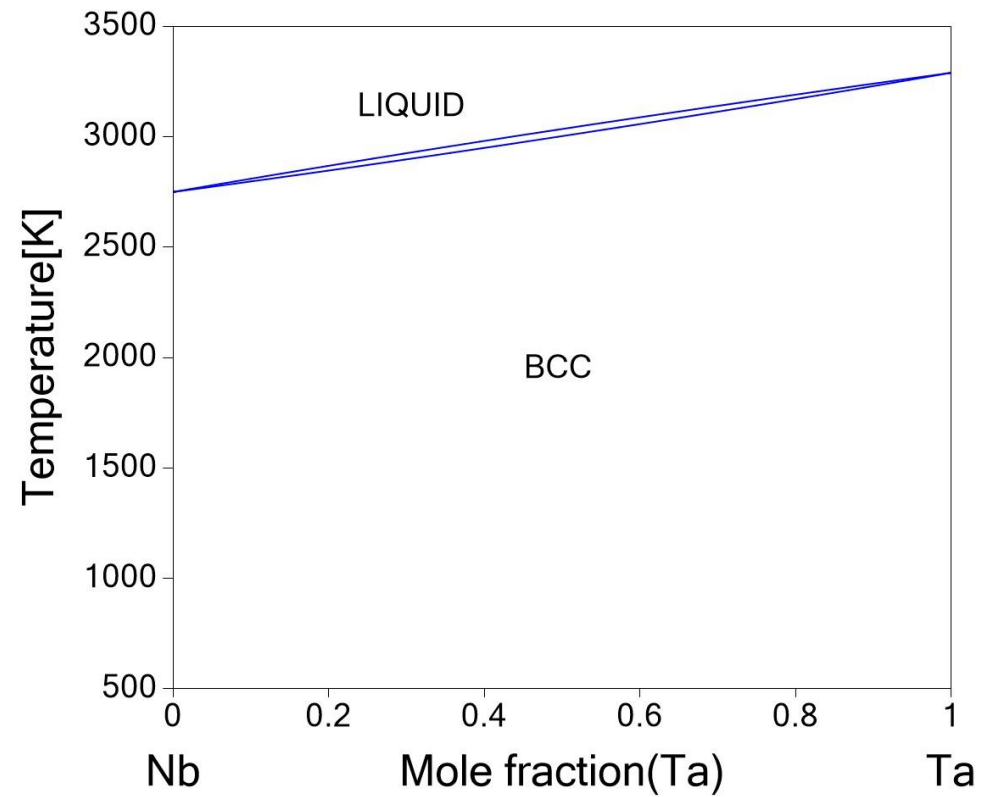
Introduction to the B-Nb-Ta System



- *Ternary refractory metal–boron system*
- *Relevant for the development of advanced high-temperature and wear-resistant materials*
- *Formation of Nb and Ta borides characterized by:*
 - *high melting temperatures*
 - *high hardness, mechanical strength, and wear resistance*
 - *high thermal stability and good chemical stability*
- *Limited information on the ternary B–Nb–Ta system*
- *Aim: experimental investigation of phase equilibria and development of a thermodynamic description of the ternary system*

Binary subsystems

Nb-Ta

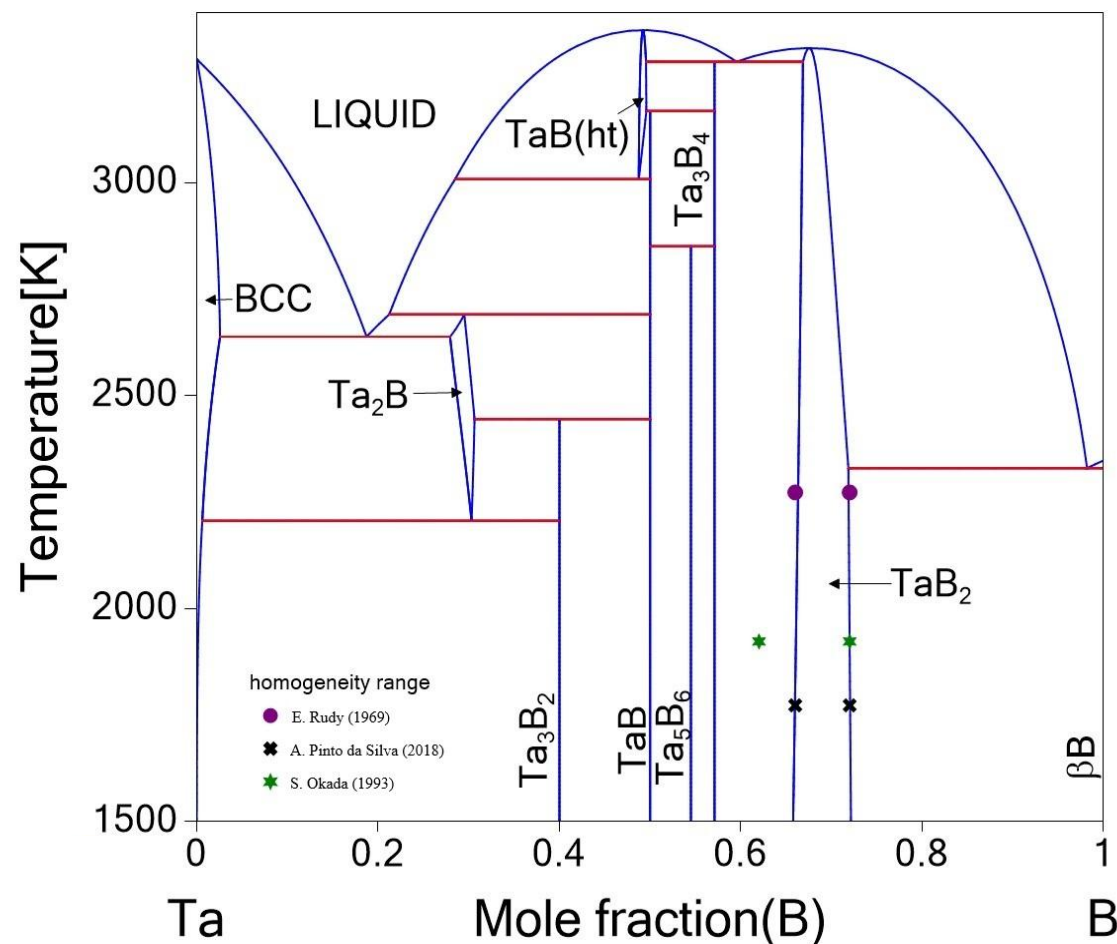


Data used for the calculation were taken from K. C. H. Kumar, T. Van Rompaey, P. Wollants, Thermodynamic Calculation of the Phase Diagram of the Co-Nb-Ta System, Z. Metallkunde, 93 (2002), 1146-1153



Binary subsystems

B-Ta

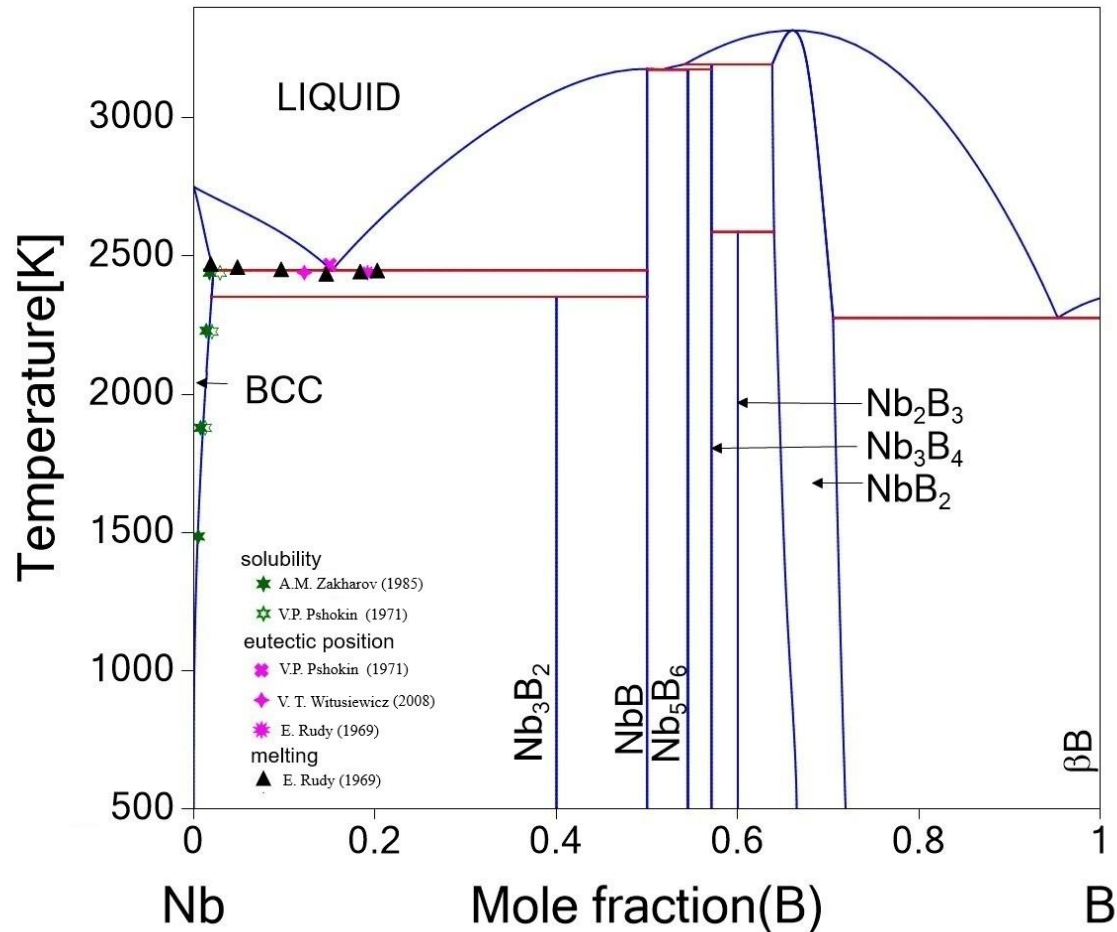


- Starting parameters: A. A. Pinto da Silva, F. Ferreira, B. B. de Lima-Kühn, G. C. Coelho, C. A. Nunes, P. Vilasi, J.-M. Fiorani, N. David, M. Vilasi, The Ta-B system: Key experiments and thermodynamic modeling, Calphad 63 (2018), 107-115
- The parameters for TaB₂ were optimized to achieve compatibility with NbB₂

Phase	Pearson symbol	Space group	Structure type
βB	hR105	R3m	B
Ta-bcc	cI2	Im $\bar{3}$ m	W
Ta ₃ B ₂	tP10	P4/mbm	U ₃ Si ₂
TaB	oC8	Cmcm	CrB
TaB(ht)	oP8	Pnma	FeB
Ta ₅ B ₆	oC22	Cmmm	Ta ₅ B ₆
Ta ₃ B ₄	oI14	Immm	Ta ₃ B ₄
Ta ₂ B	tI12	I4/mcm	Al ₂ Cu
TaB ₂	hP3	P6/mmm	AlB ₂

Binary subsystems

B-Nb



- Starting parameters: Y. Nakama, H. Ohtani, M. Hasebe, Thermodynamic Analysis of the Nb–Ti–B Ternary Phase Diagram, Mater. Trans. 50 (2009), 984-993
- BCC was re-modeled from $(\text{Nb},\text{B})_1(\text{Va})_3$ to $(\text{Nb})_1(\text{B},\text{Va})_3$
Boron was modeled as an interstitial element in the BCC solid solution
- Nb_3B_2 was slightly modified

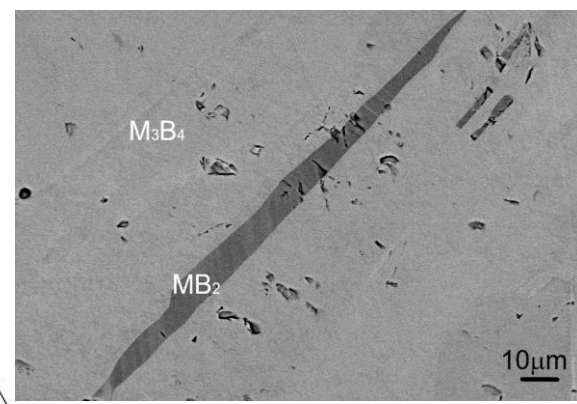
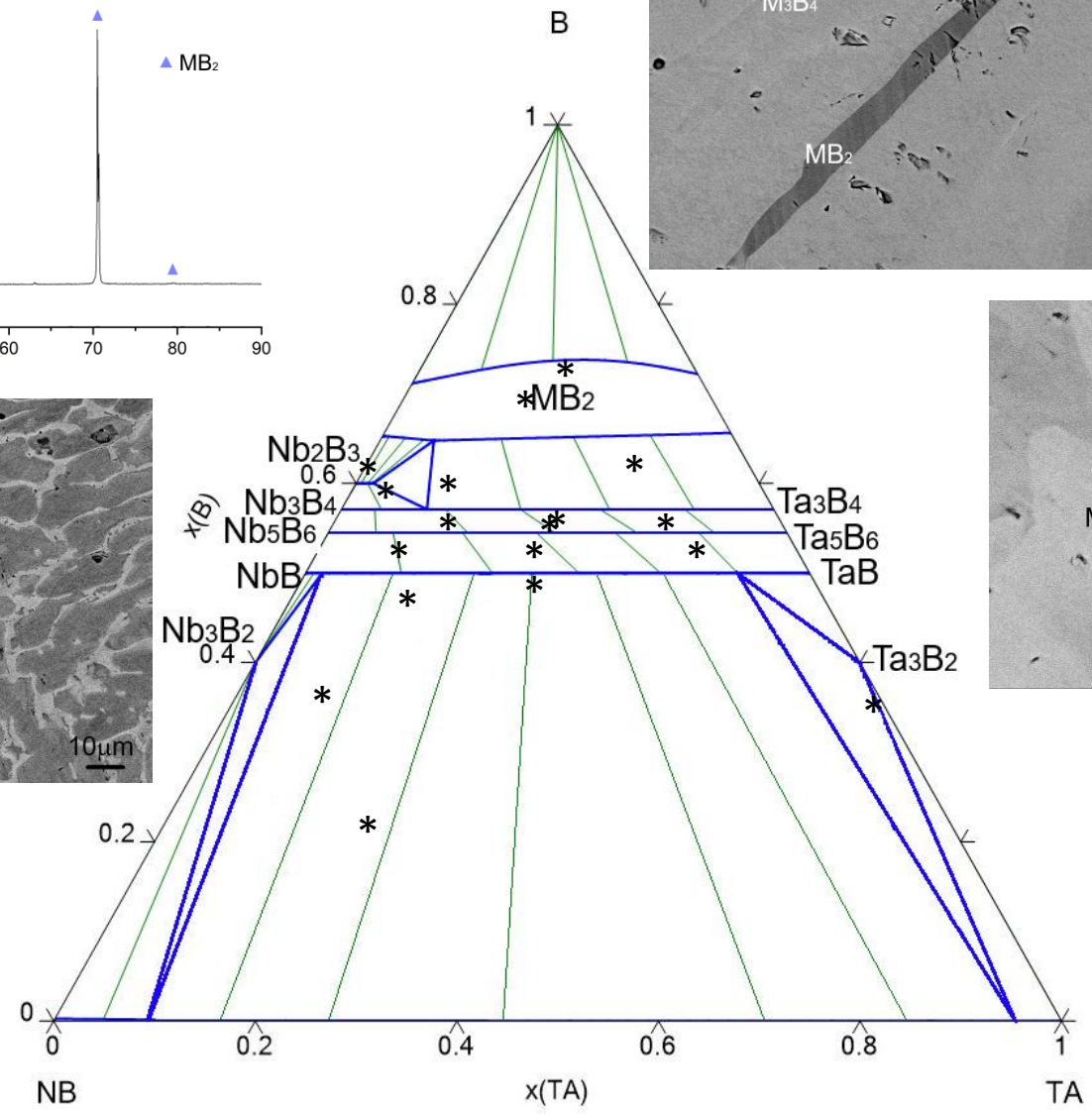
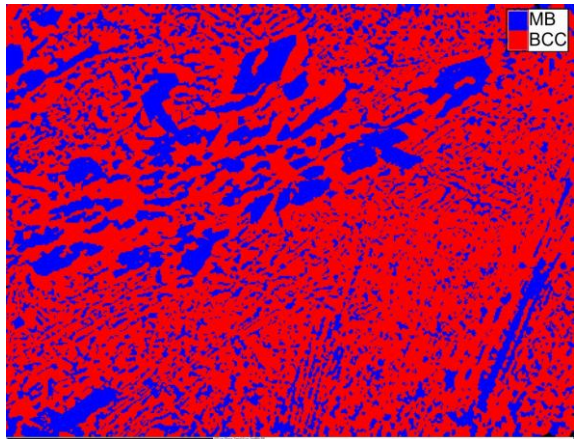
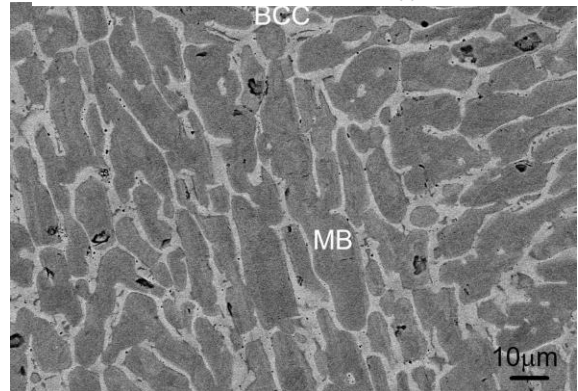
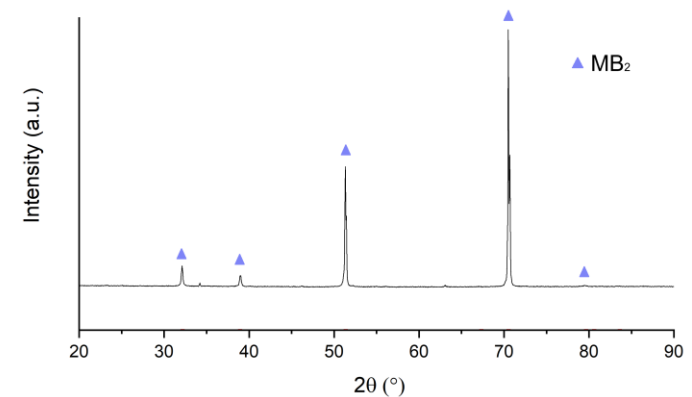
Phase	Pearson symbol	Space group	Structure type
βB	hR105	R3m	B
Nb-bcc	cl2	$\text{Im}\bar{3}\text{m}$	W
NbB	oC8	Cmcm	CrB
Nb_2B_3	oC20	Cmcm	V_2B_3
NbB_2	hP3	$\text{P6}/\text{mmm}$	AlB_2
Nb_5B_6	oC22	Cmmm	V_5B_6
Nb_3B_2	tP10	$\text{P4}/\text{mbm}$	U_3Si_2
Nb_3B_4	ol14	Immm	Ta_3B_4

Materials and Experimental Procedure

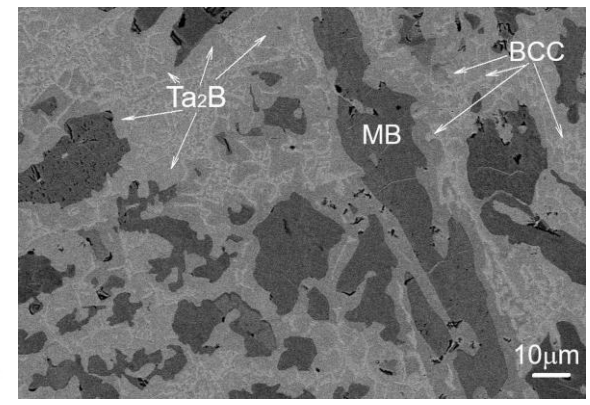
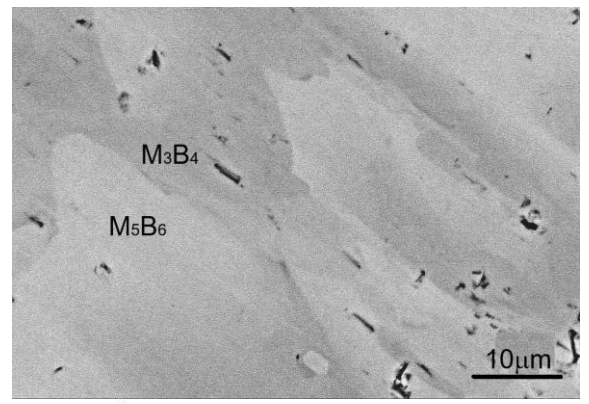
- **Preparation of model alloys:**
 - powder purity: B 99.9%, Nb 99.9%, Ta 99.98%
 - model alloys preparation: Ar arc furnace, multiple re-melting
 - two sets of alloys (32 alloys in total)
- **Heat treatment:**
 - 1323K/2940h
 - 973K/3200h
- **Experimental methods:**
 - SEM/EDX: BSE imaging mode, 10 kV
 - EBSD map
 - XRD: Co-K α radiation, ICSD database

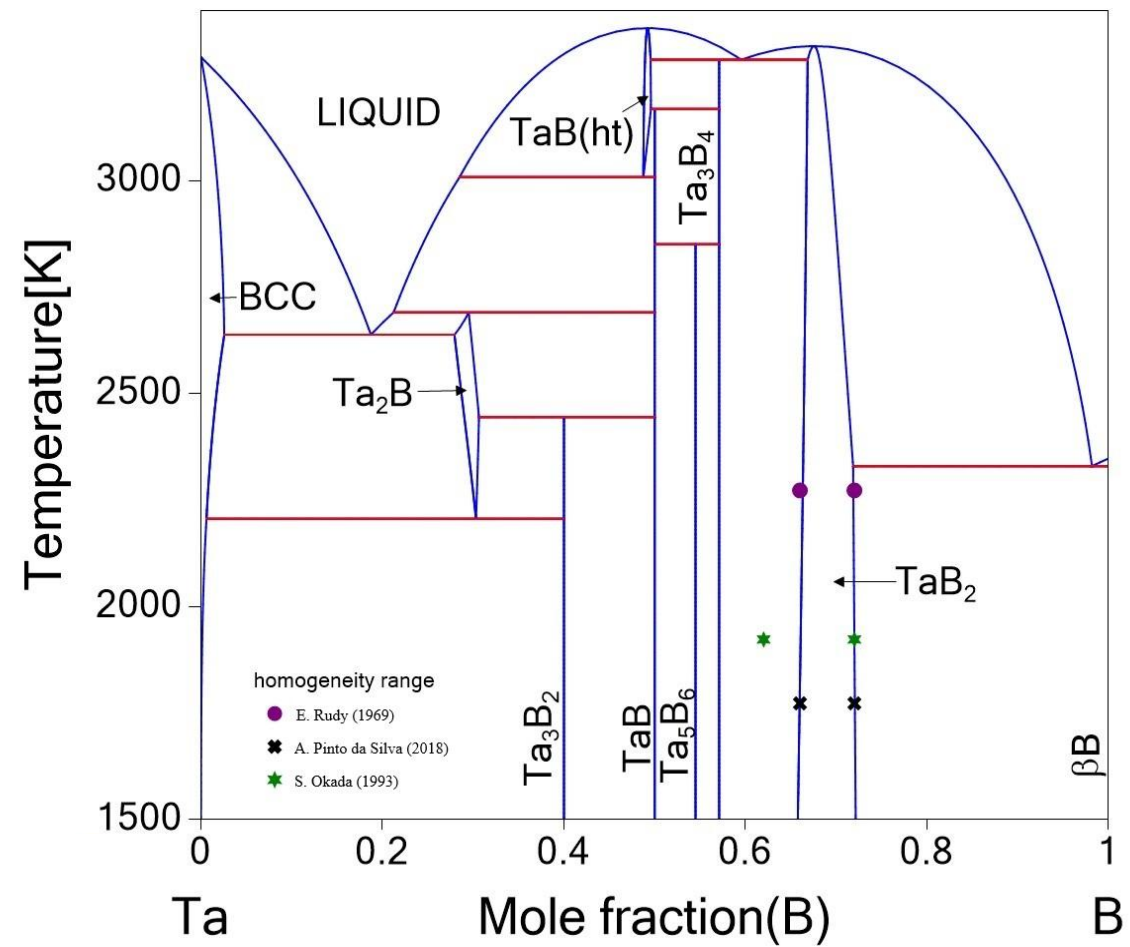
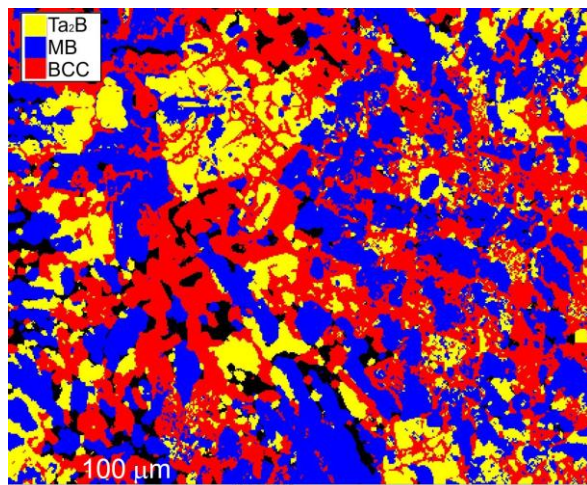
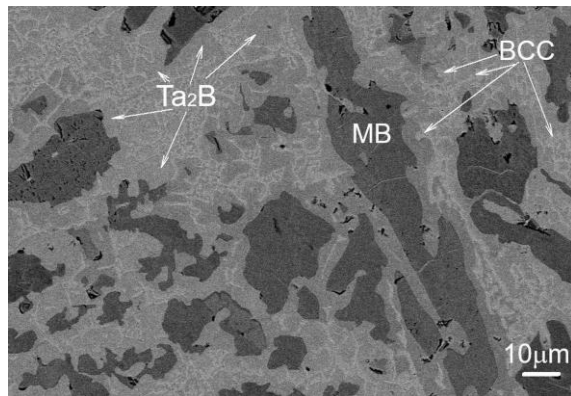


B-Nb-Ta

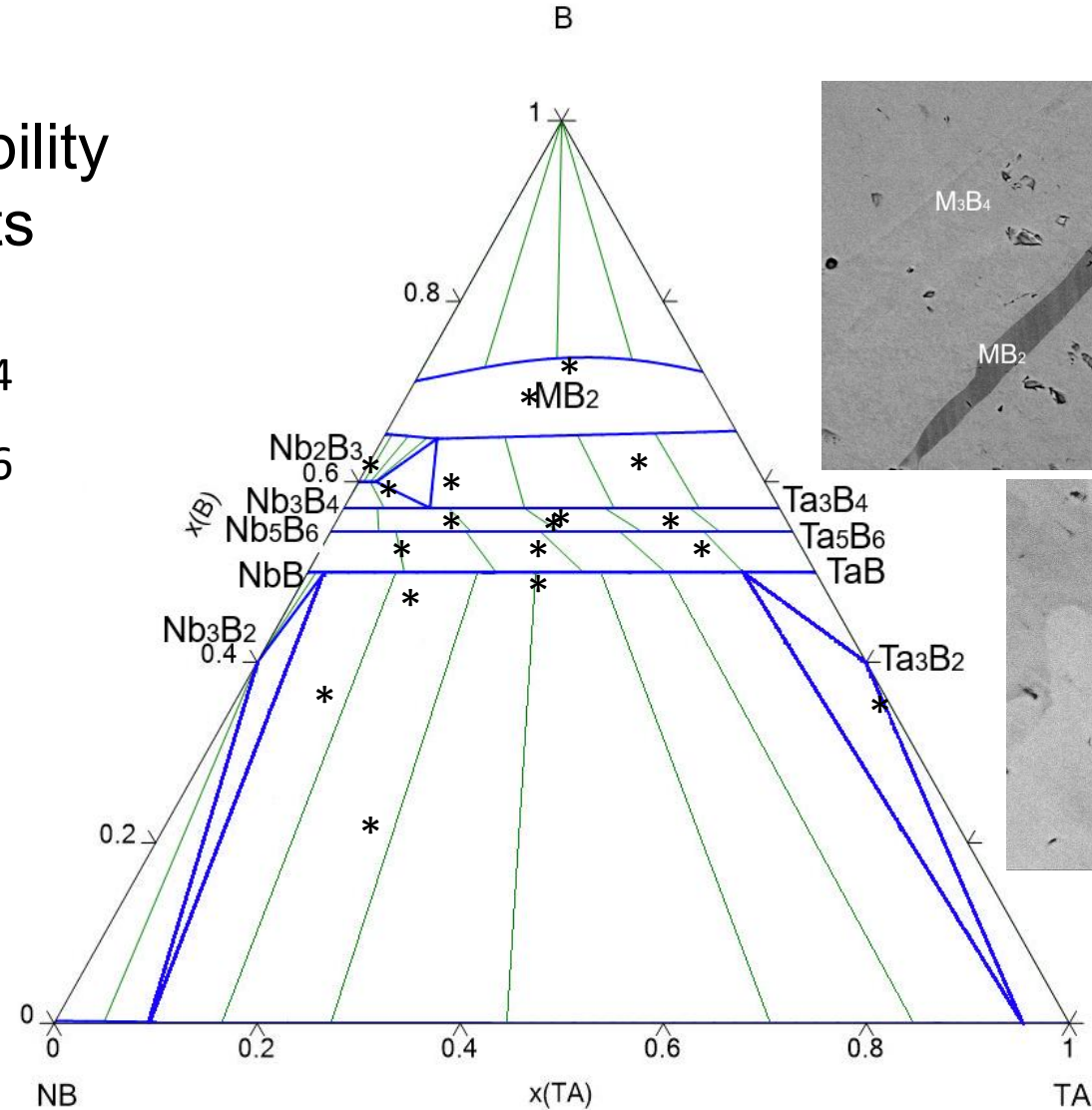
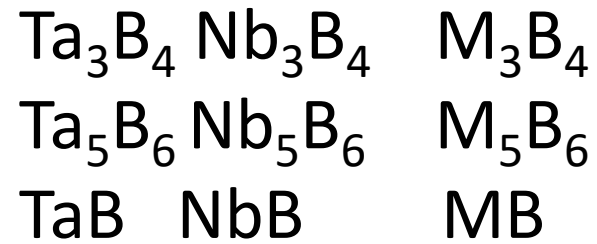


1323K

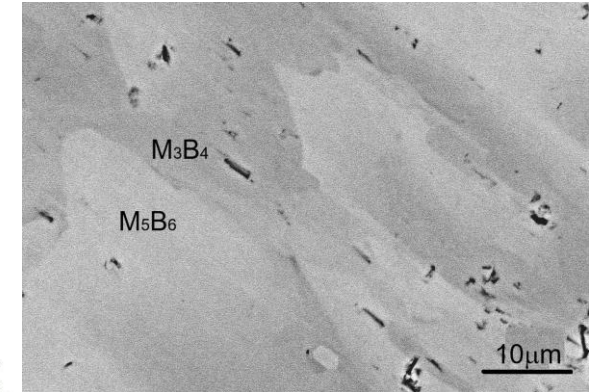
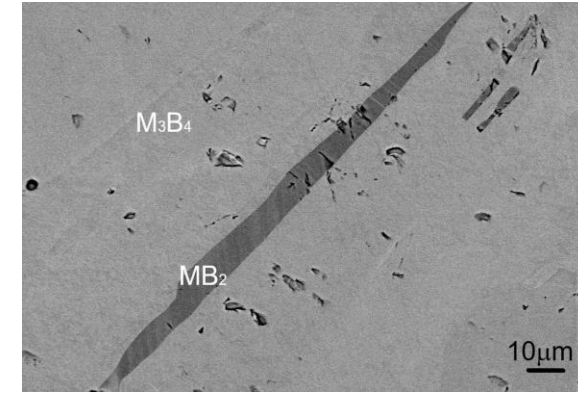




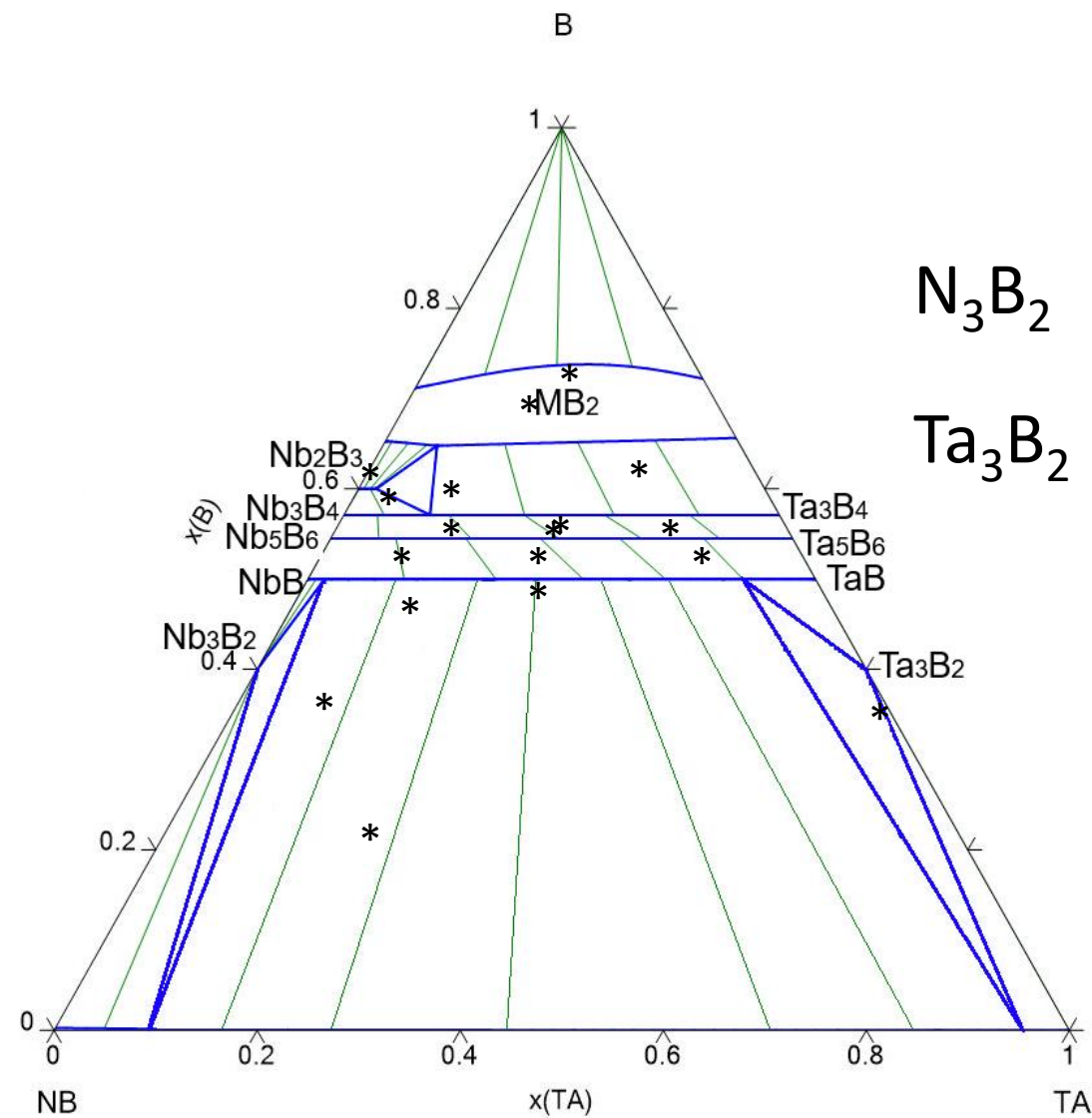
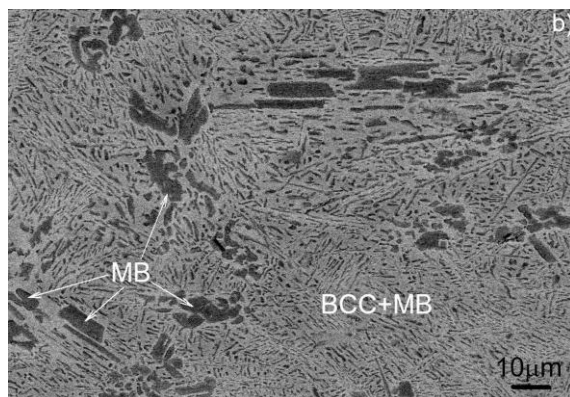
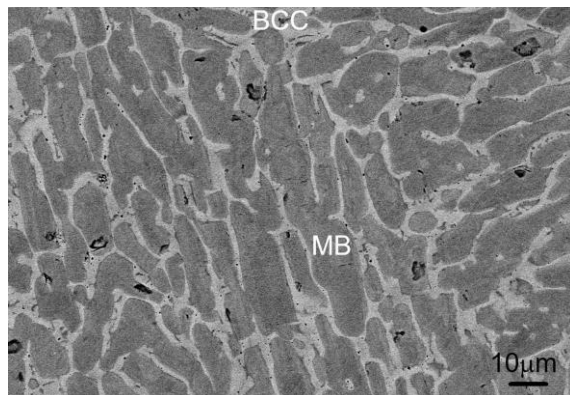
- complete mutual solubility of the metallic elements



1323K



1323K

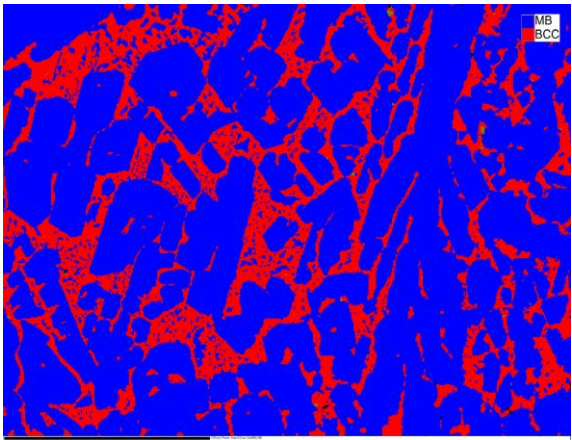
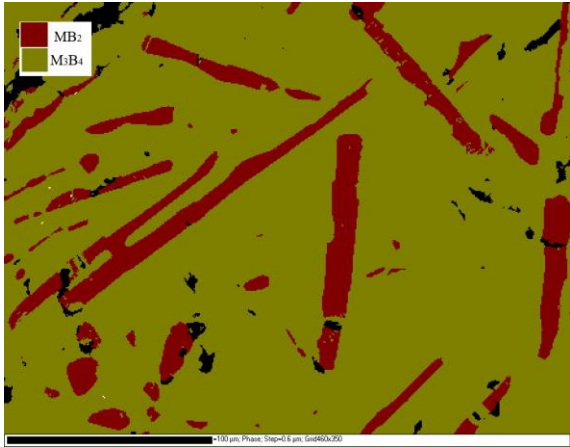
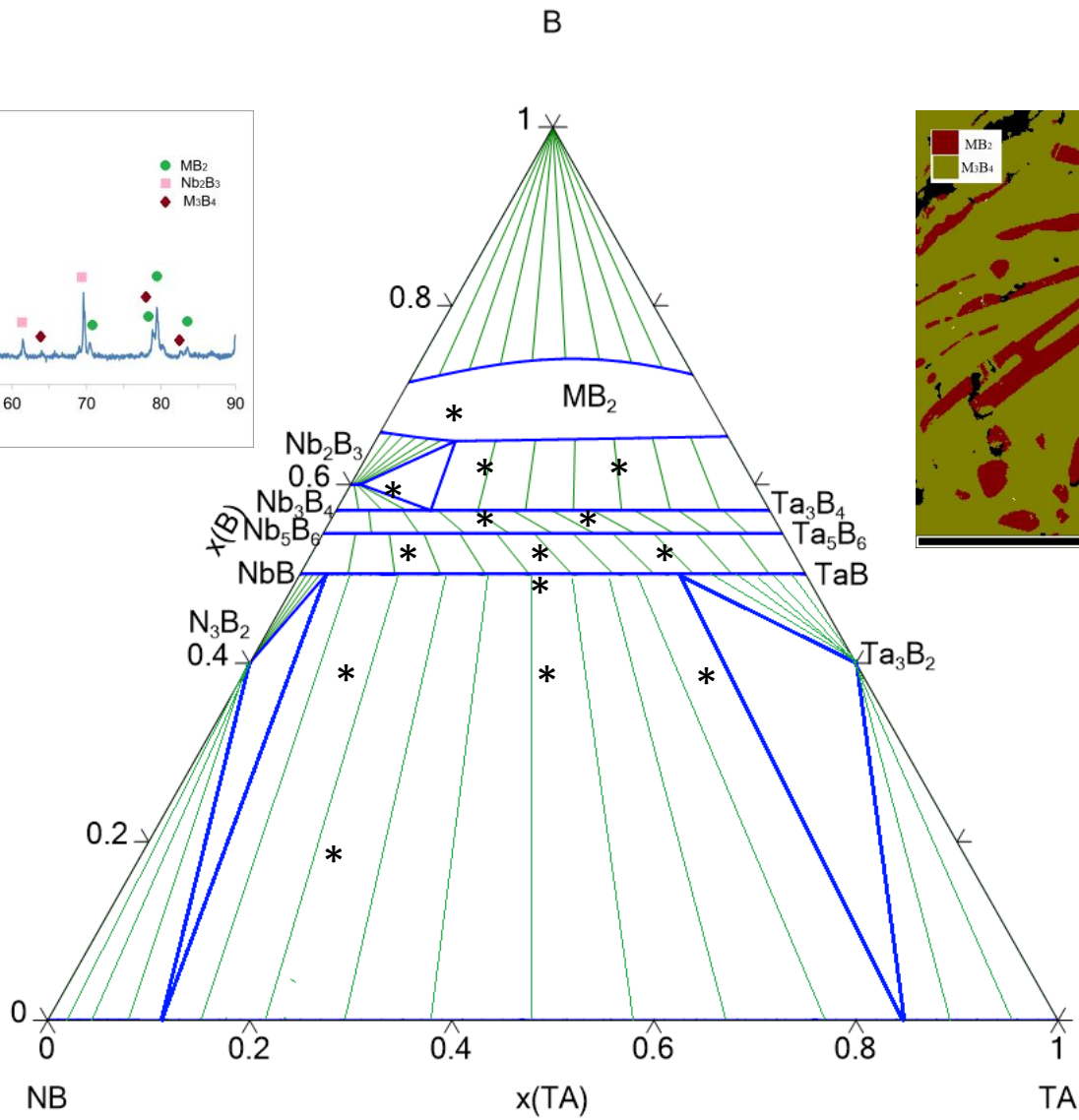
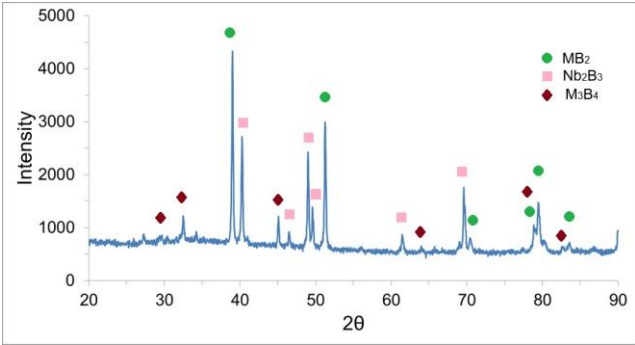


Nb_3B_2 P4/mbm tP10 U_3Si_2

Ta_3B_2 P4/mbm tP10 U_3Si_2

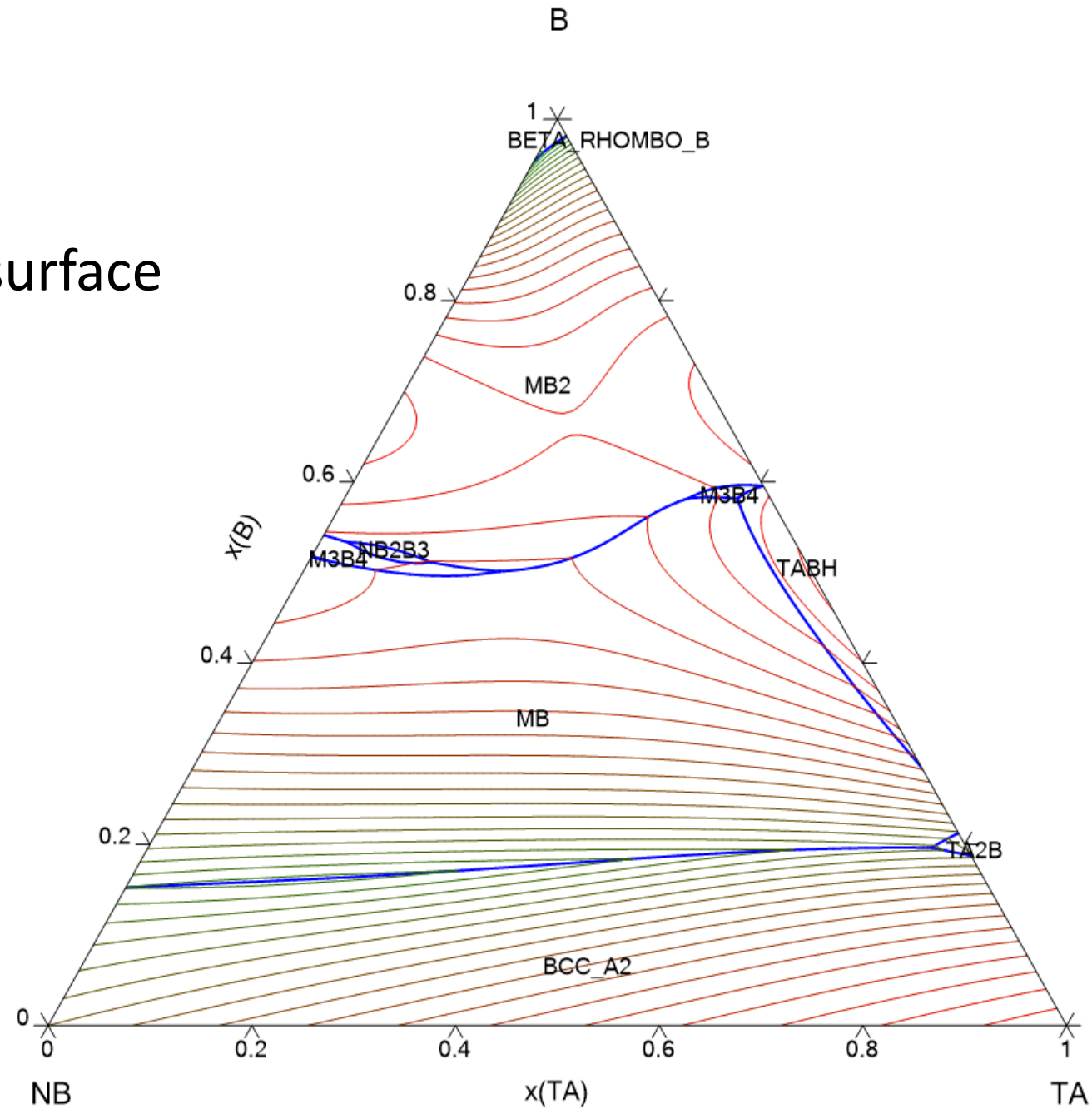
B-Nb-Ta

973K



B-Nb-Ta

Calculated liquidus surface



Conclusions

- The thermodynamic models and parameters of the BCC solid solution, MB_2 and Nb_3B_2 boride phases in the Ta–B and Nb–B binary systems were modified to ensure consistency across all subsystems.
- Boron was modeled as an interstitial element in the BCC phase.
- Two isothermal sections of the B-Nb-Ta phase diagram were experimentally determined
- The Ta_2B boride was observed in the ternary alloy after 2900 h of annealing at 1323 K, despite being stable only at significantly higher temperatures in the corresponding binary system. Therefore, it is likely that Ta_2B formed during alloy production and did not dissolve completely during the subsequent long-term annealing.
- Nb_3B_2 and Ta_3B_2 were modeled as two separate phases, since the observed BCC + MB phase equilibrium indicates that they are distinct phases, despite having the same crystal structure..
- The thermodynamic dataset for the B-Nb-Ta system was developed and good agreement between the experimental data and calculations was achieved.
- The developed thermodynamic dataset provides a solid basis for the design and optimization of materials for demanding high-temperature applications.



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Thank you for your attention.

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