Multi-Scale Computational Design and Synthesis of Protective Smart Coatings for Refractory Metal Alloys

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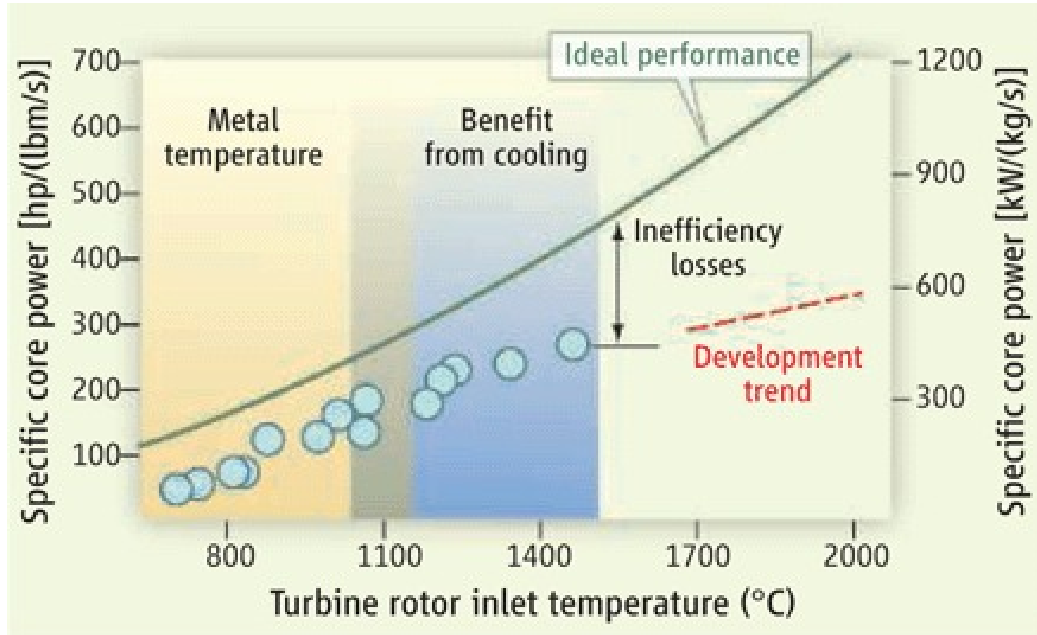
Outline

- Background
- Research Accomplishments
  - Mo-Si-B coating development for Nb alloys
  - Zr additions to Mo-Si-B coating
- Future Work
- Concluding Remarks

Background

- Ni-based superalloys provide the necessary structural strength while at the same time remaining oxidation resistant in combustion systems
- Other high temperature materials must be explored because Ni-based superalloys are reaching their limit in operational temperature
- Protective coatings necessary for increased oxidation performance



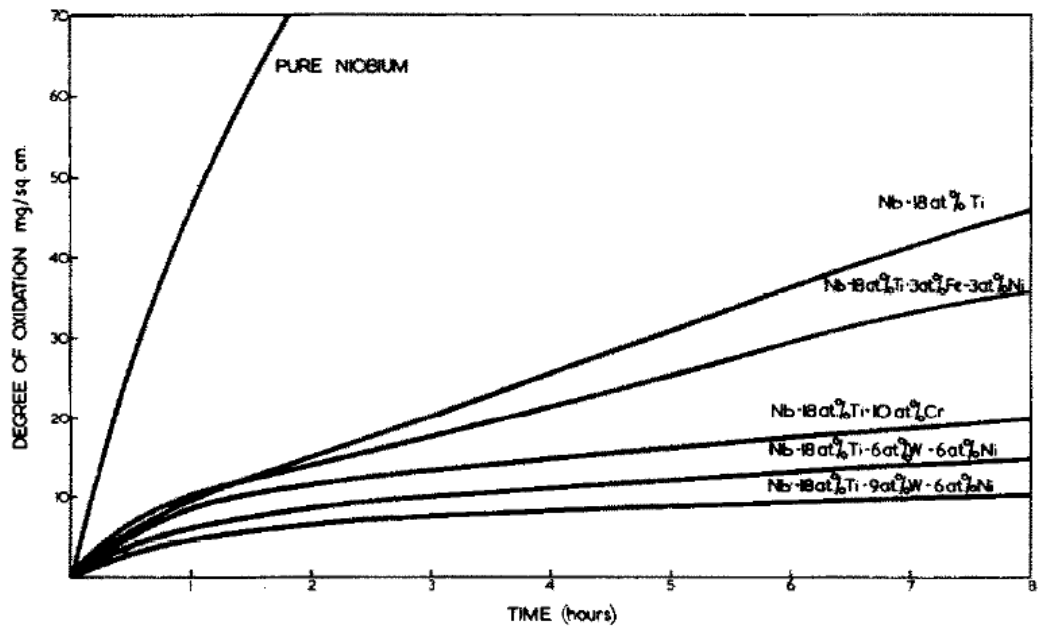
Core power output vs. inlet temperature for gas turbine engines [1]

[1] J.H. Perepezko, Science, 326 (2009) 1068-1069.

Background

- Refractory metals are have higher melting points than current nickel-base superalloys.
- Refractory metals readily oxidize at high temperatures forming metal oxides that drastically reduce the integrity of the metal
- Prospective alloys are Nb-based alloys consisting of Hf, Ti, Cr, Ge, Al, B, and Si additions

Main alloying addition	Function
Si	Aid in creep and oxidation resistance resistance (Nb_5Si_3, Nb_3Si)
Ti (~25 at.%)	Formation of $Nb_2O_5 \cdot TiO_2$ to reduce oxidation rate of alloy [2]
Cr (~8 at.%)	Formation of Cr_2Nb Laves phase, aiding in oxidation resistance ($CrNbO_4$ during oxidation) [3][4]
Ge/B	Reduce viscosity of silica glass

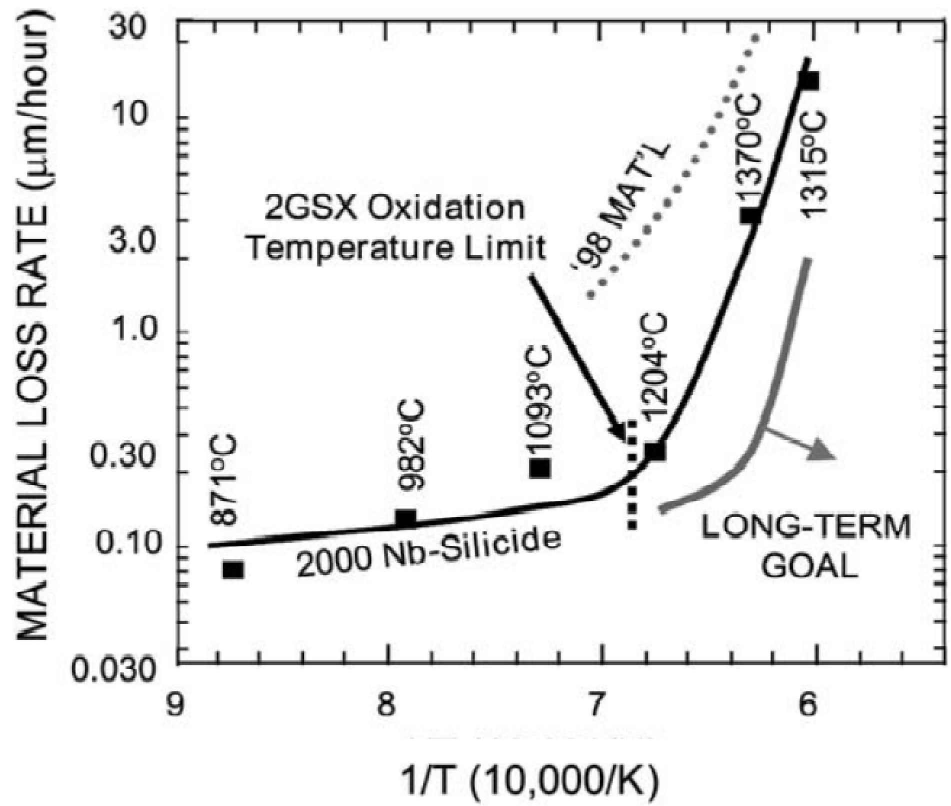


Oxidation of Nb alloys in air at 1100°C [5]

[2] R. Smith, Journal of the Less Common Metals, 2 (1960) 191-206.
[3] P.R. Subramanian, M.G. Mendiratta, D.M. Dimiduk, M.A. Stucke, Materials Science and Engineering: A, 239–240 (1997) 1-13.
[4] K.S. Chan, Metall Mater Trans A, 35A (2004) 589-597
[5] R. Smith, Journal of the Less Common Metals, 2 (1960) 191-206

Background

- While alloy additions to Nb have shown increased oxidation resistance the long term goal of these alloys is still out of reach
  - Long term goal operational temperature of 1315°C with <25μm material loss in 100 hrs
- Nb produces 3 different oxides: Nb_2O_5, NbO_2, NbO [6]
- Protective coatings necessary for increased oxidation performance
  - Retain ductility in Nb alloys



Mass Loss Rate vs. Temperature for Nb alloys [7]

[6] E.A. Gulbransen, K.F. Andrew, Journal of The Electrochemical Society, 105 (1958) 4-9

[7] B.P. Bewlay, M.R. Jackson, J.C. Zhao, P.R. Subramanian, Metal Mater Trans A, 34A (2003) 2043-2052.

Background: Current Protection Methods

- Current protection methods are based on silicide coatings that produce a protective silica layer
  - Due to selective oxidation of Si
- A study by Kurokawa et al. showed that disilicides would either form a protective SiO_2 scale or a non protective mixed oxide scale depending on the temperature during oxidation (Table 1) [8]
  - Refractory metal disilicides ($MoSi_2$, WSi_2) also form trioxide, which is either stable or volatile depending on temperature and partial pressure of O_2

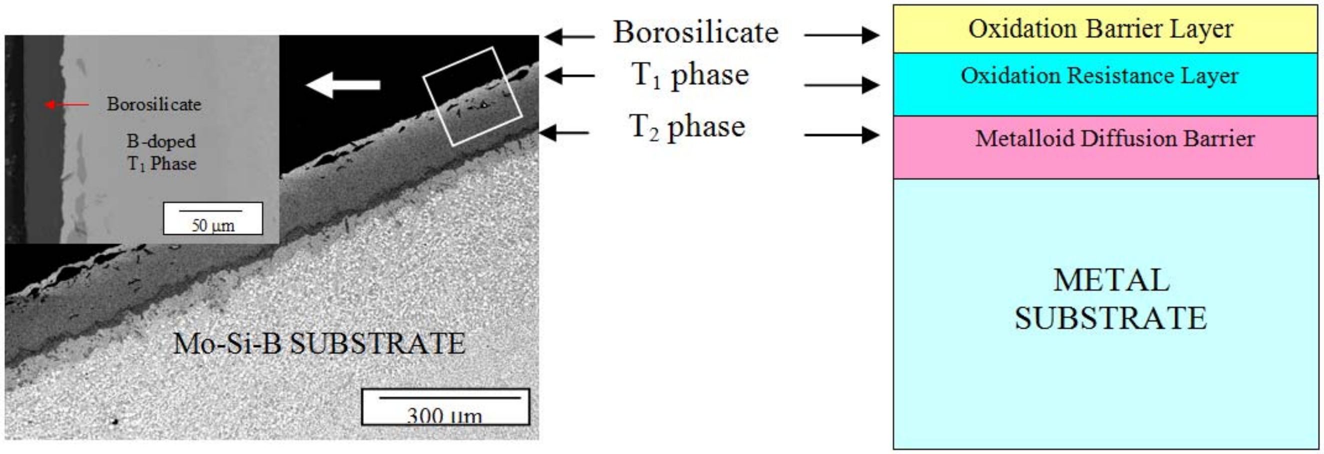
Table 1 Structure of oxide scale on disilicide and oxidation resistance.

Oxide scale structure	Silicide	Oxid. resistance	Temp. region
SiO_2 scale	$FeSi_2$	◎	<1273K
	$CoSi_2$	◎	<1273K
	$MoSi_2$	◎	>1073K
	WSi_2	◎	>1573K
	VSi_2	○	>1173K
	$ReSi_{1.75}$	△	>1273K
	$ReSi_{1.75}$	×	<1273K
Double layer scale	$CrSi_2$	◎	<1373K
		×	>1473K
Mixed oxide scale	$NbSi_2$	×	<1773K
	$TaSi_2$	×	<1773K
	$MoSi_2$	×	773−1073K
	WSi_2	×	1073−1573K
	VSi_2	○	<1173K
	$TiSi_2$	×	>773K
	Ti_5Si_3	×	>773K

◎ Excellent ○ Good △ poor × very poor

[8] K. Kurokawa, A. Yamauchi, Solid State Phenomena, 127 (2007) 227-232.

Mo-Si-B Coatings for Oxidation Protection



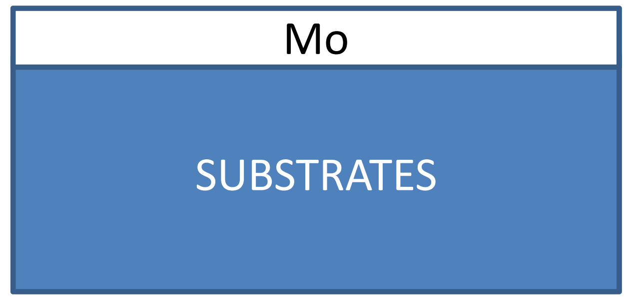
- The Mo-Si-B system has been proven to provide oxidation protection in a temperature range of 1200-2000°C
  - T_1 phase serving as a source of Si and B to enable a self-healing capability [10].
  - T_2 phase serving as a diffusion barrier to inhibit dissolution of the coating into the substrate
- Mo-Si-B coatings have been applied to other refractory metal substrates and cermets to provide enhanced oxidation protection [11,12]
  - Suggests coatings can be extended to Nb base systems

[10] R. Sakidja and J. H. Perepezko, "Phase Stability and Alloying Behavior in the Mo-Si-B System", v. 36A, Metallurgical Transaction A, (2005) pp. 507-514.
[11] O.J. Lu-Steffes, R. Sakidja, J. Bero, J.H. Perepezko, Surface and Coatings Technology, 207 (2012) 614-619.
[12] J.H. Perepezko, J.M. Bero, R. Sakidja, I.G. Talmy, J. Zaykoski, Surface and Coatings Technology, 206 (2012) 3816-3822.

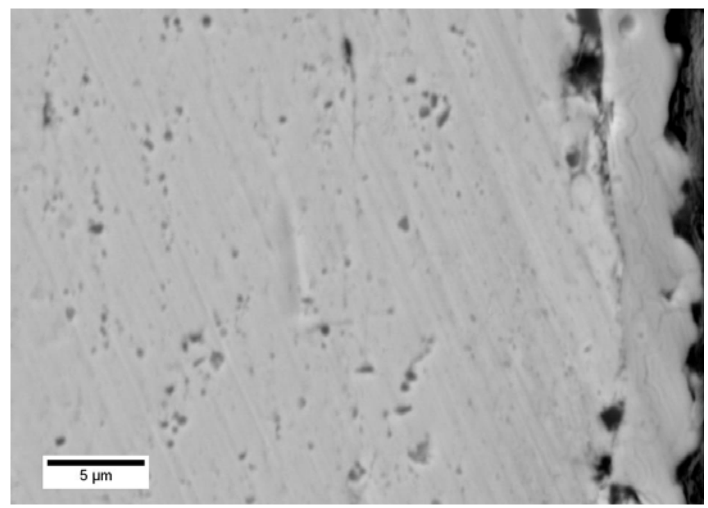
Synthesis of Mo-Si-B Coatings on RM Substrates

- 2 step processes:
  1. **Mo deposition onto substrate for < 5 minutes at 300°C using $Mo(CO)_6$ decomposition process**

$$Mo(CO)_6 \rightarrow Mo + 6CO(g)$$



Plan view SEM image of
Mo particles on Nb sample



Cross section SEM image of
Mo particles on Nb sample

Synthesis of Mo-Si-B Coatings on RM Substrates

- 2 step processes:
  2. Co-deposition of Si+B into Mo deposit and substrate ~ 50 hours at 1000°C.
- CVD technique that uses halide vapor species to diffuse to the substrate and decompose, depositing the desired elements

$3NaF + 2Si(s) \leftrightarrow 2SiF(g) + 3Na(g) + \frac{1}{2}F_2(g)$

$3NaF + 2B(s) \leftrightarrow 2BF(g) + 3Na(g) + \frac{1}{2}F_2(g)$

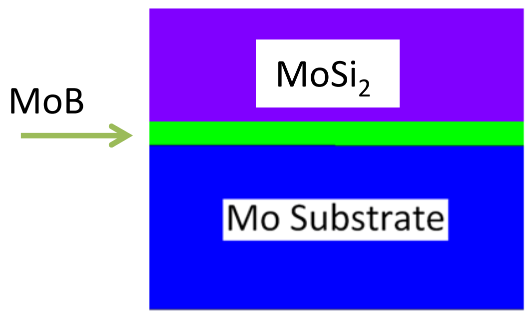
$3SiF(g) \leftrightarrow SiF_2(g) + Si(s)\downarrow$

$3SiF_2(g) \leftrightarrow 2SiF_3(g) + Si(s)\downarrow$

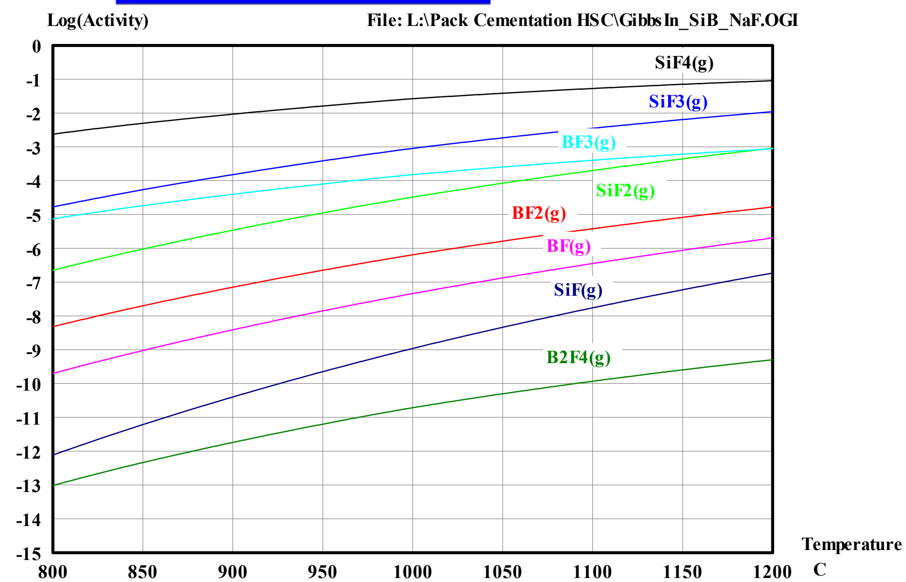
$4SiF_3(g) \leftrightarrow 3SiF_4(g) + Si(s)\downarrow$

$3BF(g) \leftrightarrow BF_2(g) + B(s)\downarrow$

$3BF_2(g) \leftrightarrow 2BF_3(g) + B(s)\downarrow$



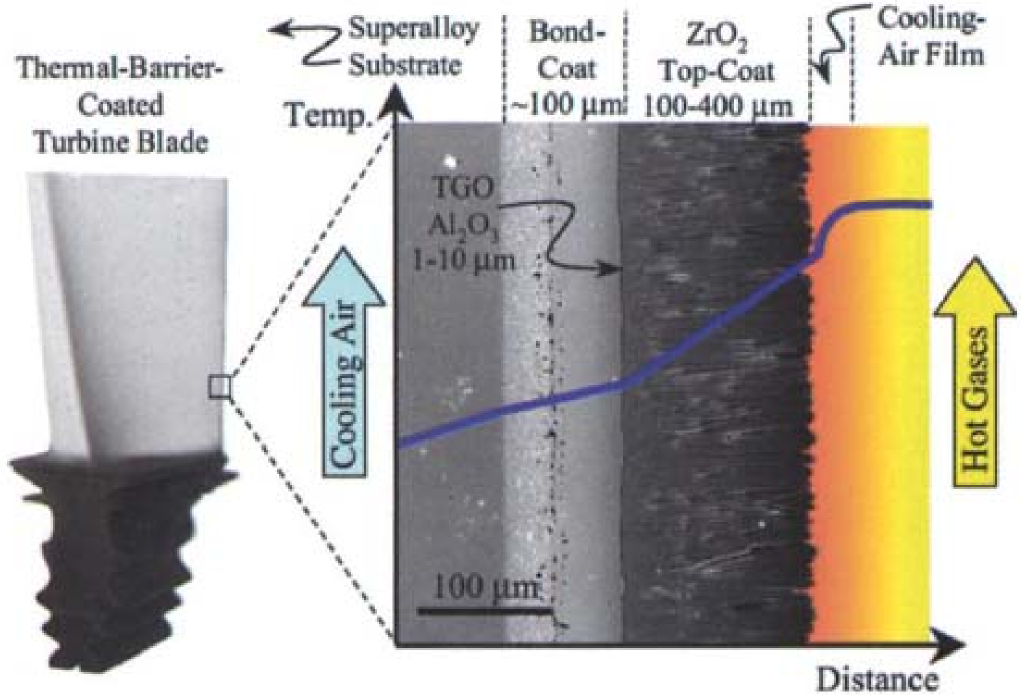
- To optimize coating structure, vary the proportion of Si and B in the pack powder



Activity of Si and B flourides (NaF activator, 35:1 Si: B ratio)

Smart Coating: Benefits of TBC

- Thermal barrier coatings (TBC) are used to limit thermal exposure
  - reduce the substrate temperature of a superalloy by as much as 300°C [13]
- CTE mismatch between the TBC and underlying layers can result in failure of the coating [14]

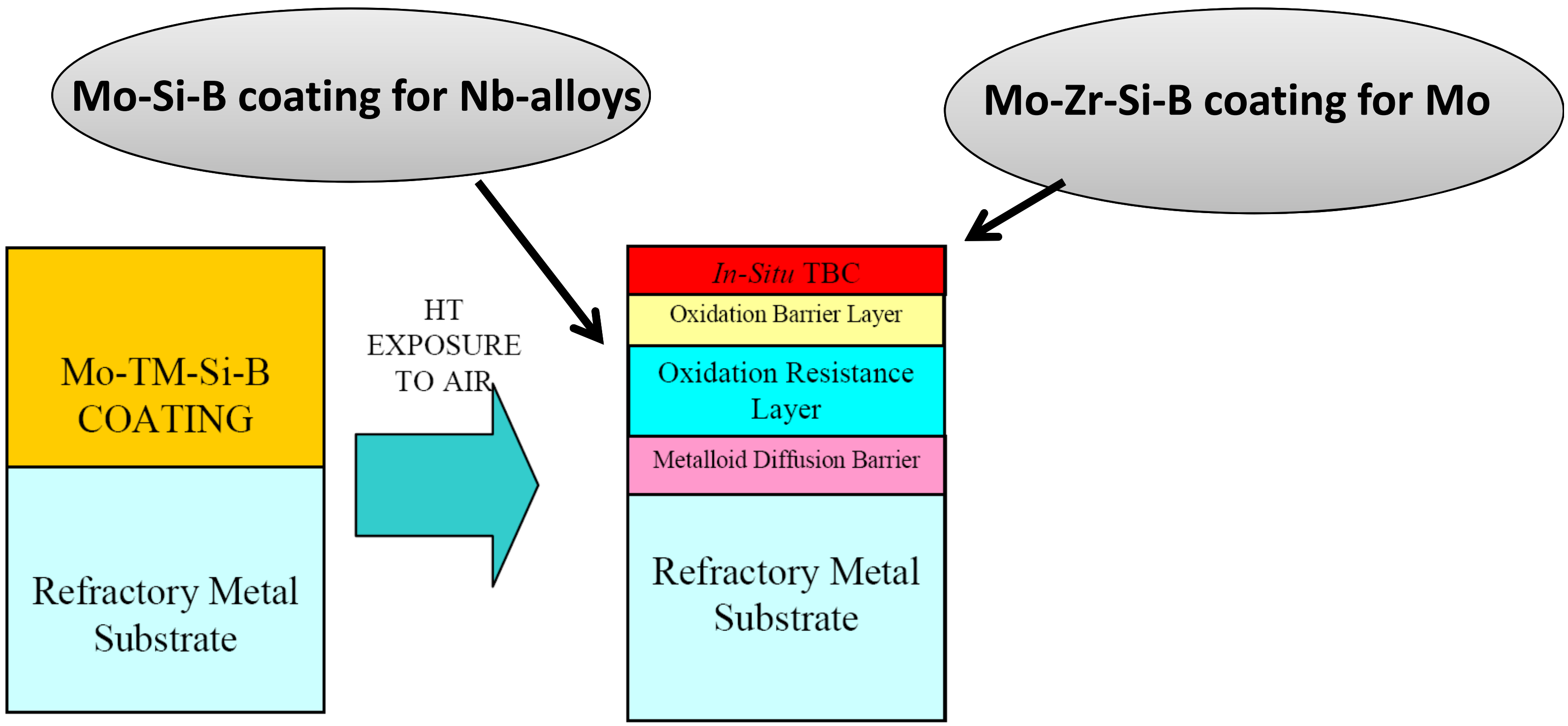


Schematic temperature profile of a turbine blade coated with a TBC [13]

[13] N.P. Padture, M. Gell, E.H. Jordan, Science, 296 (2002) 280-284
[14] W. Beele, G. Marijnissen, A. van Lieshout, Surf Coat Tech, 120 (1999) 61-67.

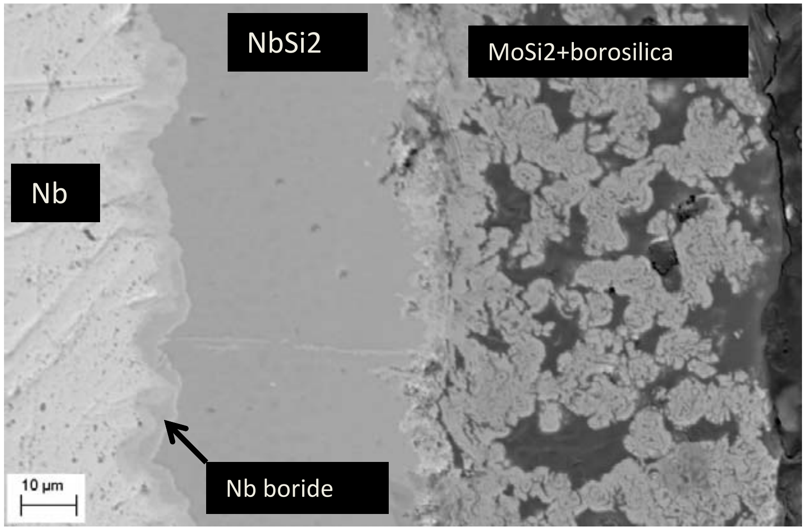
Extended coating system

- Mo-Si-B coatings provide robust oxidation resistance
- Thermal barrier coatings (TBC) are used to limit thermal exposure
- Research is focused on trying to create a coating that contains advantageous properties of both Mo-Si-B and TBC coatings
  - Divide research into two categories
    - Mo-Si-B coating for Nb alloys
    - Zr additions to Mo-Si-B on Mo

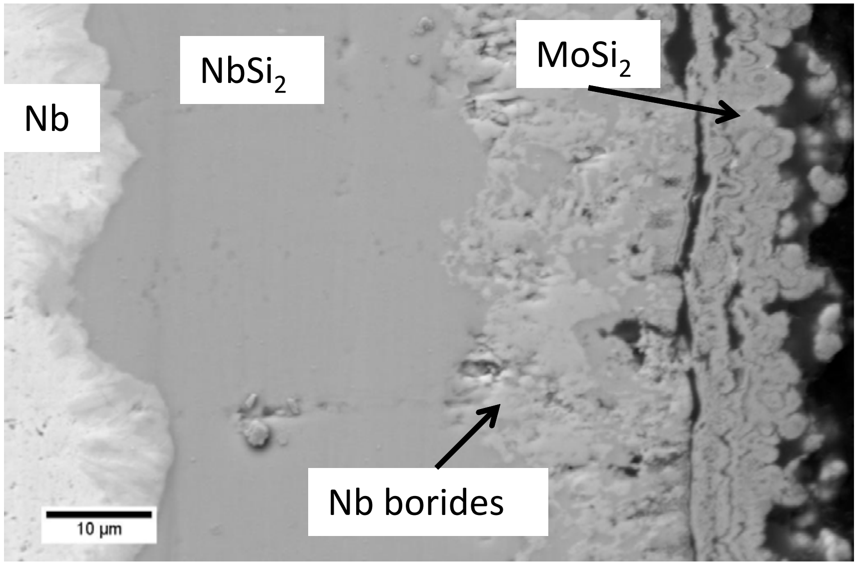


Performance of Mo-Si-B Coatings

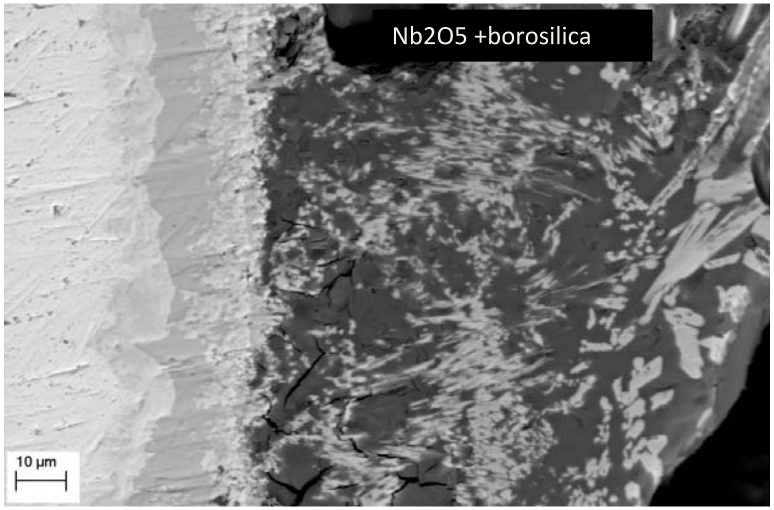
- Oxidation tests show that for a given Si:B ratio, Mo-Si-B coatings offer better protection compared to Si-B coatings
- However, the cross section of the coating reveals large amounts of Nb borides that can interfere with the formation of a protective oxidation coating



Nb-Mo-Si-B (35:1), mass change : 2.30 mg/cm^2 (1200°C 5 hours)



Cross section of as-packed coating structure on Nb substrate



Nb-Si-B (35:1), mass change: -9.10 mg/cm^2 (1200°C 5 hours)

Boride Formation in Coatings

- Study by Cockeram and Rapp produced a boron modified discilicide coating on Ti alloys and also noticed significant boride formation [15]
  - proposed following reaction for the formation of TiB_2:

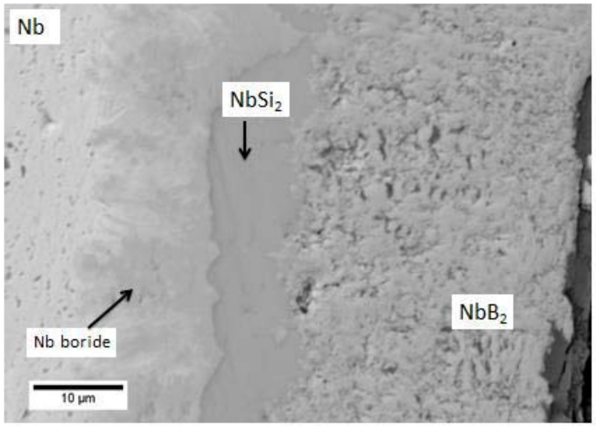
$2B + TiSi_2 \rightarrow TiB_2 + 2Si$ (1) 1000°C, ΔG=-95.64 kJ/mol

- ΔG values calculated using HSC Chemistry for $NbSi_2$ and $MoSi_2$:

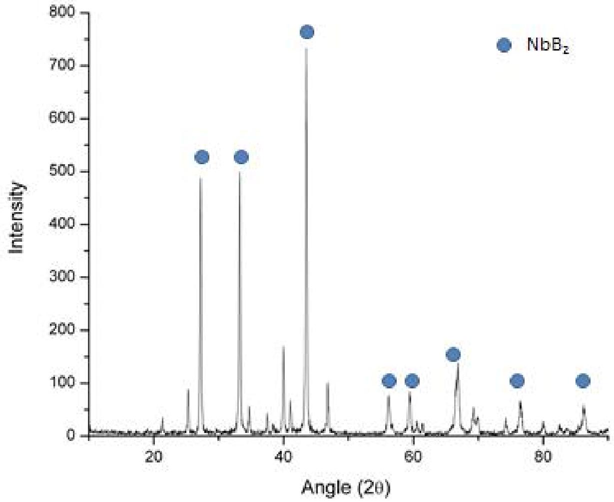
$2B + NbSi_2 \rightarrow NbB_2 + 2Si$ (2) 1000°C, ΔG=-44.33 kJ/mol

$2B + MoSi_2 \rightarrow MoB_2 + 2Si$ (3) 1000°C, ΔG=+37.50 kJ/mol

- Explains why borides are less prominent in Mo-Si-B coatings
- Boron additions in Si-B coatings all resulted in substantial boride formation



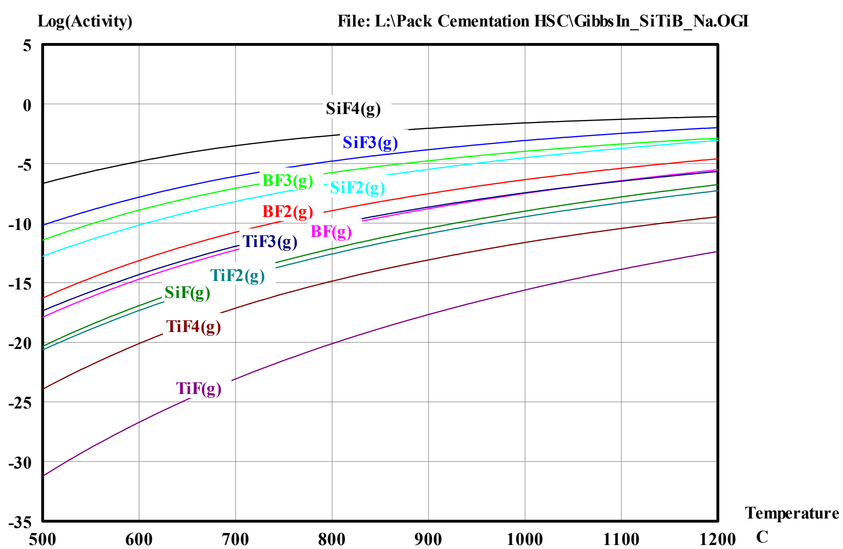
Si-B coating on Nb, Si:B ratio 10:1



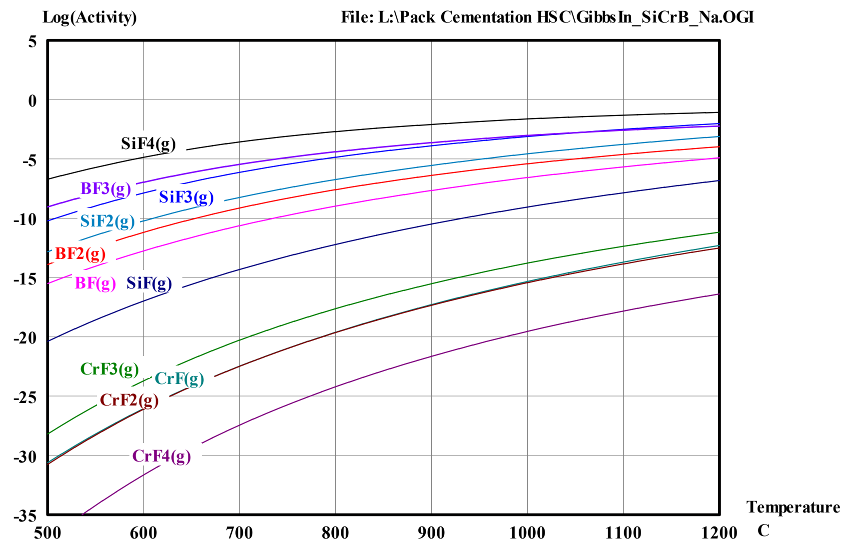
[15] B. Cockeram, R. Rapp, Oxidation of Metals, 45 (1996) 375-425

Activities of Halides

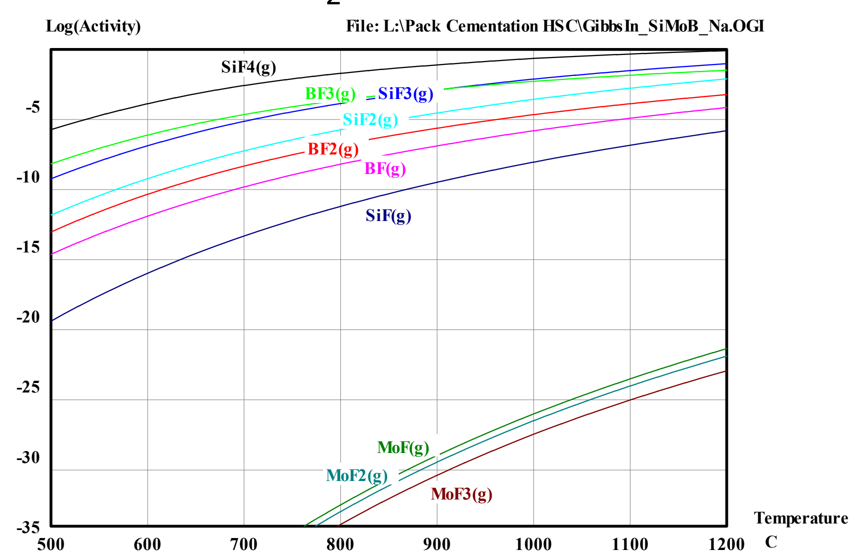
- Optimize coating structure by varying both Si:B$_{source}$ ratio as well as B source



TiB_2



CrB_2

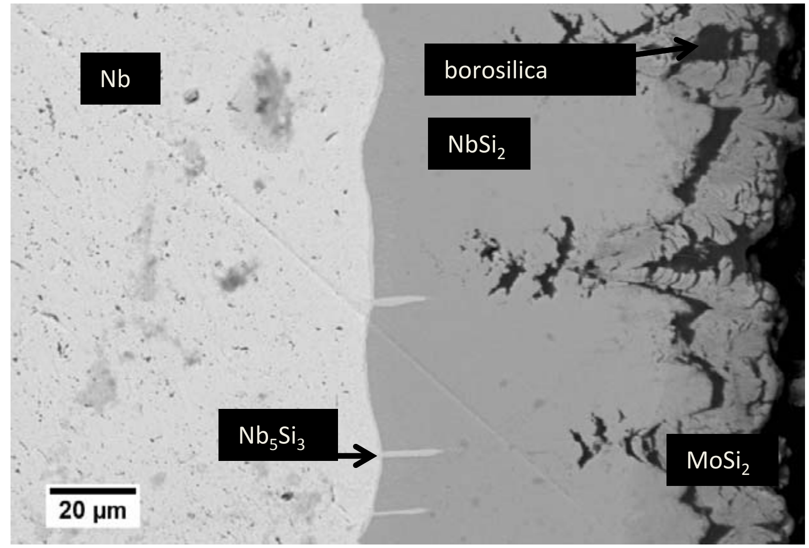


MoB

Plots have a Si: B$_{source}$ ratio of 10:1

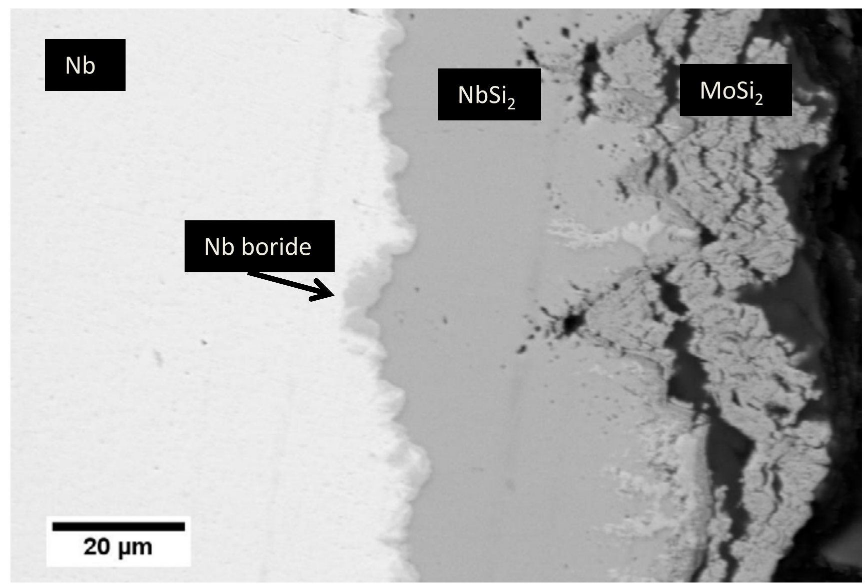
Optimize Mo-Si-B coating for Nb

- Substitution of TiB_2 in place of B in pack cementation treatment lowers the partial pressures of the boron flourides [16]
  - TiB_2 substitution in pack completely suppresses boride formation in the coating structure
- CrB_2 source shows slightly more boride formation



As- packed coating structure using Si:TiB_2 ratio of 1.8:1

	ΔG° (J/mol)	Boron activity
SiB_3	−4,990	0.656
CrB_2	−41,100	3.10×10^{-2}
TaB_2	−98,100	2.51×10^{-4}
TiB_2	−149,700	3.20×10^{-6}

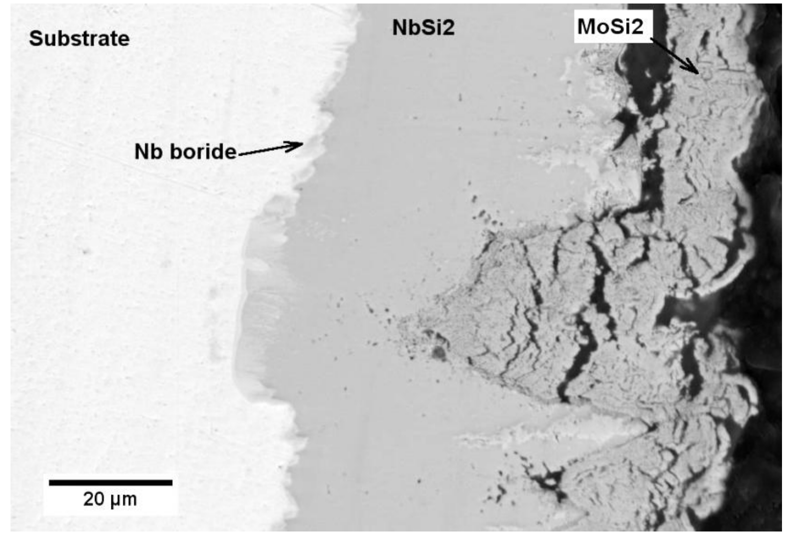


As- packed coating structure using Si:CrB_2 ratio of 10:1

[16] Brian V. Cockeram, "Growth and oxidation resistance of boron-modified and germanium-doped silicide diffusion coatings formed by the halide-activated pack cementation method", *Surface and Coatings Technology*, Volumes 76–77, Part 1, November 1995, Pages 20-27

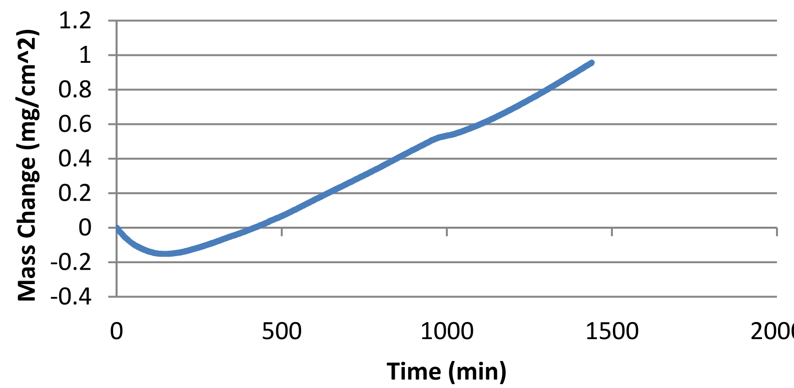
MoB substitution

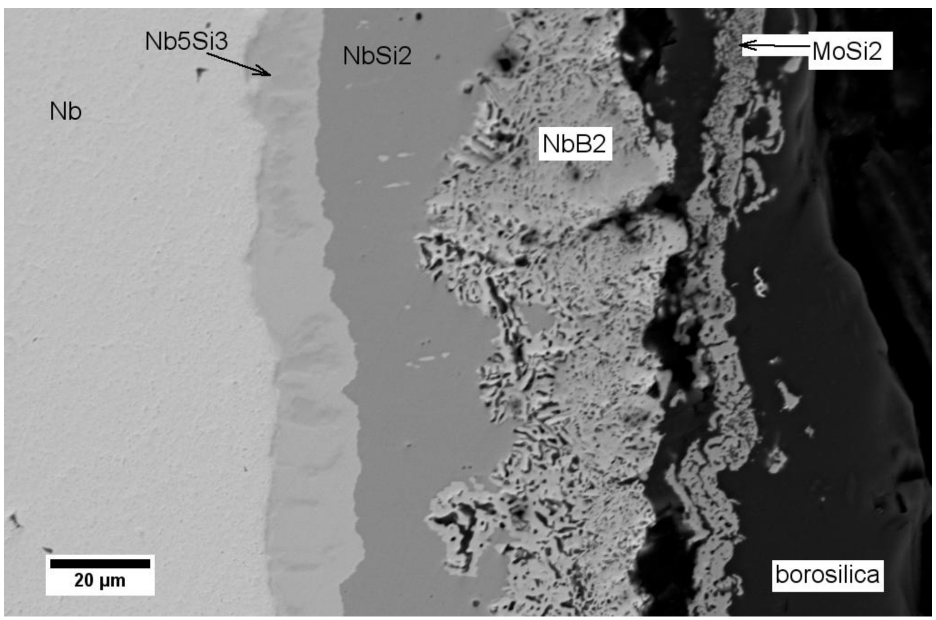
- Si:MoB ratio of 10:1 used in pack cementation process at 1000°C for 25 hours
- Heat treatment at 1200°C at 25 hours in Ar flow
- TGA results show minimal mass change (0.96 mg/cm^2)
- SEM of coating shows continuous glass formed on top of the sample, but boride phase is still present at the $MoSi_2$/$NbSi_2$ interface
- Suggests conditioning samples in Ar atmosphere prior to oxidation testing a preferred option for Nb samples



As- packed coating structure using Si:MoB ratio of 10:1

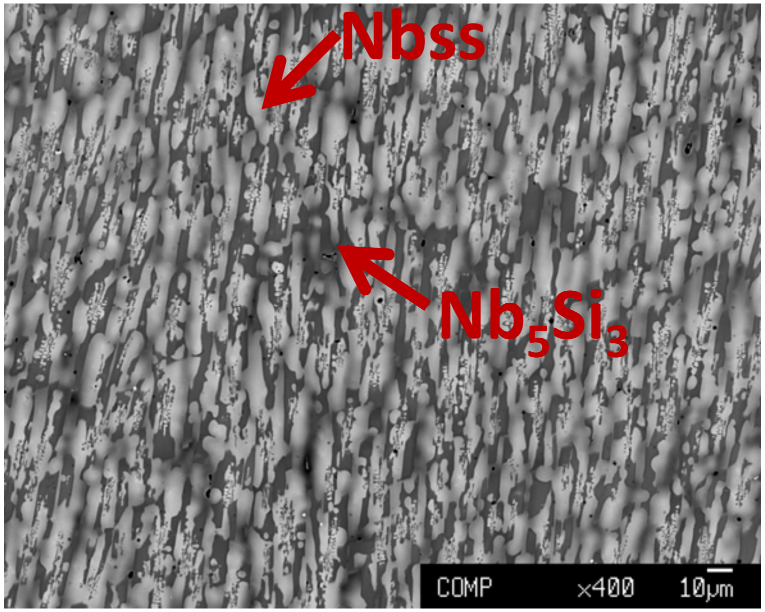
TGA 1200°C 24 hours

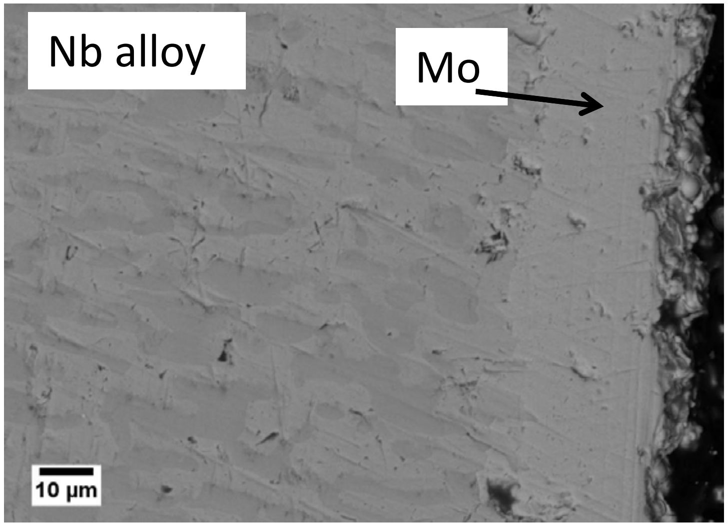




Mo-Si-B coating for Nb alloy

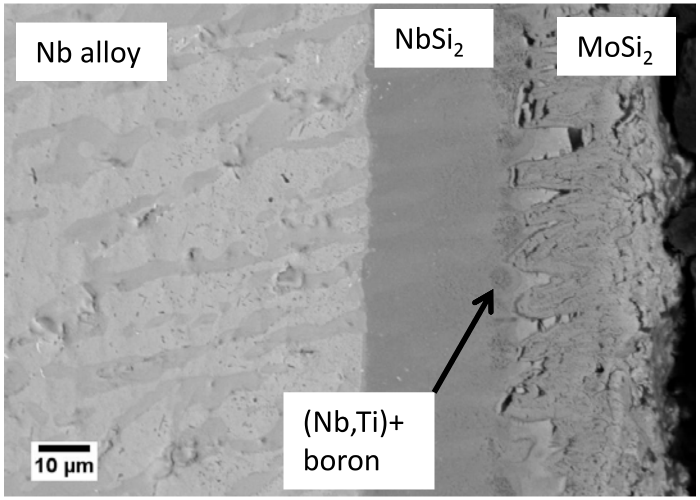
- Substrate: Nb-24Ti-15Si-4Cr-2Al-2Hf (at.%)
  - Two phases: Nb_{ss} (light regions) Nb_5Si_3 (dark regions)
- The samples were coated with Mo-Si-B in a two-step process. (1) molybdenum was deposited through the decomposition of $Mo(CO)_6$.(2) The silicon and boron/boride were deposited through a pack cementation process.
- B, CrB_2, TiB_2, MoB
- Pack condition: 1000 ^oC /25h



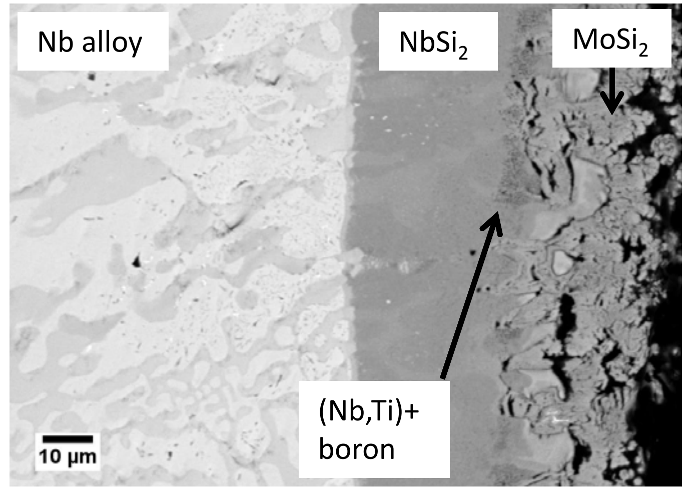


Coating structure (as-pack) for Nb alloy

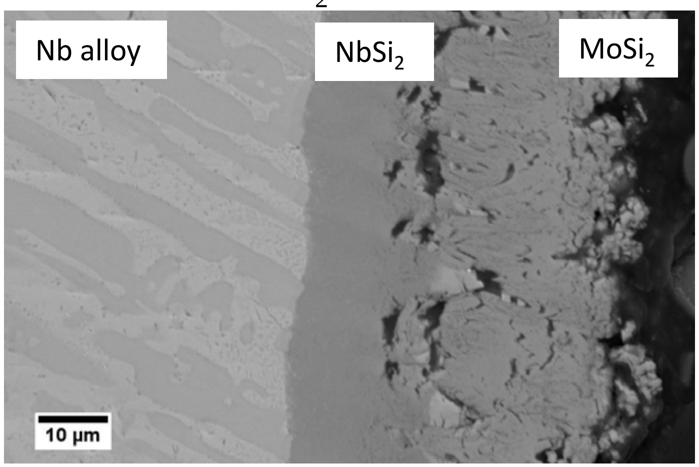
Si:B 35:1



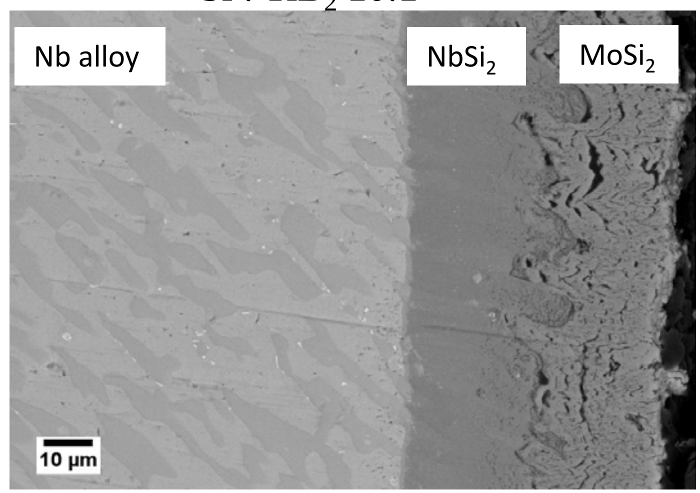
Si : MoB 10:1



Si : CrB_2 20:1



Si : TiB_2 10:1

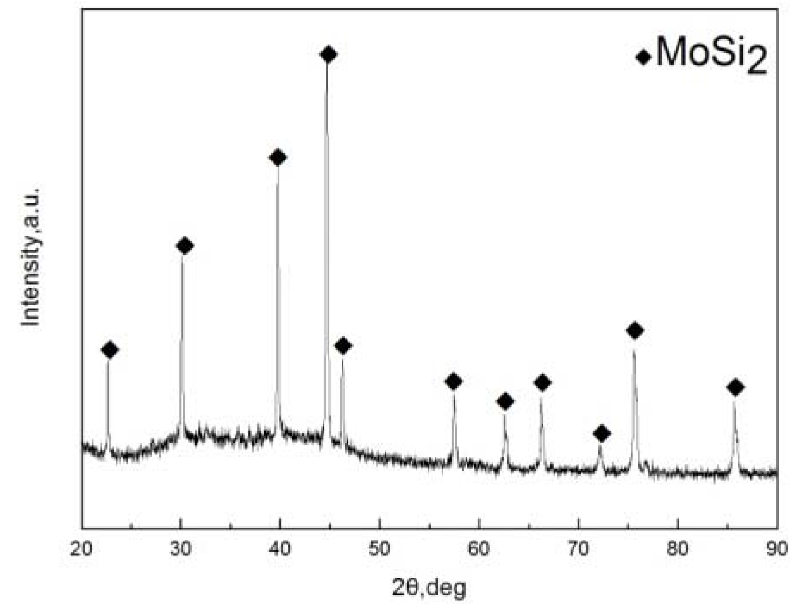


B_{source}	$NbSi_2$	Boron Zone	$MoSi_2$+glass	Total (µm)
Si:B	~30	~15	~30	~75
MoB	~40	~10	~30	~80
CrB_2	~13	~7	~30	~50
TiB_2	~20	0	~30	~50

- Boride layer reduced with TiB_2 and CrB_2 substitutions

Coating structure (as-pack) for Nb alloy

- XRD of the of sample is composed of $MoSi_2$
- EPMA shows that the boron in the "boride region" is the $(Nb,Ti)_5SiB_2$ phase
  - T_2 phase of Nb-Si-B system



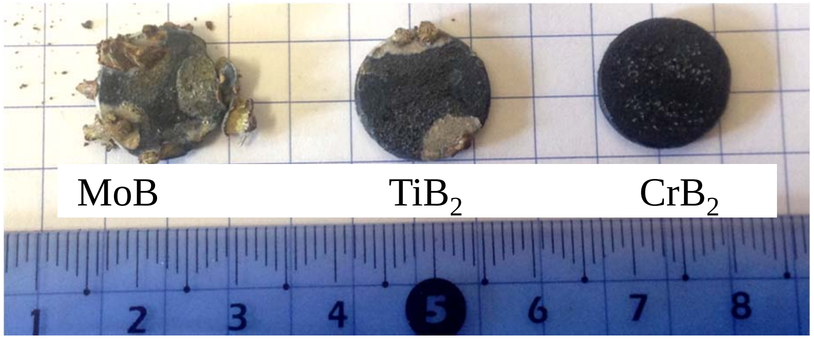
XRD results of as-pack sample using CrB_2 as B source

EPMA

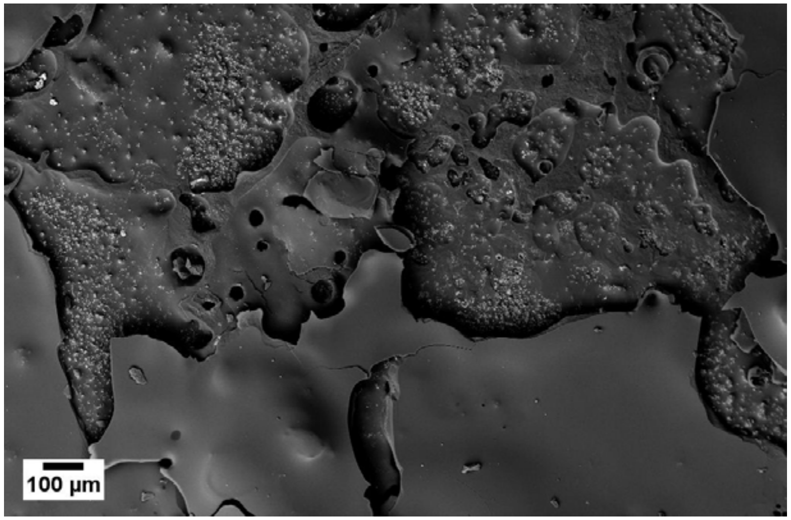
Phase	B (at.%)	Si (at.%)	Mo (at.%)	Nb (at.%)	Ti (at.%)	Na (at.%)	Al (at.%)	O (at.%)	Hf (at.%)	Cr (at.%)	Elemental total
$NbSi_2$	0	56.94	0.00	25.12	12.56	0.05	0.63	1.41	0.56	2.36	99.63
$(Nb,Ti)_5SiB_2$	31.88	14.10	0.34	29.90	14.99	0.04	1.22	4.35	0.62	2.54	99.11
$MoSi_2$	0	62.84	29.28	0.01	0.02	0.89	0.63	6.97	0.00	0.10	98.41

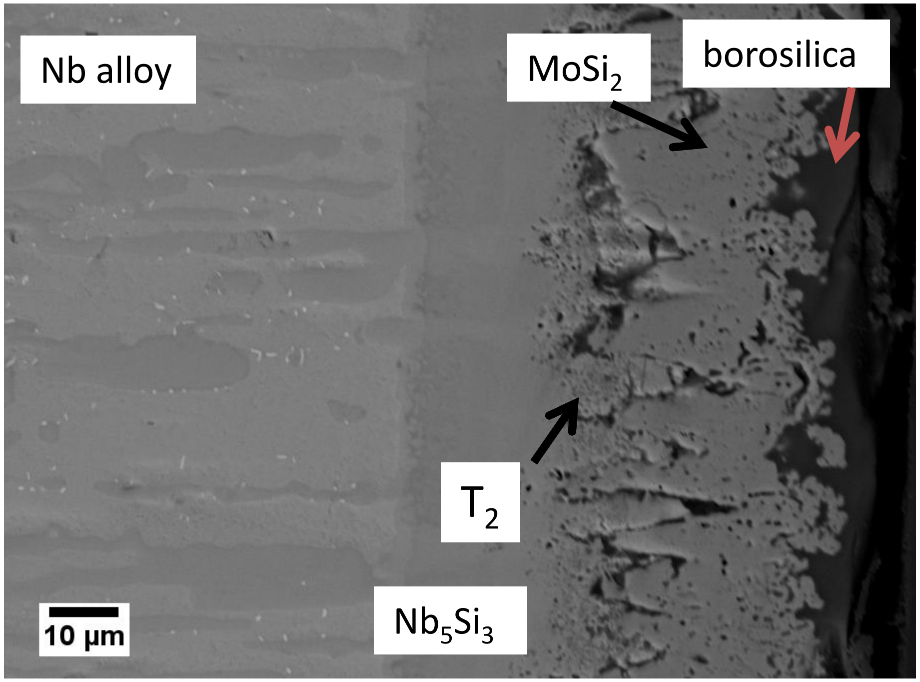
Oxidation: 1300°C 2 hours in air

B_{source}: Si ratio	Weight gain(mg/cm^2)
MoB:Si (1:10)	1.46
CrB_2:Si (1:20)	0.81, 0.82
TiB_2:Si (1:10)	1.03, 2.37
B:Si (1:20)	1.52



- CrB_2 B source shows the lowest mass gain
- Surface of sample is composed of borosilica and $MoSi_2$
- $NbSi_2$ converted to Nb_5Si_3 during oxidation



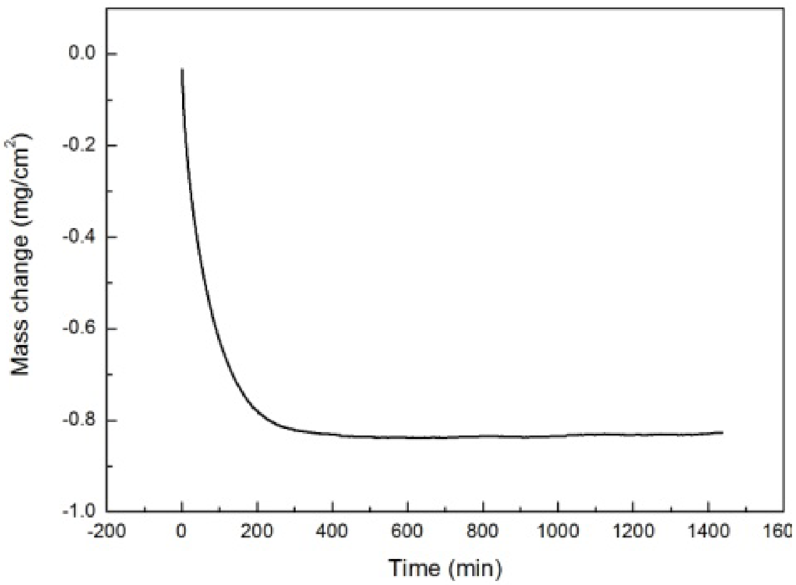


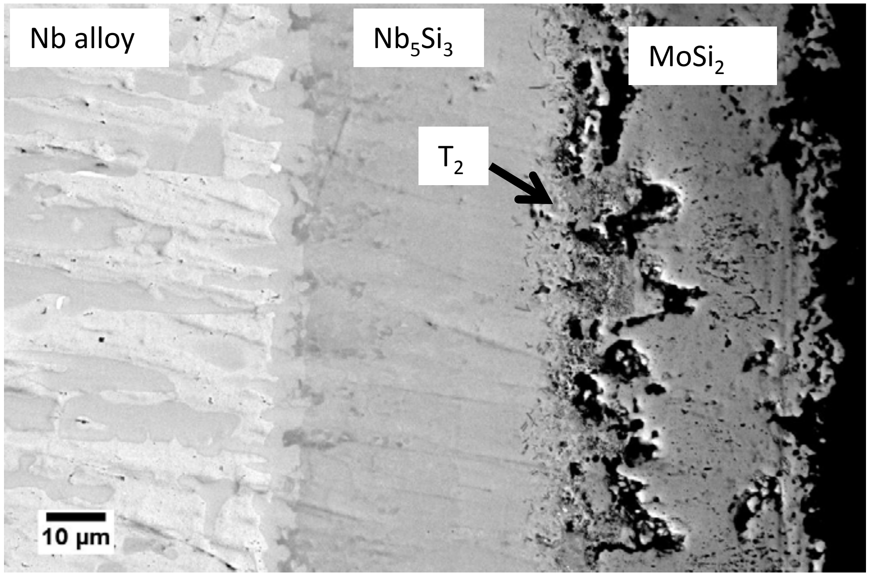
Oxidation in air 1300 °C /2h CrB_2 sample

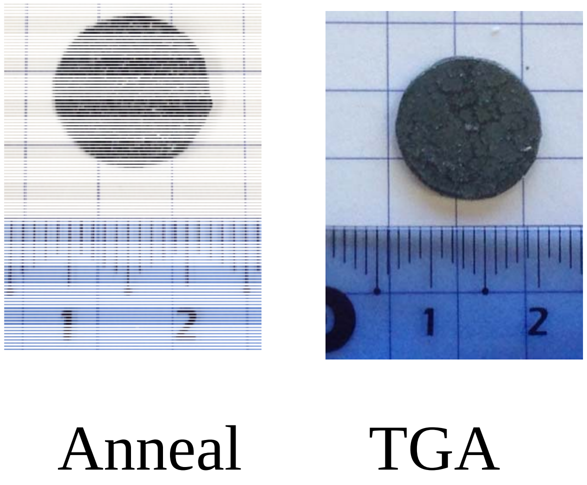
Oxidation: 1300°C 24 hours in air

- Prior to TGA testing, sample was first annealed in Ar atmosphere at 1200°C for 25 hours, then oxidized in air at 1300°C for 2 hours
  - Annealing step allows for $NbSi_2$ to convert to Nb_5Si_3 for better coating compatibiilty
- TGA testing was conducted on coated Nb alloy (CrB_2 B source) at 1300°C for 24 hours
  - Mass change: -0.83 mg/cm²
  - Initial transient stage (volatilization of MoO_3) followed by steady state oxidation
  - TGA curve shows a coating that prevents catastrophic oxidation of the alloy

Phase	Crystal Structure	CTE in a direction (C^{-1})	CTE in c direction (if applicable) (C^{-1})
MoSi2	Tetragonal I4/mmm (139)	1.04E-05	
Mo5Si3	Tetragonal I4/mcm (140)	$6.14x10^{-6}$	$1.10x10^{-5}$
NbSi2	Hexagonal P62 22 (180)	9.81E-06	1.13E10-5
Nb5Si3	Tetragonal I4/mcm (140)	~9.0E-06	

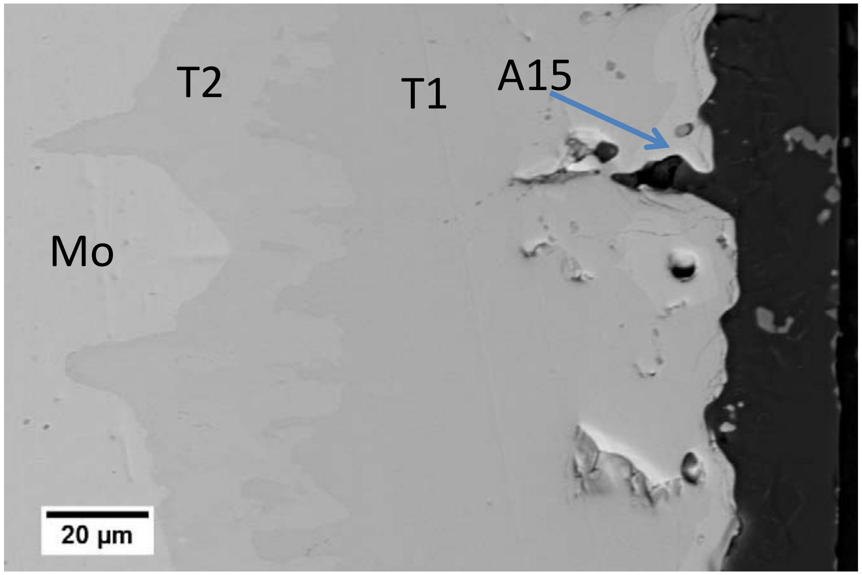


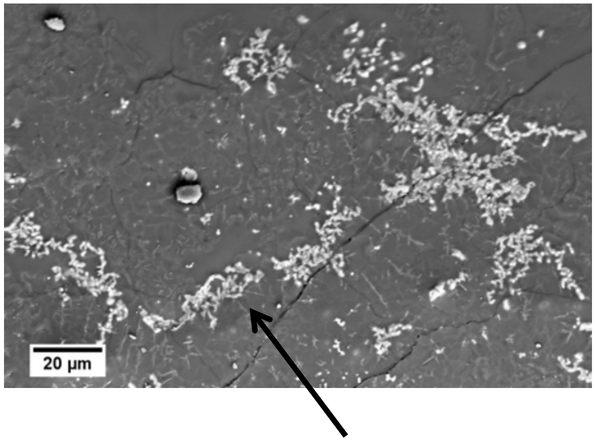




Zr additions to Mo-Si-B coating

- Zr additions were made first by arc melting Mo-Zr alloys (1, 2at.%Zr)
  - Apply Si-B pack cementation treatment
- Static oxidation tests and TGA testing of coated Mo-Zr alloys
  - Samples conditioned at 1500°C for 2 hours prior to testing
- Mo-1at.% Zr 1500°C 50 hours mass change: -0.047 mg/cm^2
- Zr rich particles seen in cross section and plan view of silica

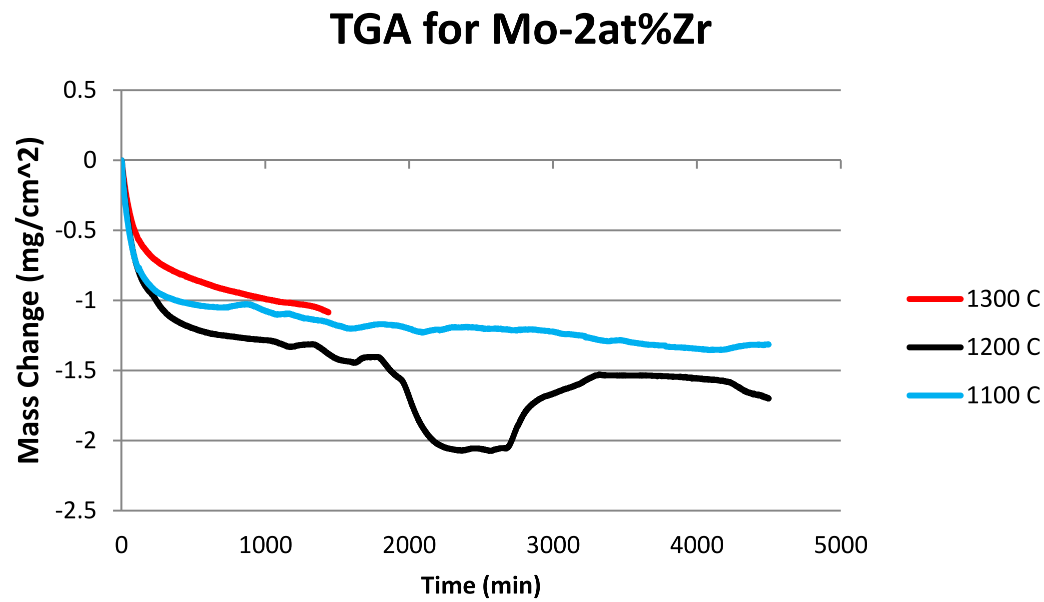


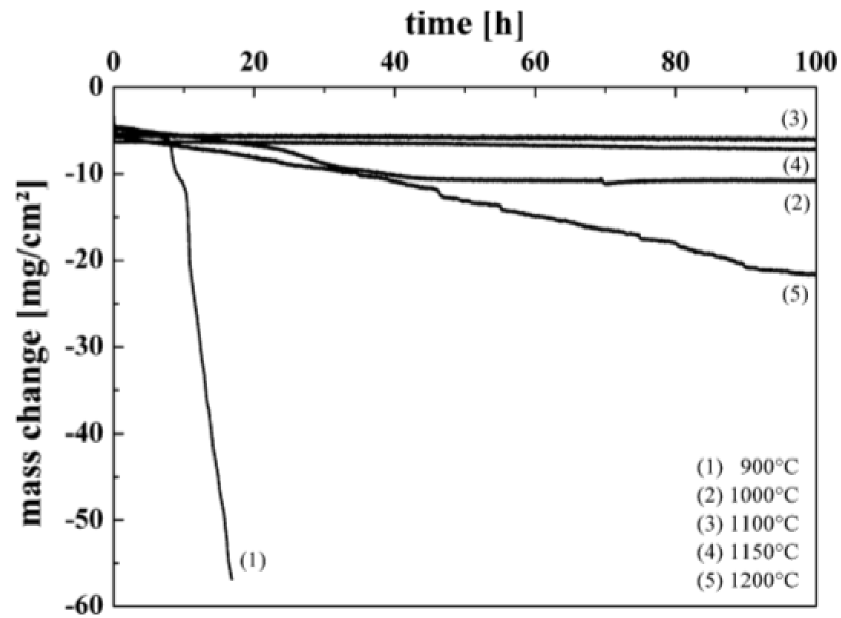


Element Line	Atom %	Atom % Error
O K	45.94	+/- 0.43
Na K	0.62	+/- 0.05
Al K	0.56	+/- 0.04
Si K	33.34	+/- 0.13
Zr L	19.54	+/- 0.09
Total	100.00	

TGA Results

- TGA Results of Si-B coated Mo-2atZr show reasonable oxidation
  - Zr additions do not inhibit the formation of an oxidation resistant coating
- Mass change less than those obtained from Mo-Si-B-Zr alloy [17]
  - Oxidation protection not obtained at temperatures above 1300°C



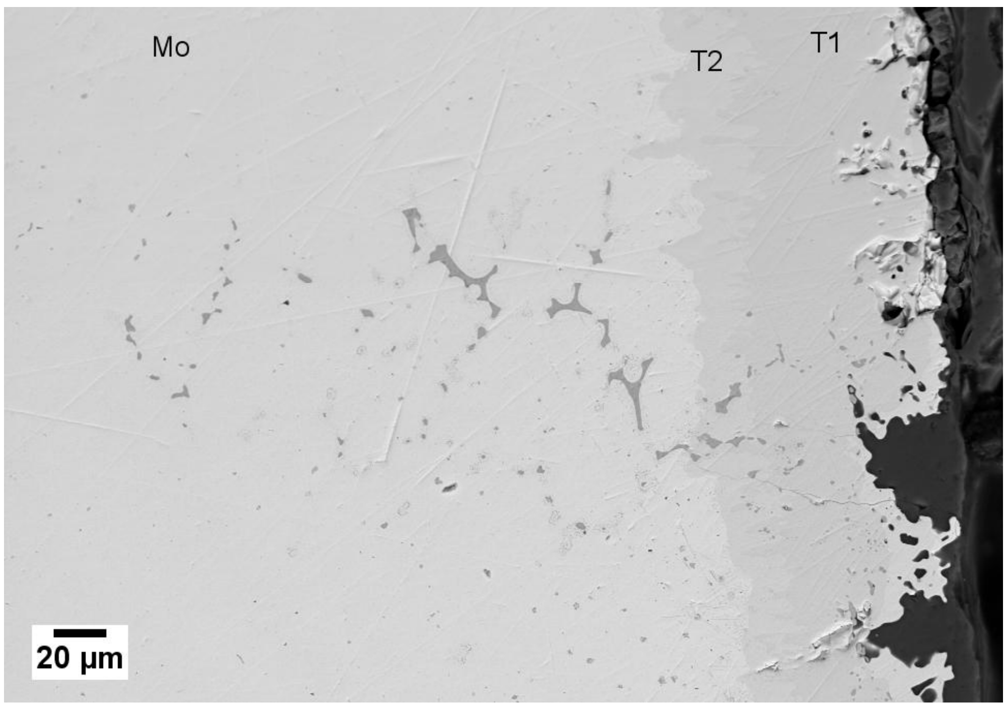


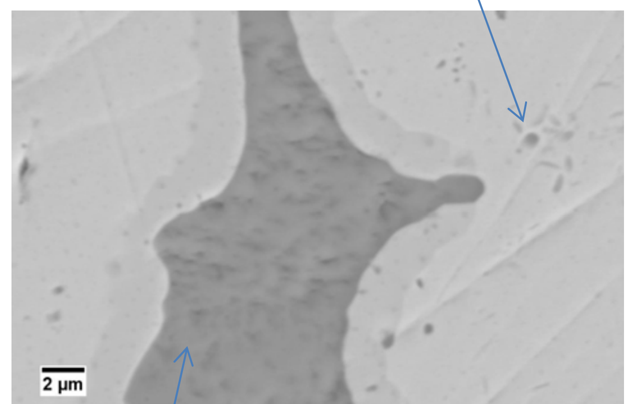
Calculated oxidation rates for MoSiB and MoSiB-1Zr alloys [13]

[17] S. Burk, B. Gorr, V. Trindade, H.-J. Christ, Oxidation of metals, 73 (2010) 163-181.

SEM: Mo-2Zr (1500°C, 24 hr)

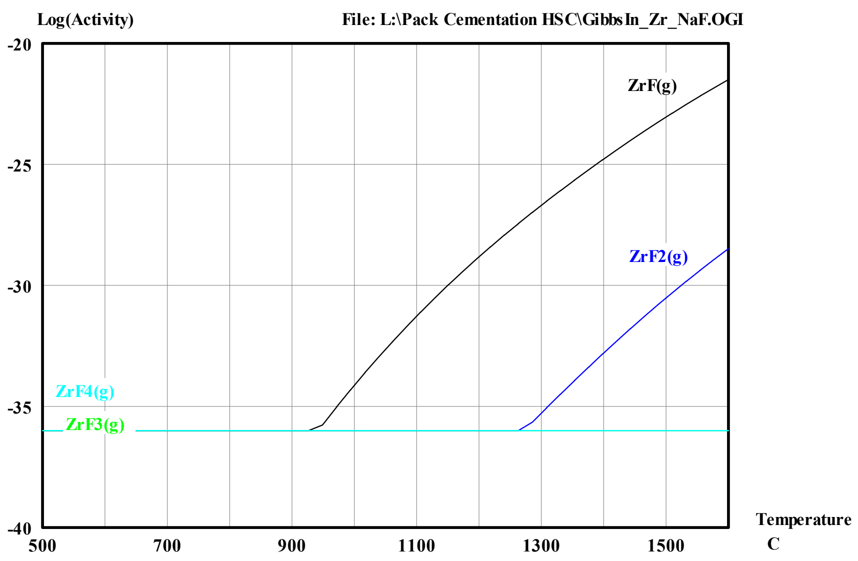
- Mass change: 1.40 mg/cm^2
- Zr-O phase seen within the substrate (~250 µm from the surface)
  - Zr additons increasing oxygen diffusion through coating



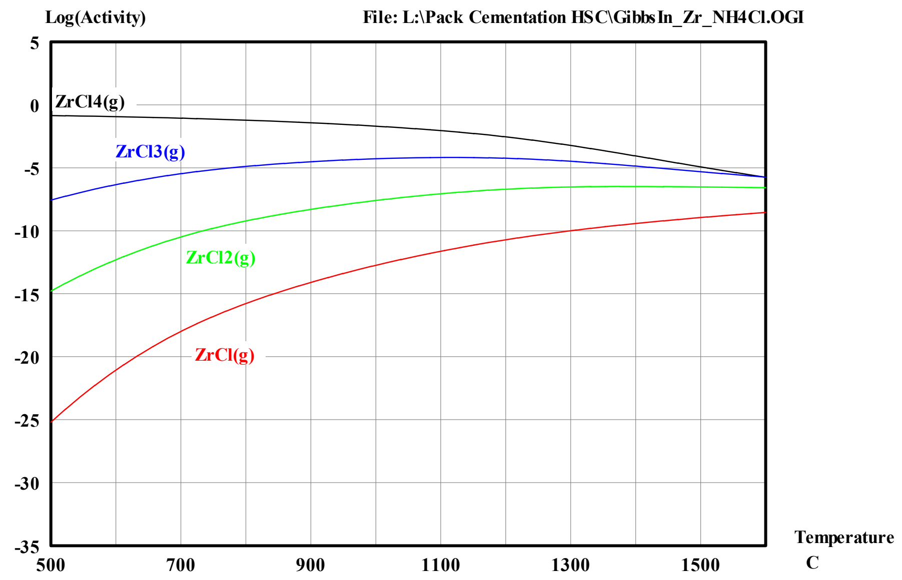


Zr additions to Mo-Si-B coating

- Zr additions should be focused within the coating as opposed to the substrate
  - Could produce unwanted phases compromising the properties of the substrate
- Pack cementation treatment to infuse Zr into the Mo-Si-B coating
  - Check vapor pressures to assess feasibility
- $ZrCl_x$ much more active compared to ZrF_x



NaF activator



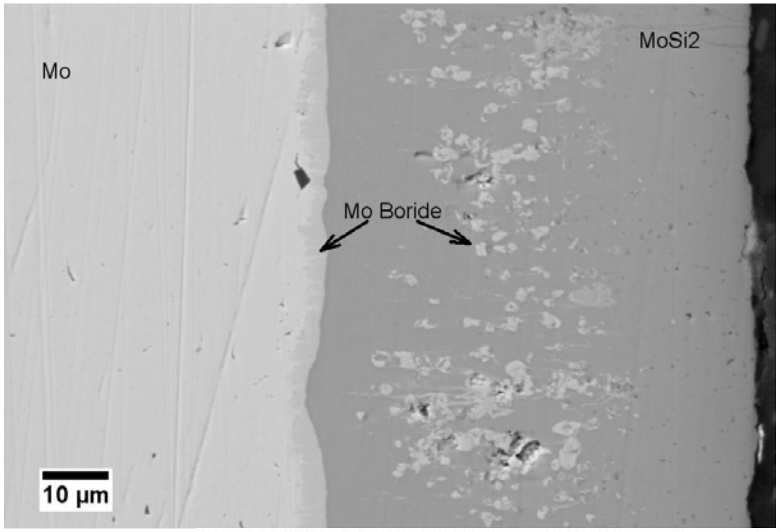
NH_4Cl activator

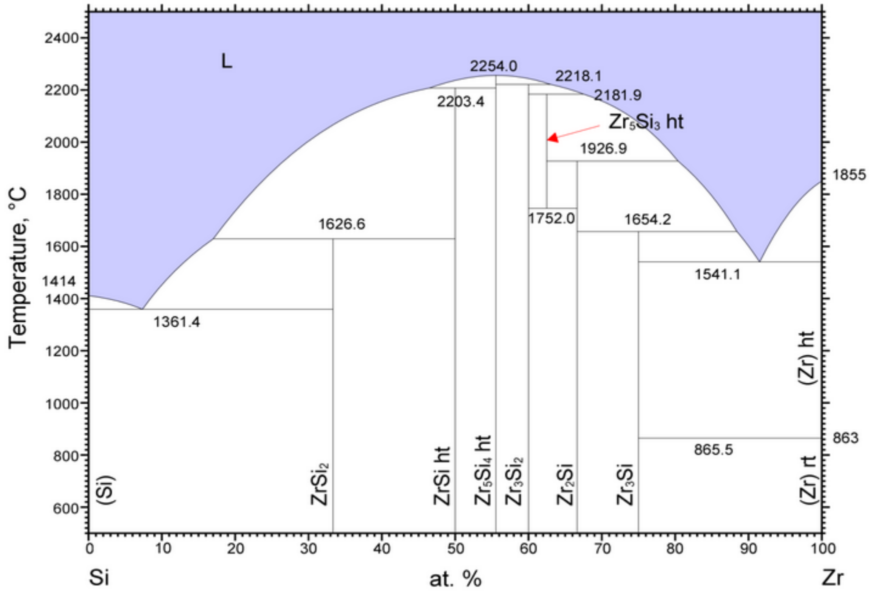
Zr additions to Mo-Si-B coating

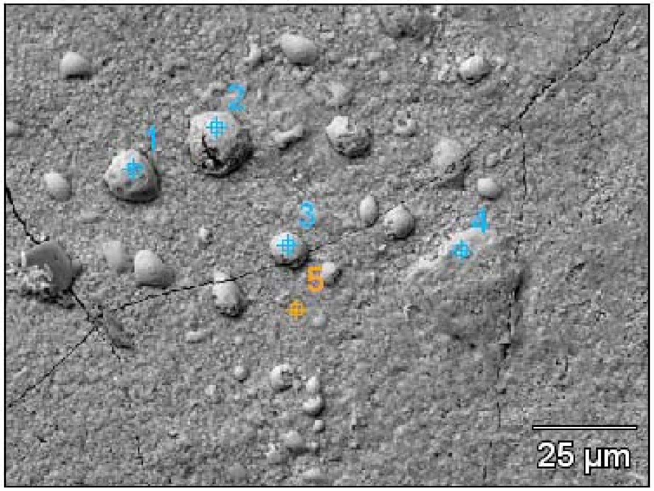
- Si-B pack cementation applied to polished Mo coins (2mm thickness)
  - 1000°C 50 hrs
- Samples were ultrasonic cleaned and packed in Zr pack
  - 5 wt.% Zr
  - 2.5 wt.% NH_4Cl
  - Bal. Al_2O_3
  - 1000°C 10 hr
- Samples oxidized at 1500°C

Zr additions to Mo-Si-B coating

- As- Packed
  - Coating composed of $MoSi_2$ and Mo boride (standard as-pack structure)
- EDS on the surface suggest formation of Zr silicides



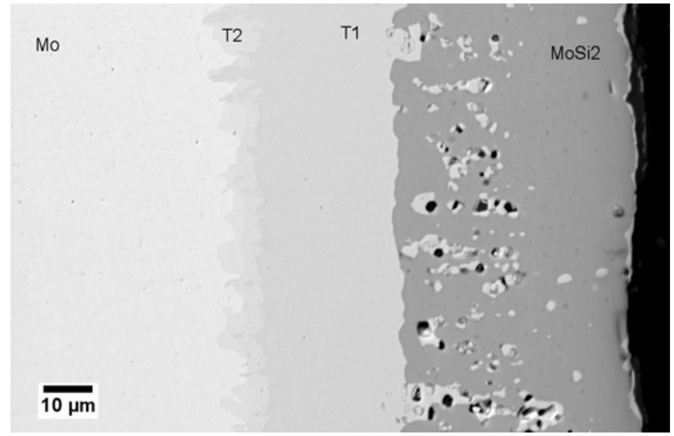


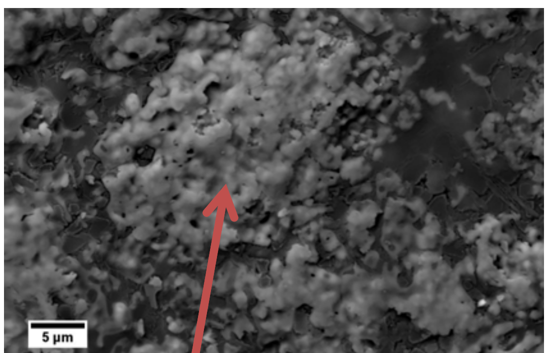


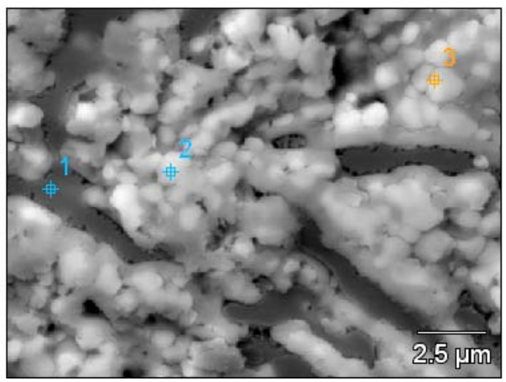
	O-K	Na-K	Al-K	Si-K	Zr-L	Mo-L
pt1	12.20		4.68	30.53	52.59	
pt2	15.86	0.71	0.23	33.70	49.49	
pt3	22.50		0.84	30.75	45.92	
pt4	25.04			27.57	47.38	
pt5				75.69		24.31

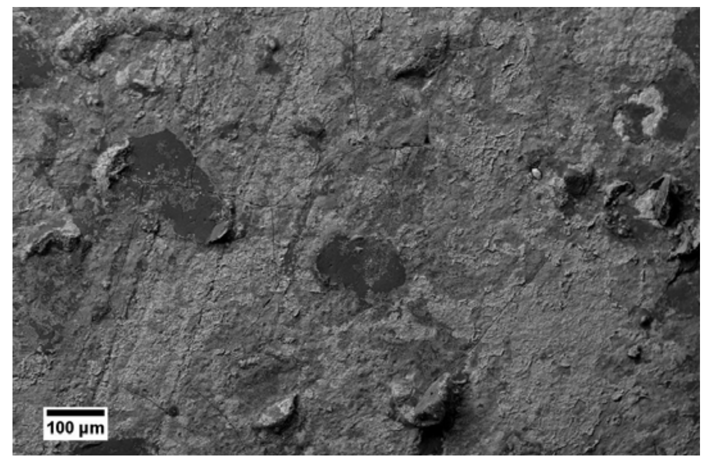
Zr additions to Mo-Si-B coating: oxidation (1500°C 2hr)

- Mass change: 0.25 mg/cm^2
- Cross section after oxidation shows Mo-Si-B coating has converted some of the $MoSi_2$ into T_1 and T_2
- Surface of sample appears to be completely covered by Zr-O particles
  - EDS detects regions containing both ZrO_2 as well as Zircon ($ZrSiO_4$)









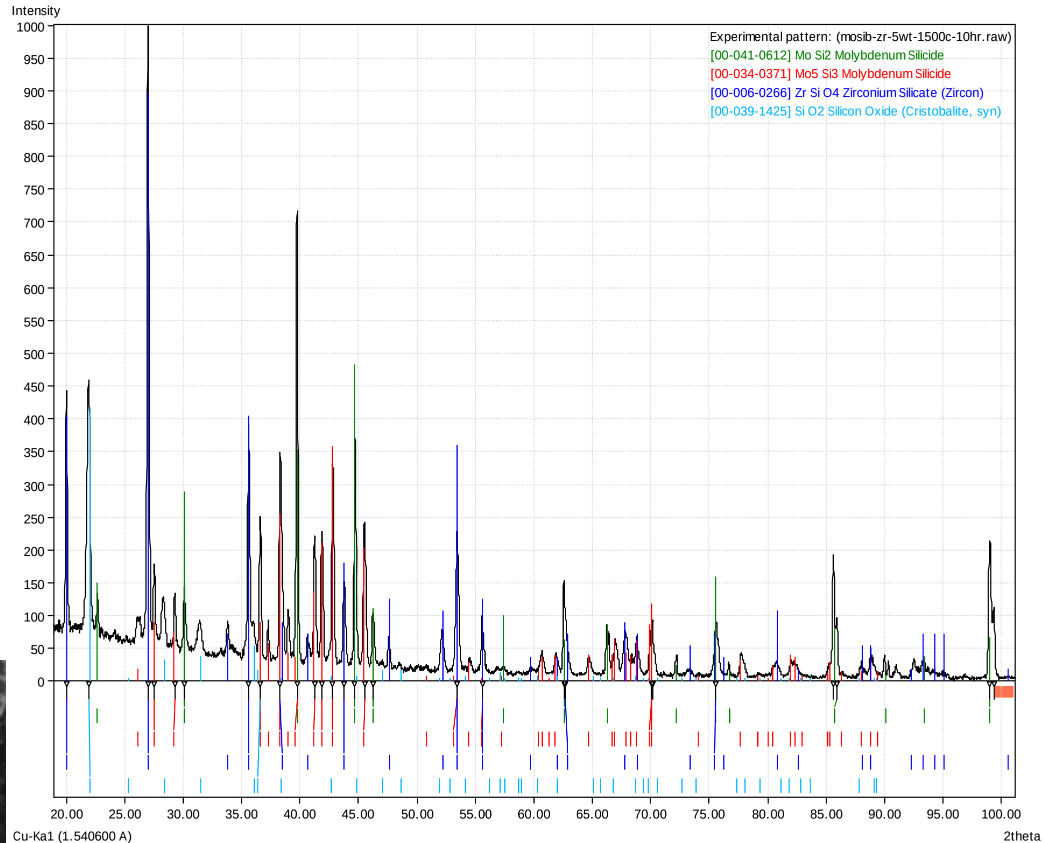
250 X

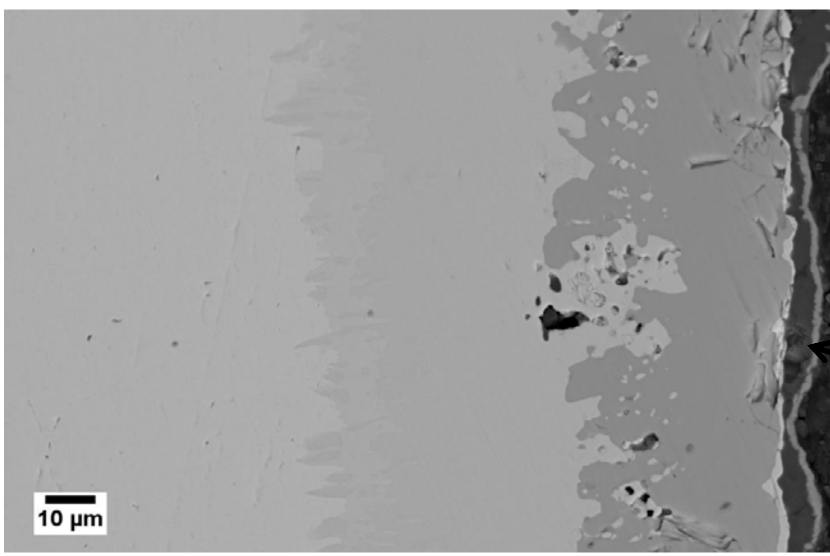
Element Line	Atom %
O K	62.69
Al K	0.37
Si K	19.87
Si L	---
Zr L	17.07
Zr M	---
Total	100.00

	O-K	Na-K	Al-K	Si-K	Zr-L
Base(209)_pt1	55.56	0.73	0.47	26.77	16.47
Base(209)_pt2	54.93			9.42	35.65
Base(209)_pt3	56.17			6.98	36.85

Zr additions to Mo-Si-B coating: oxidation (1500°C 10hr)

- 1500 C 10 hr, mass change: 1.30 mg/cm^2
- XRD shows peaks corresponding to Zircon, $MoSi_2$ and T_1
- SEM shows a layer of Zircon formation on top of the borosilica

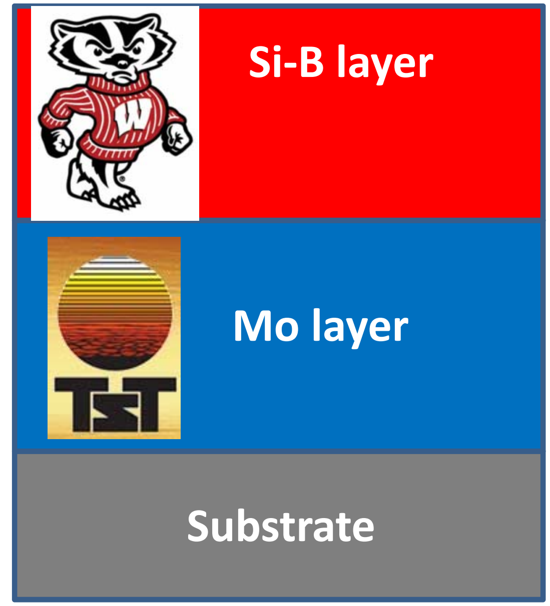




Element Line	Atom %
O K	63.40
Al K	0.20
Si K	18.14
Si L	---
Zr L	18.26
Zr M	---
Total	100.00

Future Work: Utilize plasma spray deposition

- Thermal spray process combined with Si-B pack cementation technique is an effective process to produce Mo-Si-B coatings on larger samples [18]
  - Plasma spray deposition of Mo allows for samples to be scaled up in size and complexity
- Formation of a larger coating allowing for more aggressive oxidation testing for Nb and Nb alloys

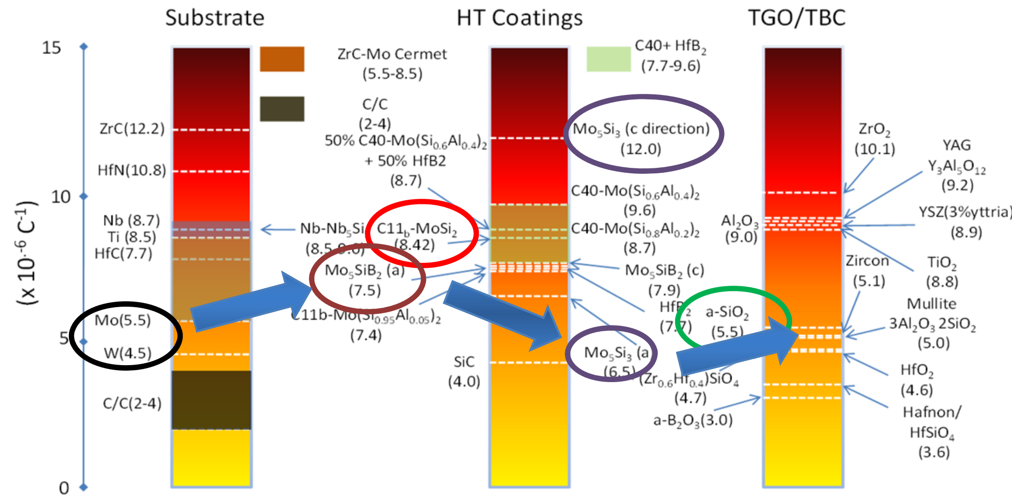


[18] P. Ritt, O. Lu-Steffes, R. Sakidja, J. H. Perepezko, W. Lenling, D. Crawmer, J. Beske. "Application of Plasma Spraying as a Precursor in the Synthesis of Oxidation Resistant Coatings." *Journal of Thermal Spray Technology.* (2013)

Future Work: Formation of Smart Coating

- Optimization of parameters for the CVD coating processes
- Integration of the smart coating into an expanded range of other TM-based alloys with emphasis on Nb-based alloys.
- Coatings with a compositional gradient decrease residual stresses [19]
  - Sharp changes in stresses may result in delamination of the coating
- Object Oriented FEA (OOF2) is public domain finite element analysis (FEA) software created by NIST to investigate the properties of microstructures
  - utilizes actual microstructure images as the basis for the finite element mesh
  - Obtain a coating structure that minimizes the residual stresses due to CTE mismatch of the coating and substrate

CTE Compatibility in
Ultra-high Temperature System



COMPOSITE AND GRADED APPROACHES TO HT COATING DESIGN

In thermodynamically compatible systems, the thermal expansion of the phase mixture as a first estimate is monotonic: $CTE(A_xB_{1-x}) = xCTE(A) + (1-x)CTE(B)$

TBC Temperature (°C)	BC Temperature (°C)	Temperature Nb-Silicide (°C)
1370	1225	1090
1510	1315	1150
1650	1405	1200
1790	1490	1260

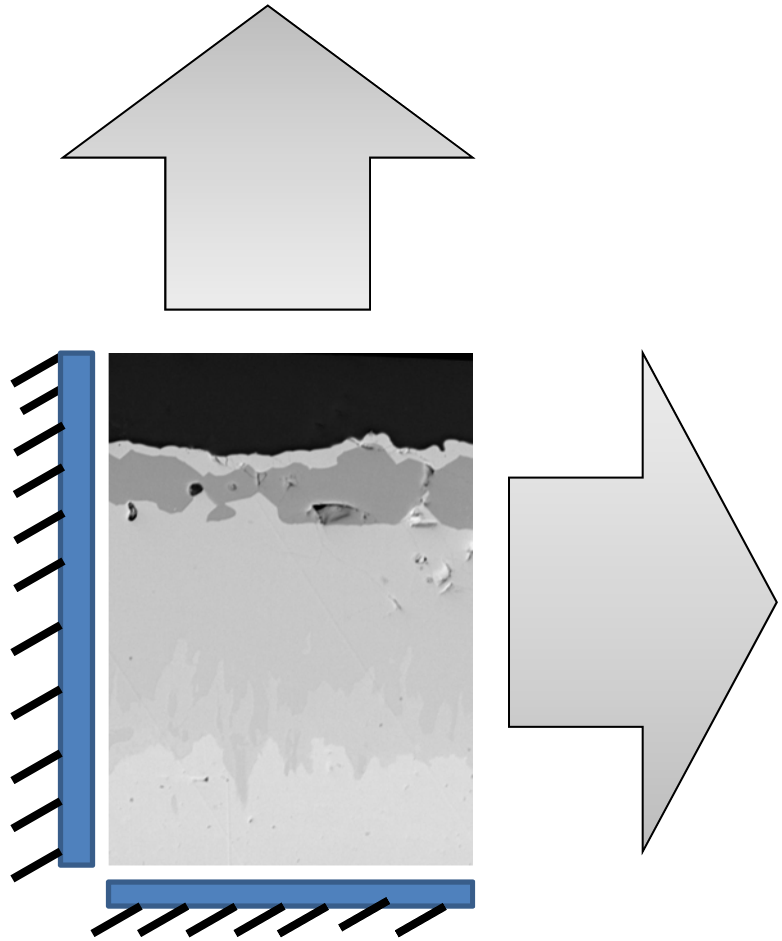
Temperatures of the TBC, BC, and Nb-Silicide as Measured during the JETS Test; the BC Temperature Was Calculated Using Measurements of the Temperatures of the TBC and Nb-Silicide Substrate, Together with Thermal Conductivity Measurements [20]

[19] X.C. Zhang, B.S. X u, H.D. Wang, Y. Jiang, Y.X. Wu, Thin Solid Films, 497 (2006) 223-231

[20] Bewlay, B. P., Jackson, M. R., Subramanian, P. R., & Zhao, J. C. (2003). A review of very-high-temperature Nb-silicide-based composites. *Metallurgical and Materials Transactions A*, *34*(10), 2043-2052.

OOF-2: Boundary Conditions

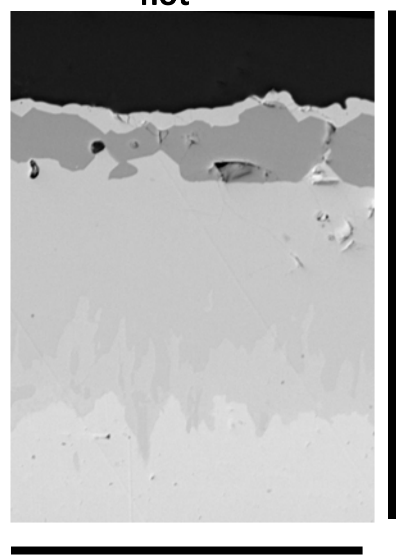
- Bottom
  - Y=0 (substrate)
  - X free to move (infinite plane)
- Left side
  - X=0
  - Y free to move (no constraints on top of coating)
- Right side
  - X= allow for free expansion such that $\sum \sigma_x = 0$
  - Want non-free surfaces to expand in a planar fashion
    - Run simulation first under no constraints to provide estimate of expansion taking place



OOF-2: Materials and BC

- Isotropic values
- Assume at 1000°C the coating is in a relaxed state (temperature at which coating forms).
- Boundary Conditions
  - T_{hot}= 300
  - T_{cold} = 0
  - Y_{bottom} =0
  - X_{left} =0
  - X_{right} = 2.23x10^{-8} m

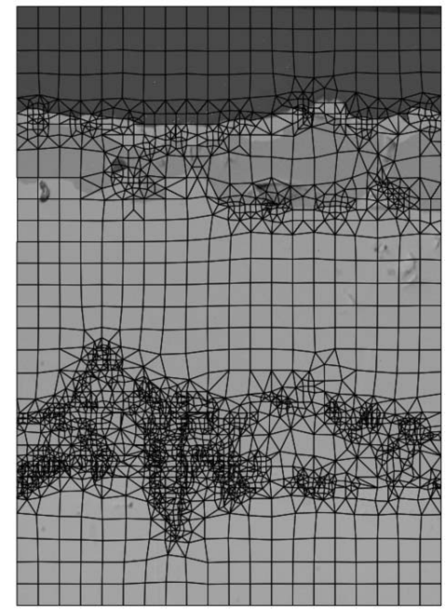
T_{hot}



138.35 microns

T_{cold}

98.28 microns

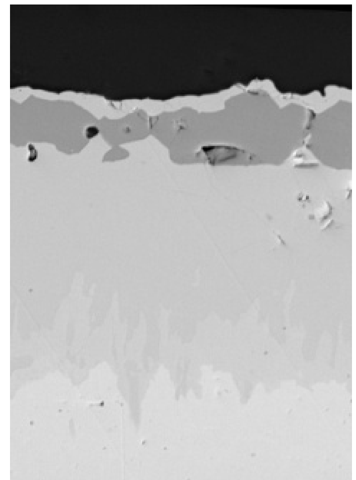


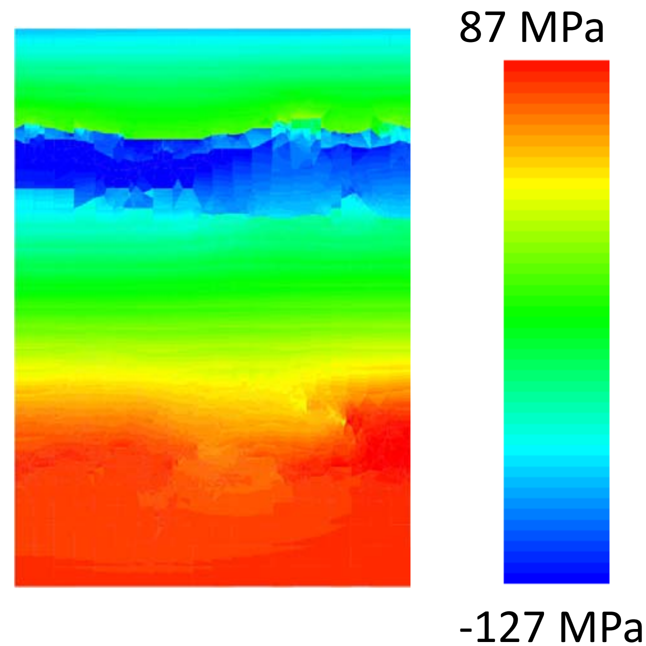
FEM mesh generated in OOF-2

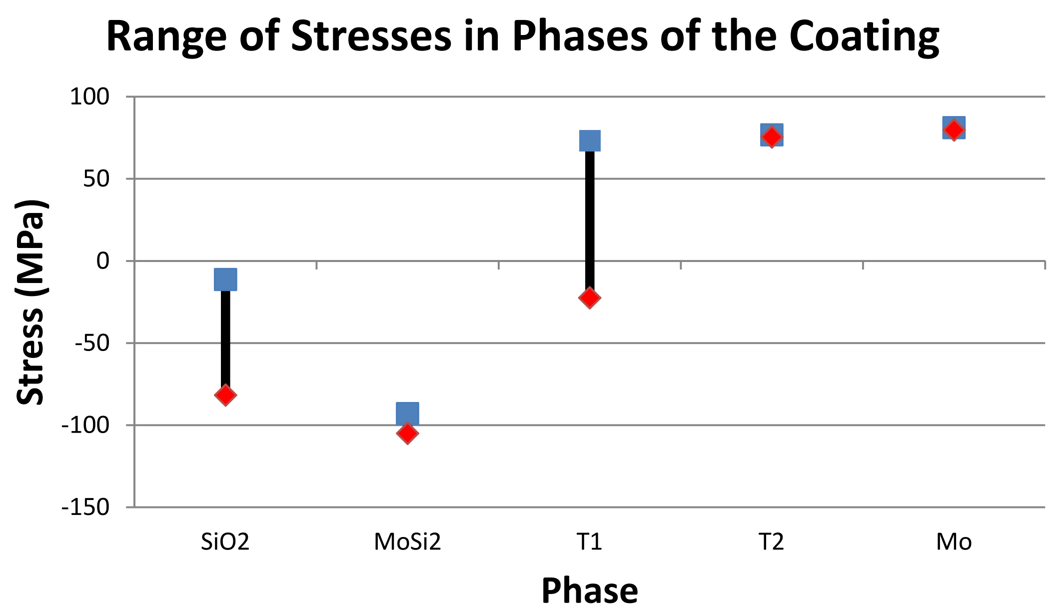
Material	Density (kg/m^3)	Young's Modulus (GPa)	Poisson Ratio	Thermal Cond (W/mK)	CTE (C^{-1})
Mo	10200	324.8	0.293	138	6.50x10^{-6}
MoSi2	6300	432	0.151	28.6	1.04x10^{-5}
Mo5Si3 (T1)	8190	363	.268	19	8.35x10^{-6}
Mo5SiB2 (T2)	8800	383	0.27	28	8.5x10^{-6}
borosilicate glass	2400	64	0.19	1.1	4.00x10^{-6}

OOF-2: Stesses

- Top portion of coating is in compression while bottom (substrate) is in tension
- Compressive yield stress for $MoSi_2$: 769 MPa
  - Suggests that coating will be intact under these conditions







Concluding Remarks

- Mo-Si-B coating applied to Nb alloys to provide oxidation resistance
  - Can be synthesized first by applying a Mo layer via decomposition of molybdenum hexacarbonyl followed by a Si-B co-pack cementation process
  - Boride formation during pack cementation process within Nb produces undesirable coating structure, but can be optimize using different boride source
  - Enhanced oxidation protection by reducing the formation of Nb oxides in favor for a protective borosilica coating
- Coated Mo-Zr alloys show promise that the transition metal oxide can develop within the Mo-Si-B coating to provide further environmental protection.
  - Zr can be added to Mo-Si-B coating via pack cementation technique
    - Upon oxidation, oxidation resistant silica and zircon/zirconia form
  - Coating provides the necessary components for the development of a smart coating for refractory metal alloys.

Thank You!

List of papers published, conference presentations, students supported under grant FE0007377

- Publications:
  - Lu-Steffes, O. J., Sakidja, R., Bero, J. & Perepezko, J. H. Multicomponent coating for enhanced oxidation resistance of tungsten. *Surface and Coatings Technology* **207**, 614-619, doi:10.1016/j.surfcoat.2012.08.011 (2012)
  - P. Ritt, O. Lu-Steffes, R. Sakidja, J. H. Perepezko, W. Lenling, D. Crawmer, J. Beske. "Application of Plasma Spraying as a Precursor in the Synthesis of Oxidation Resistant Coatings." *Journal of Thermal Spray Technology.* doi:10.1007/s11666-013-9947-2 (2013)
  - C. C. Dharmawardhana, R. Sakidja, S. Aryal, and W. Y. Ching, "Temperature dependent mechanical properties of Mo--Si--B compounds via ab initio molecular dynamics ," *APL Mater*. 1, 012106 (2013), DOI:10.1063/1.4809539
- Conferences
  - Research results were presented at the 2012 Materials Science and Technology conference in the symposium "Beyond Nickel Based Superalloys-II." The title of the presentation was "Transition Metal Doped Mo-Si-B Coatings."
  - Research results were presented at the 2012 First ACEEES International Forum. The title of the presentation was "Design and Synthesis of Zr Doped Mo-Si-B Coatings"
  - Research results were presented at the 2013 Materials Science and Technology conference in the symposium "High Temperature Corrosion and Oxidation of Materials." The title of the presentation is "Mo-Si-B Coatings on Niobium Base Systems for Enhanced Oxidation Protection"
  - Research results were presented at the 2013 Second ACEEES International Forum. The title of the presentation was "Enhanced Oxidation Protection for Niobium Base Alloys Utilizing a Mo-Si-B Coating"
  - Research Accomplishments from this project were presented at the 2012 University Coal Research/Historically Black Colleges and Universities and Other Minority Institutions Contractors Review that took place on May 31, 2012.
  - Research Accomplishments from this project were presented at the 2013 University Coal Research/Historically Black Colleges and Universities and Other Minority Institutions Contractors Review that took place on June 11-13, 2013.
- Support
  - John Perepezko; PI
  - Otto Lu-Steffes; graduate student
  - Dana Jackson; undergraduate laboratory assistant