Oxidation of thin film binary entropy alloys

Martijn Homsma, Wesley van den Beld, Robbert van de Kruijs, Marcelo Ackermann

XUV Optics Group, MESA+ Institute, University of Twente

PREDICTING ALLOY BEHAVIOUR

- General Guidelines from Metallurgy:
  Hume-Rothery (HR) rules
  1. Minimize atomic radii difference (δ) (~below 4%)
  2. Identical crystal structure of metals used
  3. Minimize Electronegativity difference (**Δχ**)
  4. Maximize valence electron concentration (VEC) and minimize the difference between metals used.

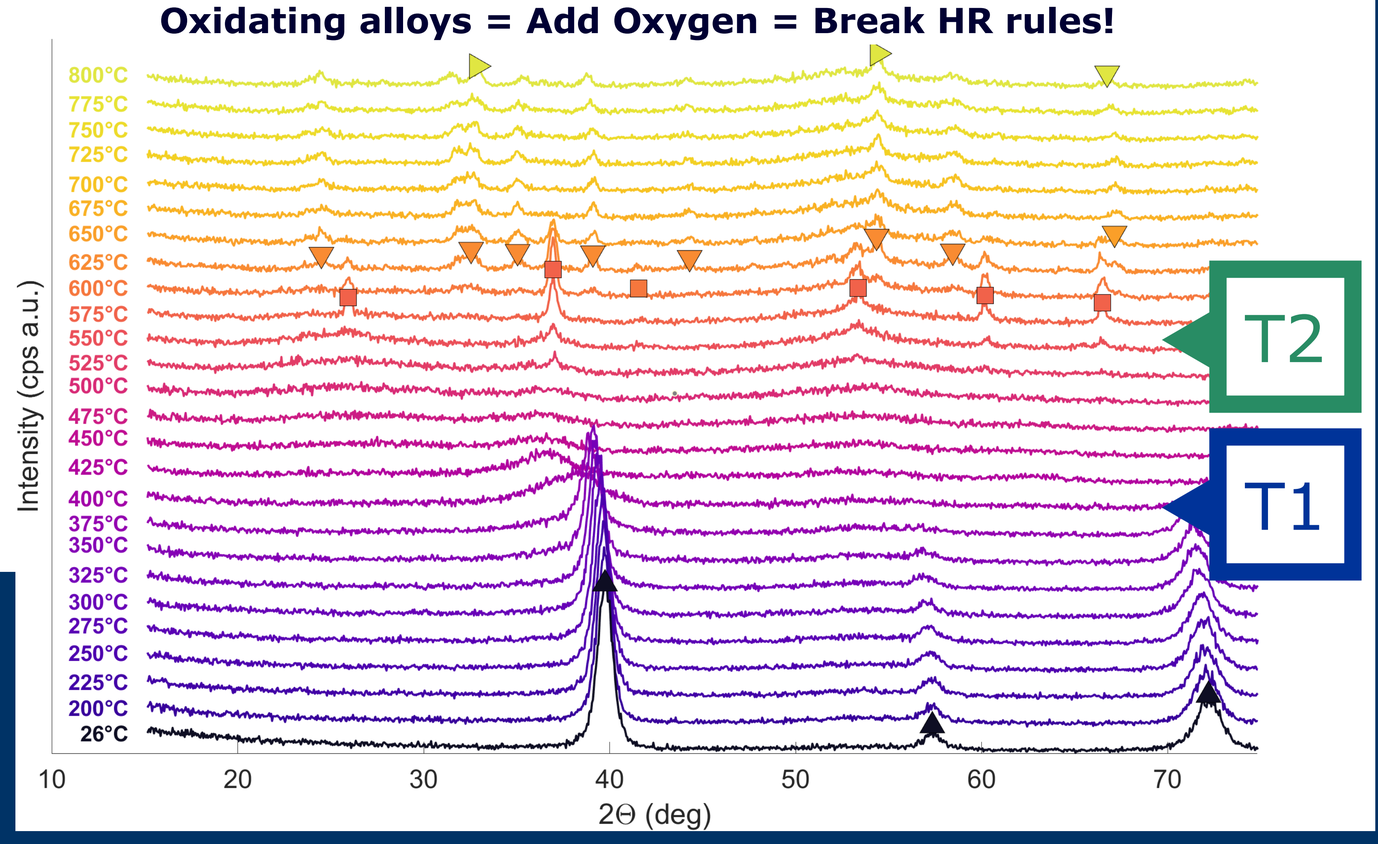
- Following rules → **Single Phase** Solid Solution
- Breaking rules → **Glass** Forming Solution

Two transition temperatures:

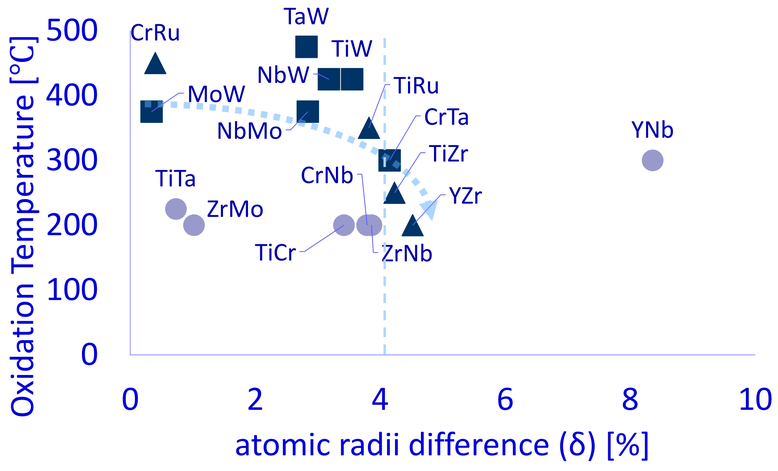
T1 = As-deposited phase into "Glass Forming Solution" Amorphous

T2 = Polycrystalline oxide formation; Demixing temperature

Oxidating alloys = Add Oxygen = Break HR rules!

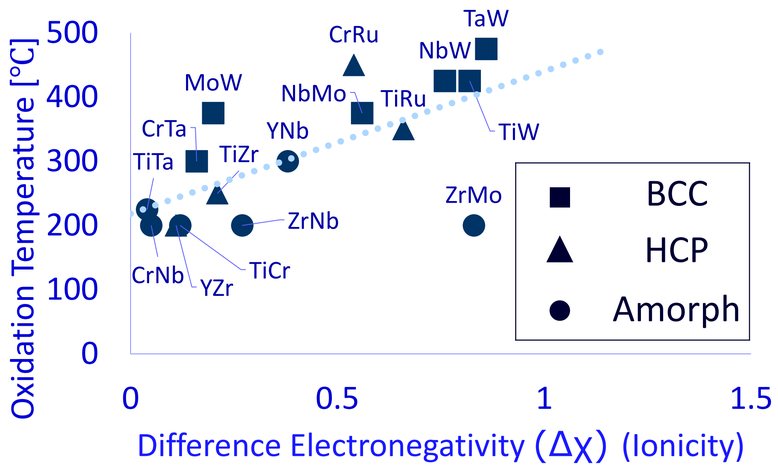


HR #1: High δ means stacking errors which increases Oxidation



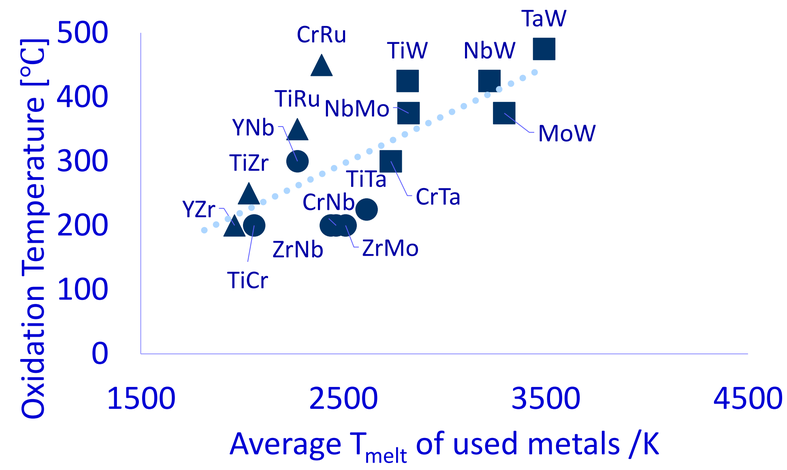
Crystal: δ >4% lower **Oxidation Temp T1**
Amorphous: poor Oxidation Temp

HR #3: High $\Delta\chi$ implies an electronegative element which prevents Oxidation



Increase $\Delta\chi$ = higher **Oxidation Temp T1**

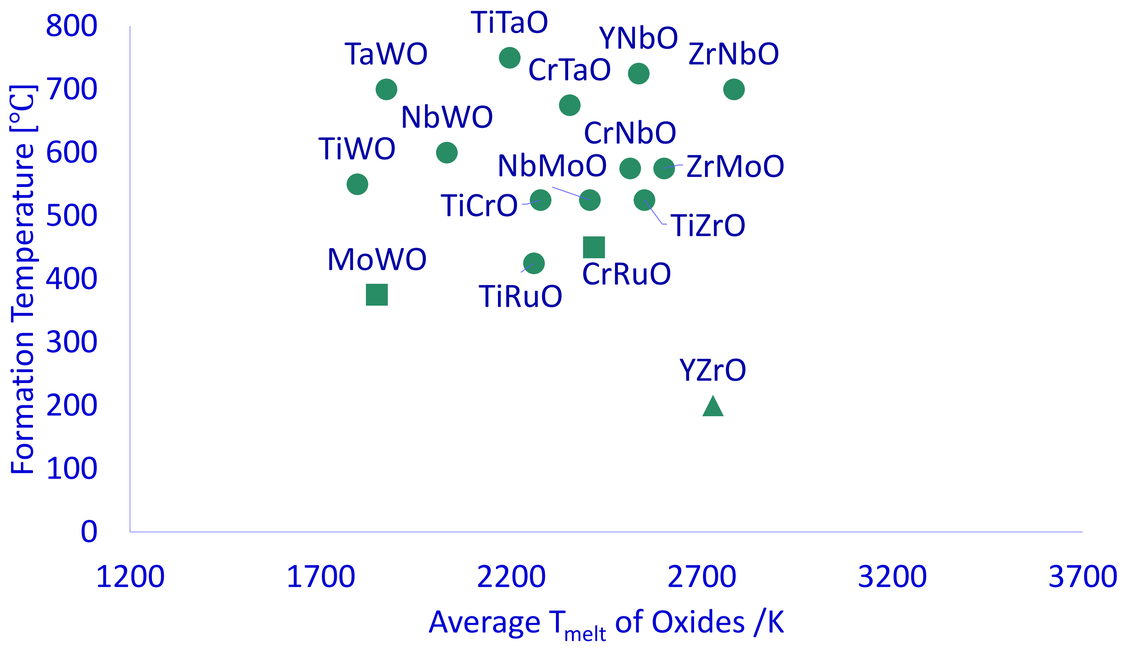
High $\langle T_{melt} \rangle$ means Stability which slows Oxidation



High $\langle T_{melt} \rangle$ = high **Oxidation Temp T1**
Sub-trends for different as-depo structures

What about Polycrystalline Oxide Formation Temperature(s) [T2]?

High $\langle T_{melt,\,Oxides} \rangle$ is the same as reduced Mobility which means a higher **Formation Temperature T2**



…But there is no trend? Same for HR rules
Research Ongoing

HR rules + $\langle T_{melt} \rangle$ explain **T1**

- Metallurgy rules still apply to thin films:
  - Lattice distorted crystals increase oxidation
  - Ionicity decreases oxidation (as does covalency)
  - Increase in melting temperatures lowers oxide temperature

None of the (HR) rules explain T2

- Using Metallurgy rules for oxides does not explain why the Formation Temp is affected.
- Help! ☹

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