UNIVERSITÄT BAYREUTH

Werkstoffe Metallische

Entropy Effects on Mechanical Properties of Single-Phase HEA (fcc, bcc and hcp)

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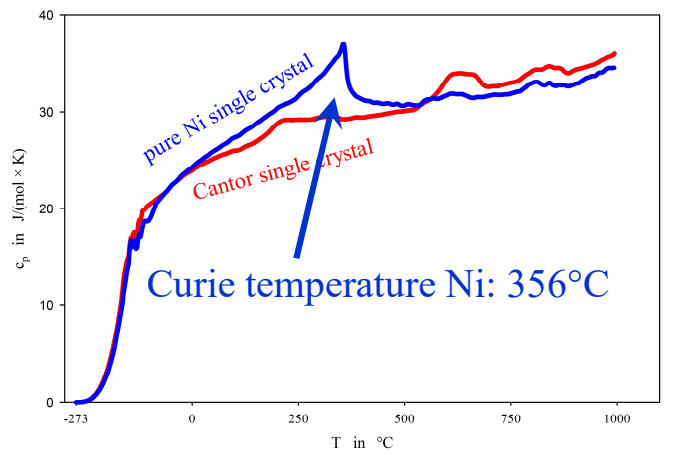
Experimental Determination of Entropy (SX!)

$$S_{total} = S_{conf} + S_{th} = S_{conf} + \int_0^T \frac{c_p}{T'}\, dT'$$

specific heat capacity:



Determined in 3 different temperature regimes:

- -170°C → +300°C with DSC204
- -50°C → +1000°C with DSC404 steel
- +200°C → +1540°C with DSC404 rhodium

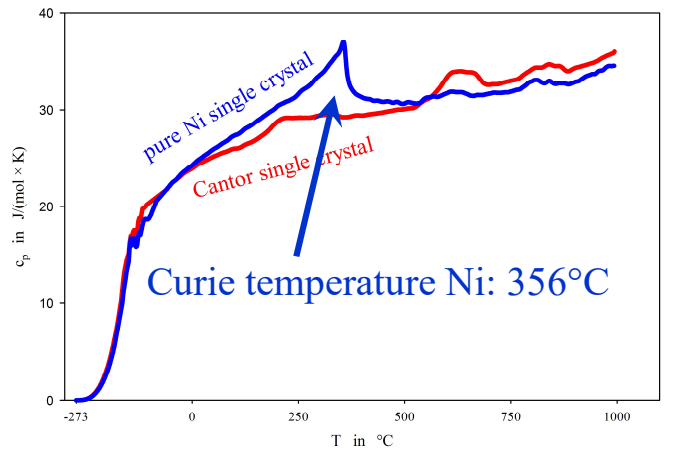
Experimental Determination of Entropy (SX!)

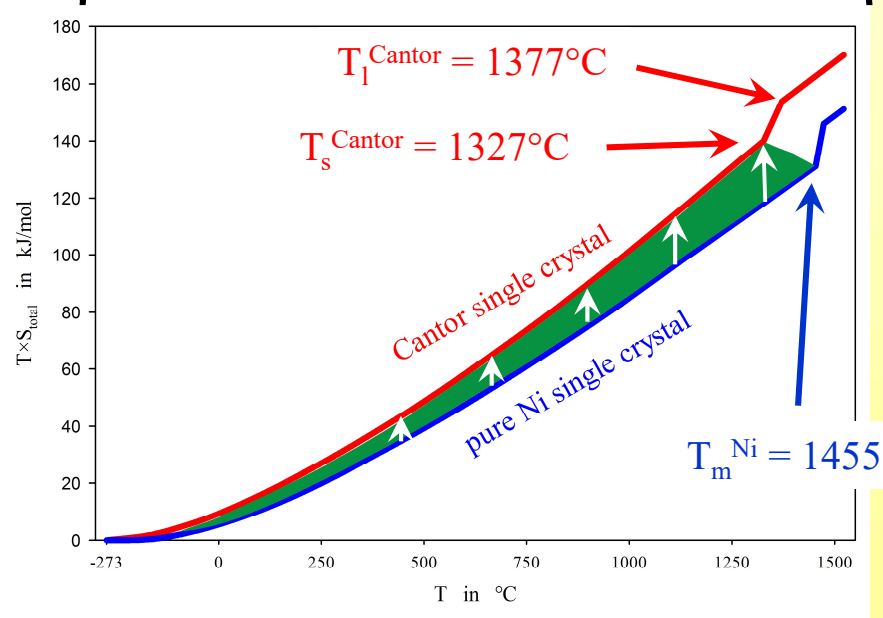
$$S_{total} = S_{conf} + S_{th} = S_{conf} + \int_0^T \frac{c_p}{T'}\, dT'$$

$$S_{conf}^{Cantor} = 1.61 \cdot R$$

$$G = H - T \cdot S_{total}$$

specific heat capacity:





To our knowledge not published in literature!

Entropy Contributions to Gibbs Free Energy:

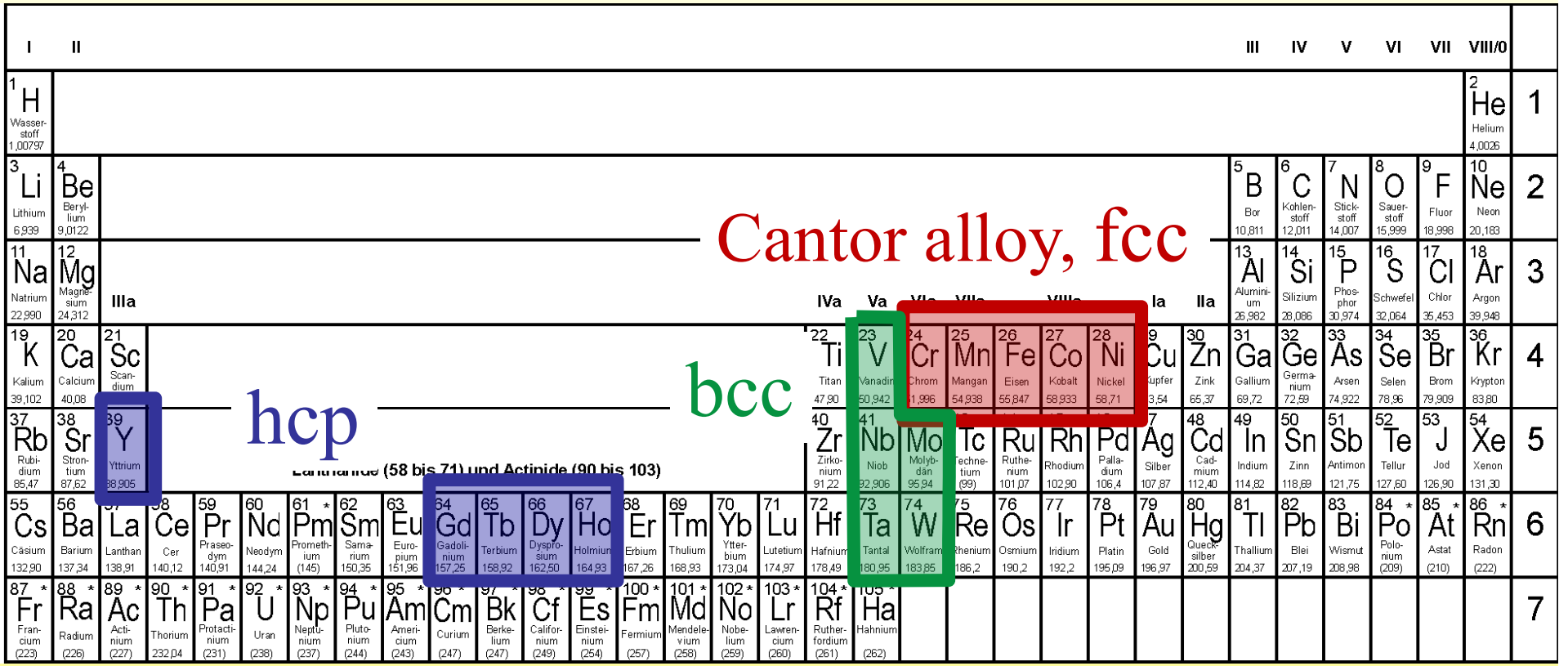
at 1400°C (in-between T_m^{Ni} and T_s^{Cantor}) in kJ/(mol atoms):

- $T \cdot S_{thermal} \approx 138$
- $T \cdot S_{conf} \approx 23$
- $T \cdot S_{impurities} \approx 0.1$
- $T \cdot S_{vacancies} \approx 0.01$

In comparison: enthalpy of formation of intermetallic phases:

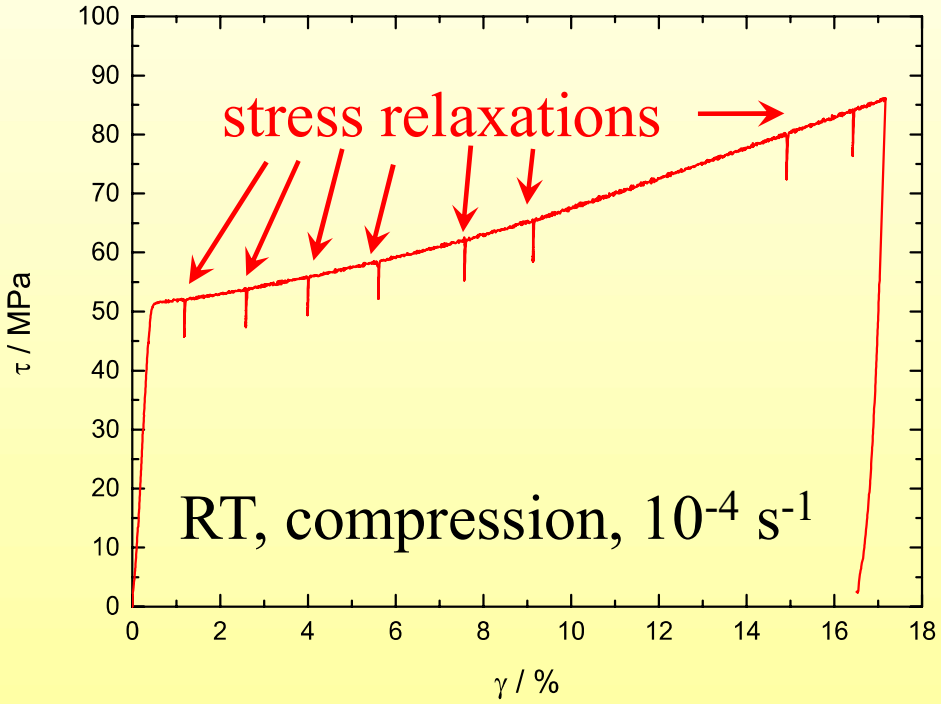
$FeAl \approx 33$ $FeAl_3 \approx 30$ $NiAl \approx 66$ $Ni_3Al \approx 41$ $PtAl \approx 97$

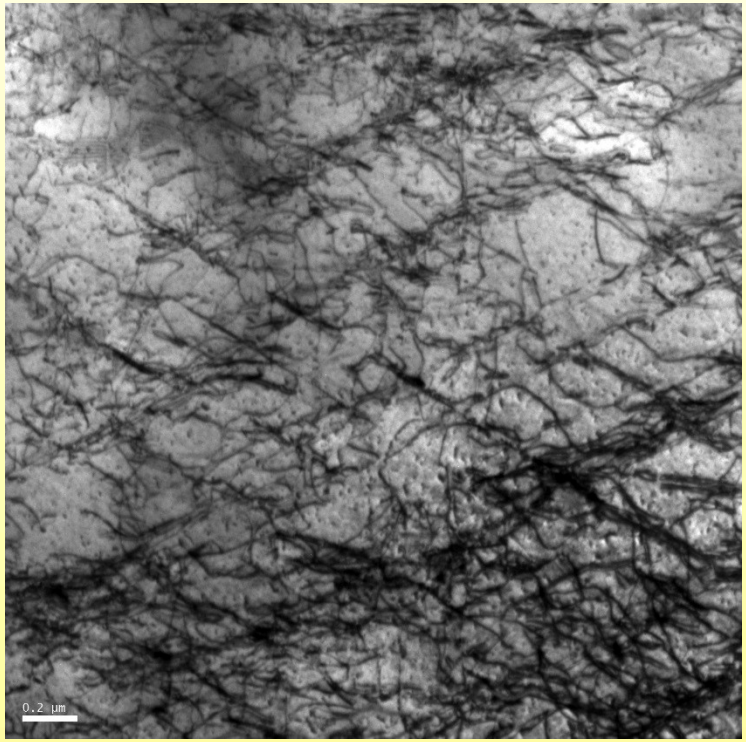
High Entropy Alloys



hcp: Y + Gadolinium + Terbium + Dysprosium + Holmium

Deformation, Microstructure of SX Cantor Alloy





(111) glide plane

Forschungszentrum Jülich

Goals and Cooperation

- work program: entropy determination, mechanical testing, draw correlations for fcc, bcc and hcp HEA (if possible single crystals)
- in direct correlation of overall goal of Priority Programme
- many cooperation planned
  - *Heidelmann, Feuerbacher*: SX
  - *Wilde*: Cantor and bcc
  - *Divinski, Grabowski*: hcp
  - *Galetz*: oxidation SX and equiaxed Cantor
  - *Liebscher*: hot tension, creep, probe corrected STEM
  - *Glatzel*: borders of HEA