



UNIVERSITÄT
BAYREUTH



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

Uwe Glatzel
Metals and Alloys
University Bayreuth

GL 181/56-1

Michael Feuerbacher
Forschungszentrum Jülich
Jülich

FE 571/4-1

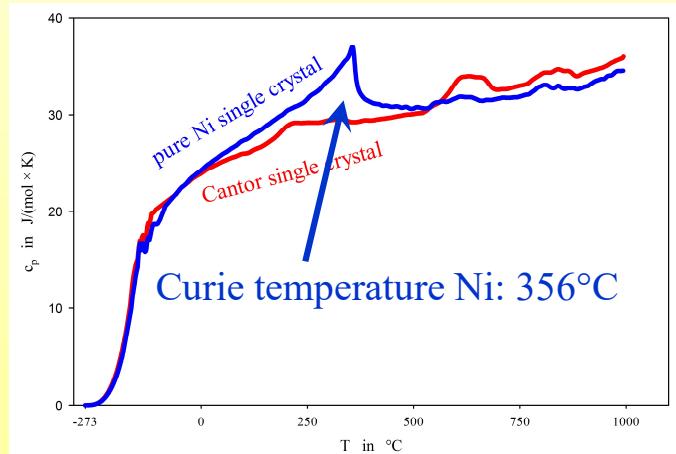


Experimental Determination of Entropy (SX!)



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

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!)

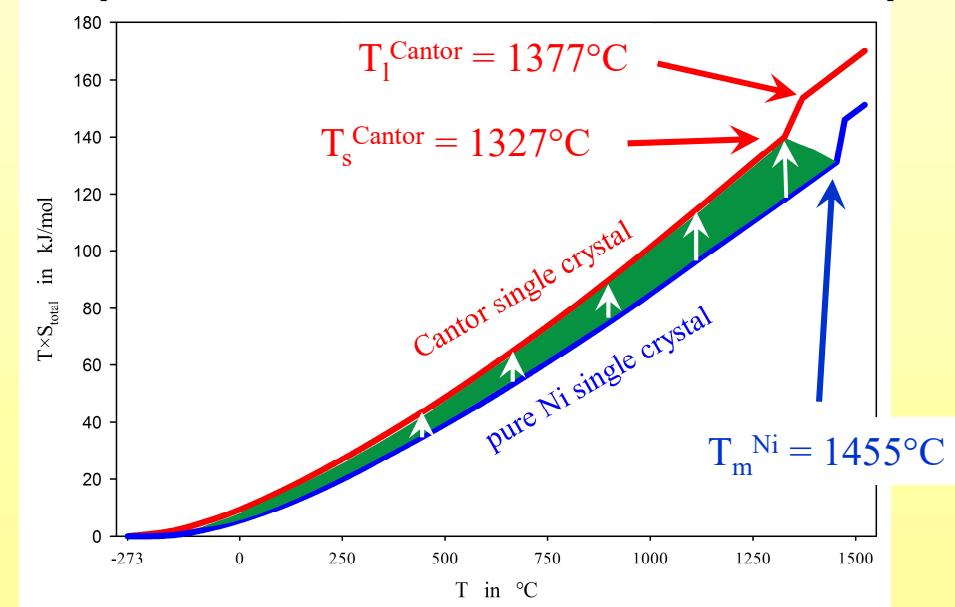
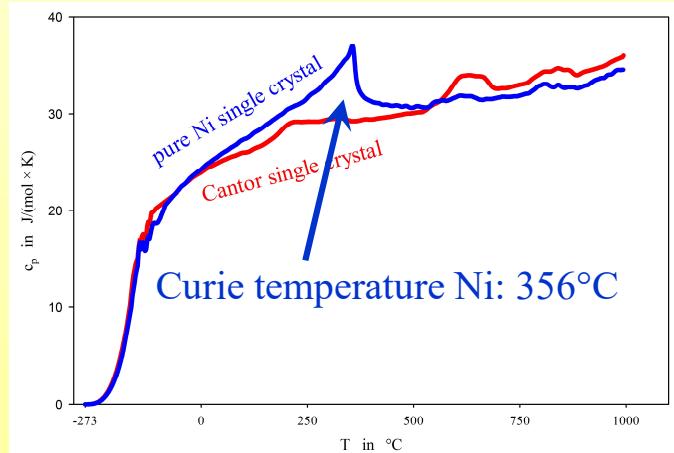


$$S_{\text{total}} = S_{\text{conf}} + S_{\text{th}} = S_{\text{conf}} + \int_0^T \frac{c_p}{T'} dT'$$

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

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

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):

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

In comparison: enthalpy of formation of intermetallic phases:

$\text{FeAl} \approx 33$ $\text{FeAl}_3 \approx 30$ $\text{NiAl} \approx 66$ $\text{Ni}_3\text{Al} \approx 41$ $\text{PtAl} \approx 97$



High Entropy Alloys



| I | II | | | | | | | | | | | | | III | IV | V | VI | VII | VIII/0 | | | | | | | | | | | | |
|--|---|---------------------------------------|-----------------------------------|---|--------------------------------------|--|--|--|--|---------------------------------------|--|---------------------------------------|--------------------------------------|---|---|--|--|---|---------------------------------------|--|--------------------------------------|---------------------------------------|--------------------------------------|--|---|--|------------------------------------|--------------------------------------|--|-------------------------------------|-------------------------------------|
| ¹ H Wasserstoff 1,00797 | | | | | | | | | | | | | | | | | | | ² He Helium 4,0026 | | | | | | | | | | | | |
| ³ Li Lithium 6,939 | ⁴ Be Beryllium 9,0122 | | | | | | | | | | | | | ⁵ B Bor 10,811 | ⁶ C Kohlenstoff 12,011 | ⁷ N Stickstoff 14,007 | ⁸ O Sauerstoff 15,999 | ⁹ F Fluor 18,998 | ¹⁰ Ne Neon 20,183 | | | | | | | | | | | | |
| ¹¹ Na Natrium 22,990 | ¹² Mg Magnesium 24,312 | | | | | | | | | | | | | ¹³ Al Aluminium 26,982 | ¹⁴ Si Silizium 28,086 | ¹⁵ P Phosphor 30,974 | ¹⁶ S Schwefel 32,064 | ¹⁷ Cl Chlor 35,453 | ¹⁸ Ar Argon 39,948 | | | | | | | | | | | | |
| ¹⁹ K Kalium 39,102 | ²⁰ Ca Calcium 40,08 | ²¹ Sc Scandium 40,92 | | | | | | | | | | | | ²² Ti Titan 47,90 | ²³ V Vanadin 50,942 | ²⁴ Cr Chrom 51,986 | ²⁵ Mn Mangan 54,938 | ²⁶ Fe Eisen 55,847 | ²⁷ Co Kobalt 58,933 | ²⁸ Ni Nickel 58,71 | ²⁹ Cu Kupfer 63,54 | ³⁰ Zn Zink 65,37 | ³¹ Ga Gallium 69,72 | ³² Ge Germanium 72,59 | ³³ As Arsen 74,922 | ³⁴ Se Selen 78,95 | ³⁵ Br Brom 79,909 | ³⁶ Kr Krypton 83,80 | | | |
| ³⁷ Rb Rubidium 85,47 | ³⁸ Sr Strontium 87,62 | ³⁹ Y Yttrium 88,905 | | | | | | | | | | | | ⁴⁰ Zr Zirkonium 91,22 | ⁴¹ Nb Niob 92,906 | ⁴² Mo Molybdän 95,94 | ⁴³ Tc Technetium (99) | ⁴⁴ Ru Ruthenium 101,07 | ⁴⁵ Rh Rhodium 102,90 | ⁴⁶ Pd Palladium 106,4 | ⁴⁷ Ag Silber 107,87 | ⁴⁸ Cd Cadmium 112,40 | ⁴⁹ In Indium 114,82 | ⁵⁰ Sn Zinn 118,69 | ⁵¹ Sb Antimon 121,75 | ⁵² Te Tellur 127,60 | ⁵³ J Jod 126,90 | ⁵⁴ Xe Xenon 131,30 | | | |
| ⁵⁵ Cs Casium 132,90 | ⁵⁶ Ba Barium 137,34 | ⁵⁷ La Lanthan 138,91 | ⁵⁸ Ce Cer 140,12 | ⁵⁹ Pr Praseodym 140,91 | ⁶⁰ Nd Neodym 144,24 | ⁶¹ *Pm Promethium (145) | ⁶² Sm Samarium 150,35 | ⁶³ Eu Europium 151,96 | ⁶⁴ Gd Gadolinium 157,25 | ⁶⁵ Tb Terbium 158,92 | ⁶⁶ Dy Dysprosium 162,50 | ⁶⁷ Ho Holmium 164,93 | ⁶⁸ Er Erbium 167,26 | ⁶⁹ Tm Thulium 168,93 | ⁷⁰ Yb Ytterbium 173,04 | ⁷¹ Lu Lutetium 174,97 | ⁷² Hf Hafnium 178,49 | ⁷³ Ta Tantal 180,95 | ⁷⁴ W Wolfram 183,85 | ⁷⁵ Re Rhenium 186,2 | ⁷⁶ Os Osmium 190,2 | ⁷⁷ Ir Iridium 192,2 | ⁷⁸ Pt Platin 195,09 | ⁷⁹ Au Gold 196,97 | ⁸⁰ Hg Quecksilber 200,59 | ⁸¹ Tl Thallium 204,37 | ⁸² Pb Blei 207,19 | ⁸³ Bi Wismut 208,98 | ⁸⁴ *Po Polonium (209) | ⁸⁵ *At Astat (210) | ⁸⁶ *Rn Radon (222) |
| ⁸⁷ * | ⁸⁸ * | ⁸⁹ * | ⁹⁰ * | ⁹¹ * | ⁹² * | ⁹³ * | ⁹⁴ * | ⁹⁵ * | ⁹⁶ * | ⁹⁷ * | ⁹⁸ * | ⁹⁹ * | ¹⁰⁰ * | ¹⁰¹ * | ¹⁰² * | ¹⁰³ * | ¹⁰⁴ * | ¹⁰⁵ * | | | | | | | | | | | | | |
| Fr (223) | Ra (226) | Ac (227) | Actinium (227) | Th (232,04) | Protactinium (231) | U (238) | Neptunium (237) | Pu (244) | Am (243) | Cm (247) | Cf (249) | Einsteinium (254) | Fm (257) | Md (258) | No (259) | Lr (260) | Rutherfordium (261) | Hs (262) | | | | | | | | | | | | | |

Cantor alloy, fcc

bcc

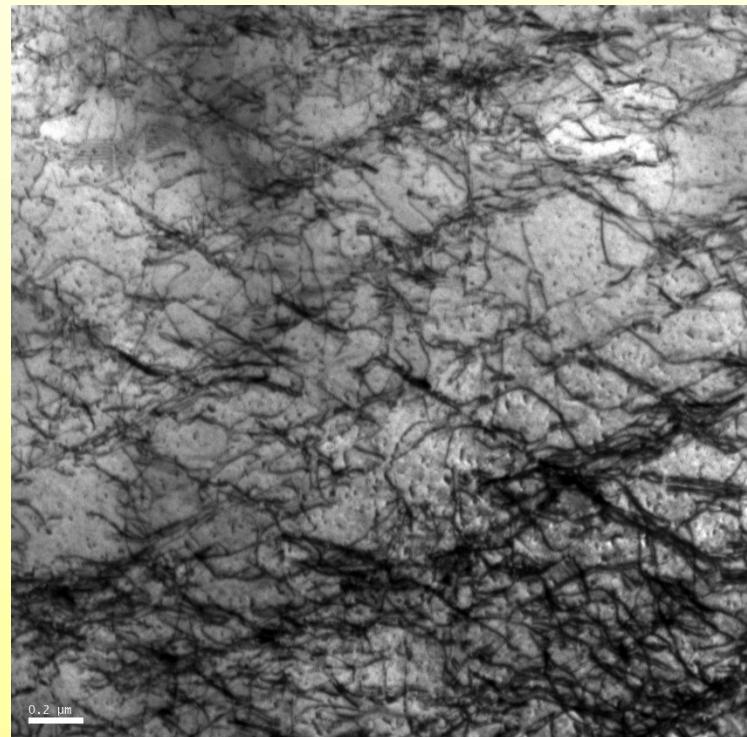
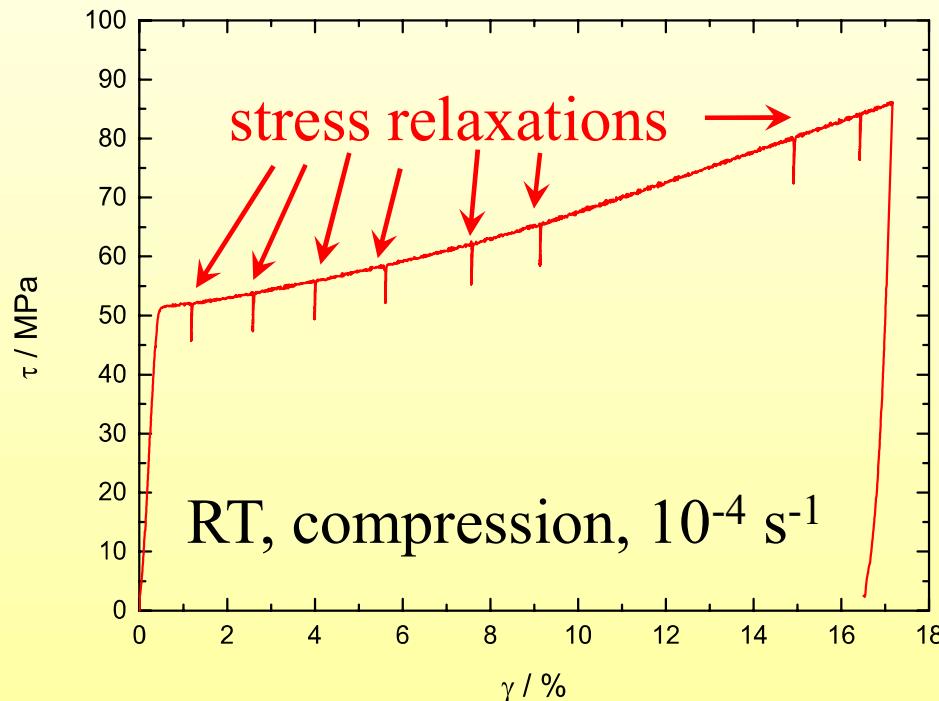
hcp

Legend: hcp (Y + Gadolinium + Terbium + Dysprosium + Holmium), bcc (V + Cr + Mn + Fe + Co + Ni + Cu + Zn), fcc (Ti + V + Cr + Mn + Fe + Co + Ni + Cu + Zn)

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