Short-range order and microhardness of the compositionally complex alloy $Al_8Co_{17}Cr_{17}Cu_8Fe_{17}Ni_{33}$

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Outline

Introduction

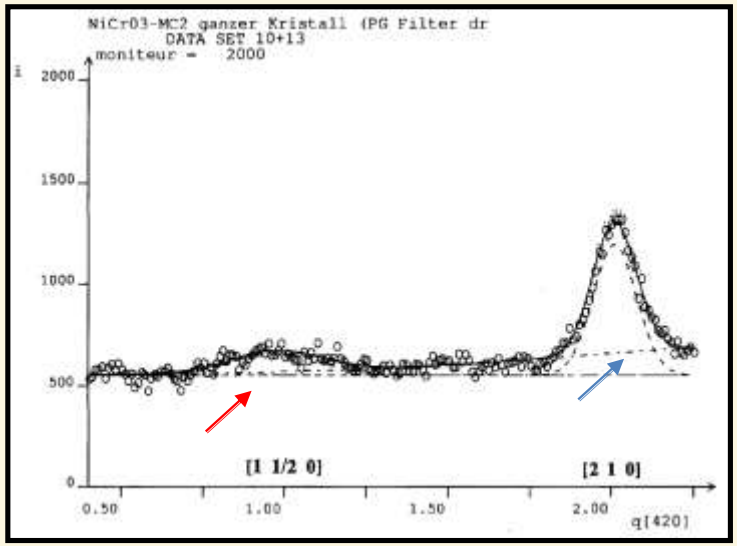
Experimental

Results
- Soft X-ray absorption spectroscopy
- Extended X-ray absorption spectroscopy
- Hardness
- Molecular dynamic simulations

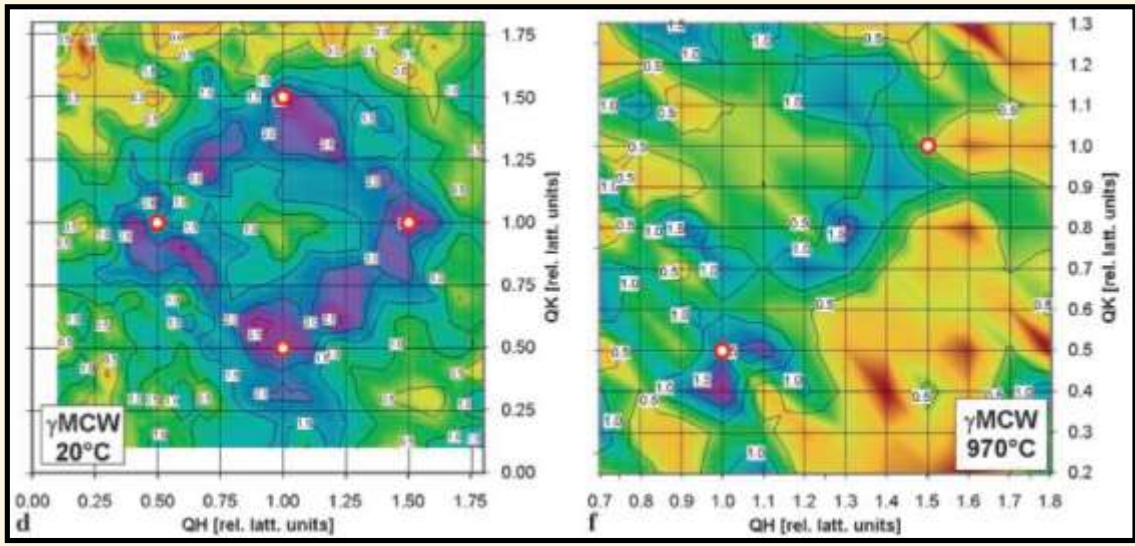
Conclusions and outlook

Short-range order in superalloys

by neutron scattering



MC-2, RT
(*Glas et al., Acta Mater 1996*)

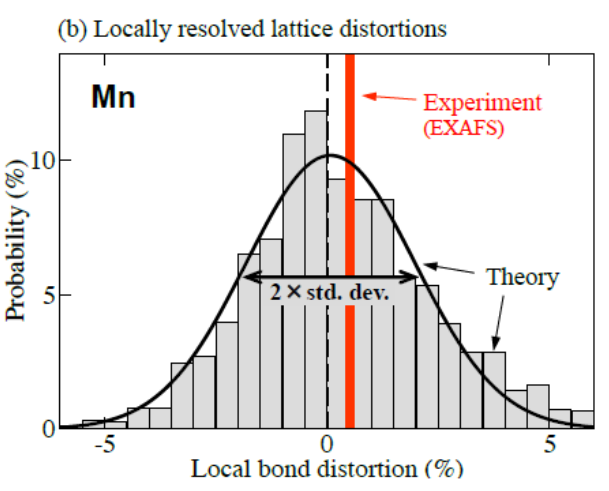


MCW at 20°C, 970°C
(*Prem et al., Appl. Phys. 2002*)

- Diffuse scattering hints of Short-Range Order
  - superstructure peak at [1 ½ 0]
  - diffuse background at [2 1 0]
- ~ 1.5 nm ordered domains at room temperature (MC-2)
- Short-Range Order dissolves above T = 600 °C (MCW)

Short-Range Order in Compositionally Complex Alloys?

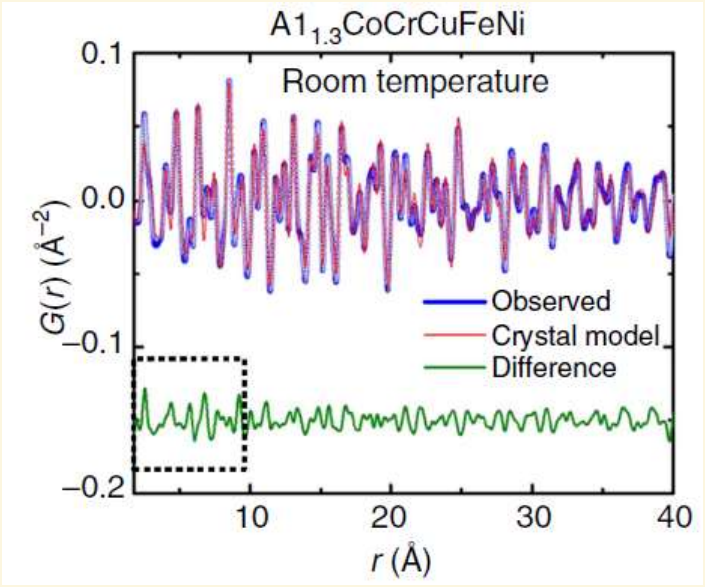
Short-range order in compositionally complex alloys



FeCoNiCrMn

Entropy 2016, 18, 321

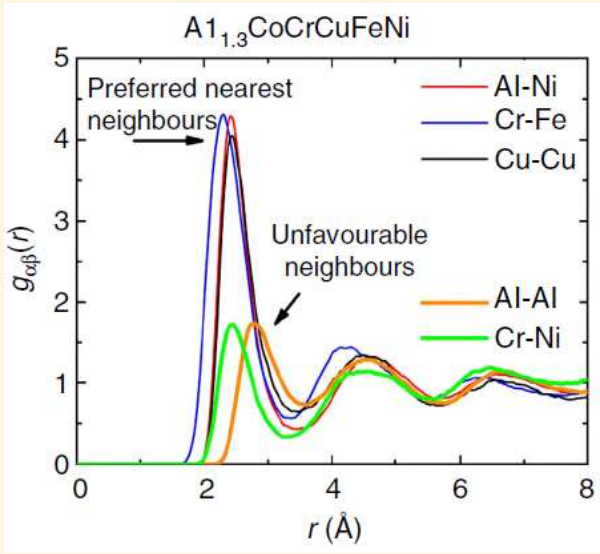
- Small element-resolved mean lattice distortions (~0.1%)
- High local fluctuations of lattice distortions (~2-3%)



Al1.3CoCrCuFeNi

Nat. Comm. 2015, 6, 5964

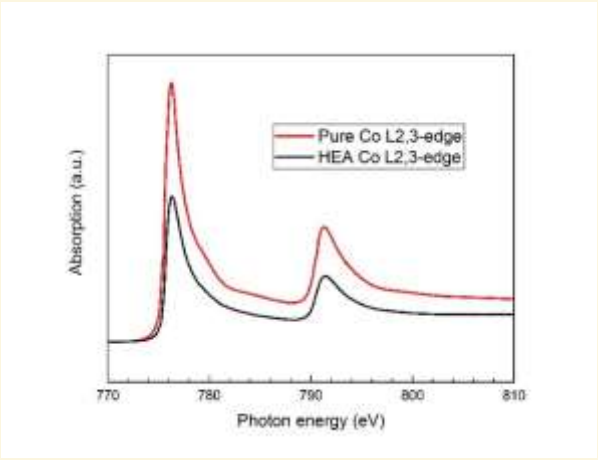
- Structure <10 Å not well modelled by cubic fcc
- AIMD simulations show preferred nearest neighbors



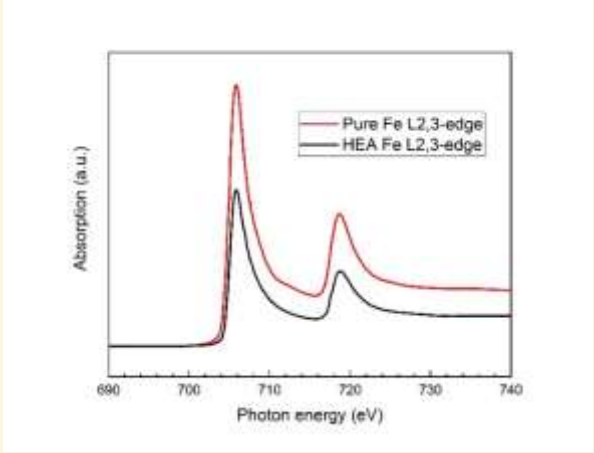
Experimental

X-ray absorption spectroscopy 5 KeV < E < 10 KeV	BESSYII: beamlines KMC-2 and KMC-3 • Mode: fluorescence • Temperatures: 20 K – 300 K
Soft X-ray Absorption Spectroscopy 100 eV < E < 1500 eV	BESSYII: Russian-German beamline Mode: total electron yield (<10nm information depth) in ultra-high vacuum
Hardness measurements	• Vickers indentation • Nanoindentation
Ab-initio molecular dynamics simulations	Dr. Yao Liu (Shandong University) Vienna ab initio simulation package
$Al_8Co_{17}Cr_{17}Cu_8Fe_{17}Ni_{33}$ specimens 2-to-4 components precursors	Bulk (Single crystal, polycrystal) Splat

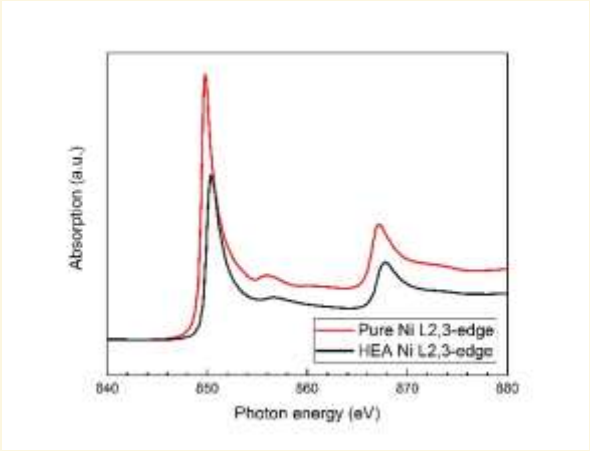
Results: Soft X-ray absorption spectroscopy



$L_{2,3}$ absorption spectra of Co in pure Co (red line) and in CCA (black line)



$L_{2,3}$ absorption spectra of Fe in pure Fe (red line) and in CCA (black line)



$L_{2,3}$ absorption spectra of Ni in pure Ni (red line) and in CCA (black line)

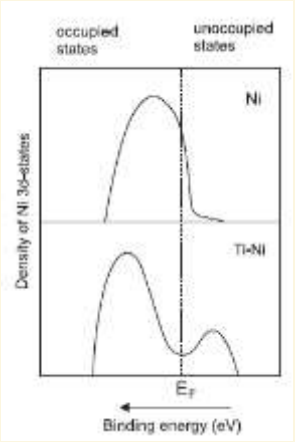
Spin-orbit splitting visible in all spectra (ΔE(Co): ≈ 15 eV), ΔE(Fe): ≈ 13 eV, ΔE(Ni): ≈ 17 eV)

- Absorption spectrum of Co/Fe in CCA similar to absorption spectra of Co/Fe pure metals

⇒ Electronic structure of Co/Fe in CCA similar to that of Co/Fe metals

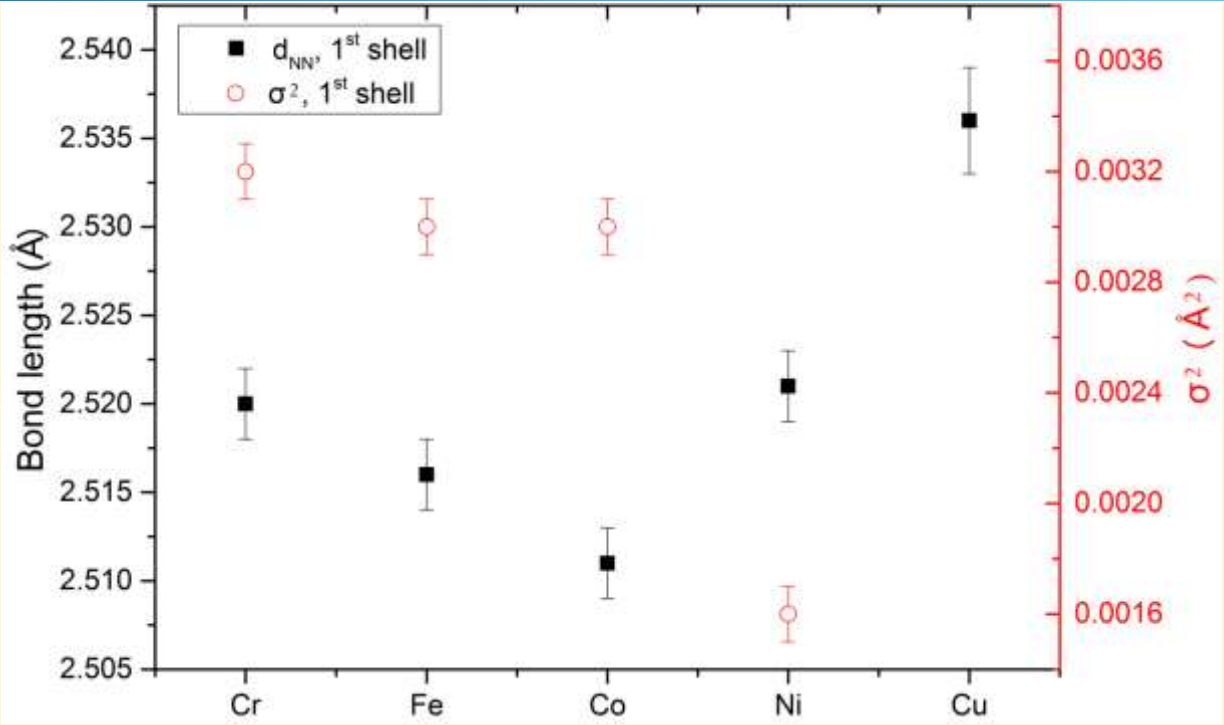
- Absorption spectrum of Ni in CCA shifted to higher energy compared with Ni in Ni metal

⇒ Electronic structure of Ni in Ni dissimilar to Ni in CCA
(i) higher binding energy of Ni 2p levels in CCA
(ii) shift in density of empty Ni d-states



Senkovskiy et al.,
J. Alloys and Compounds 537 (2012)

Results: Extended X-ray Absorption Fine Structure



Al missing. Al-K edge logistically difficult to measure (few beamlines available)

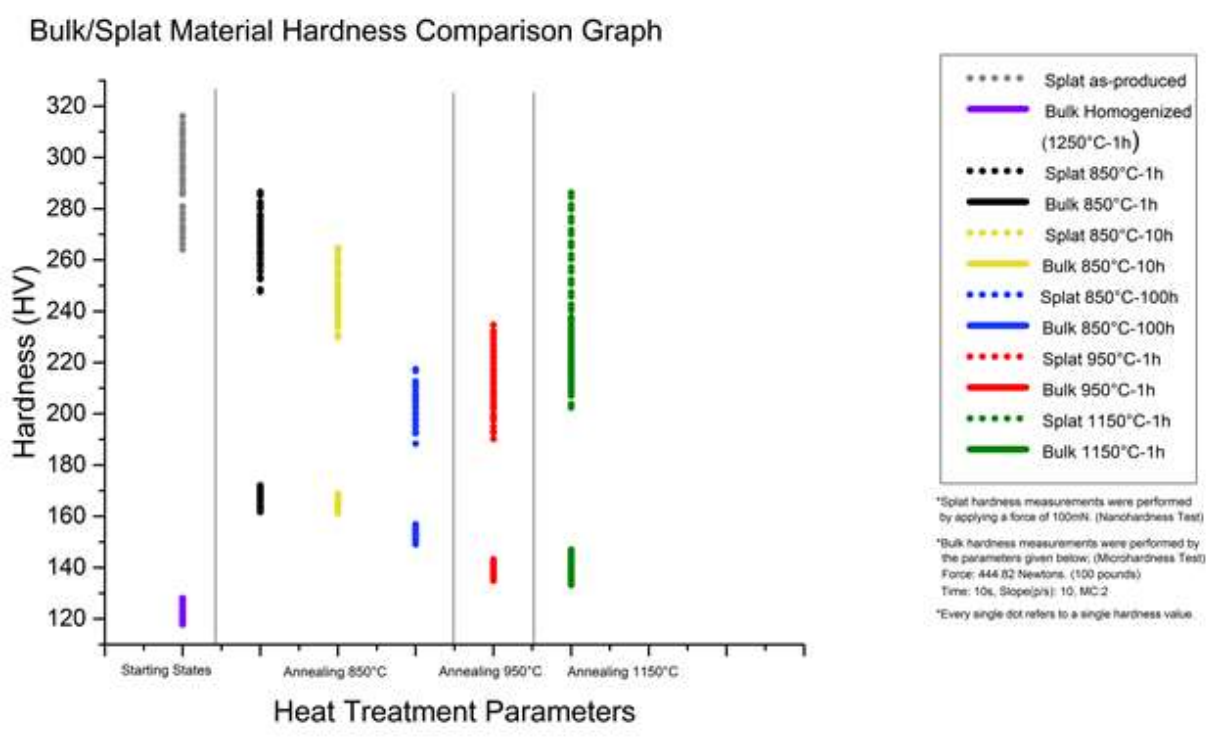
1st shell bond lengths depend on the element (Short-range order!)

- Lowest for Co (2.510(2) Å, extrapolation for T < 50K)
- Highest for Cu (2.536(3) Å, extrapolation for T < 50K)

σ^2 for Ni-1st shell is half the value compared to that of Cr, Fe and Co

- 1st shell around Ni more ordered (highest at.% of Ni in CCA a possible reason)
- Noisy spectra at Cu-K edge do not allow reliable σ^2 refinement

Results: hardness

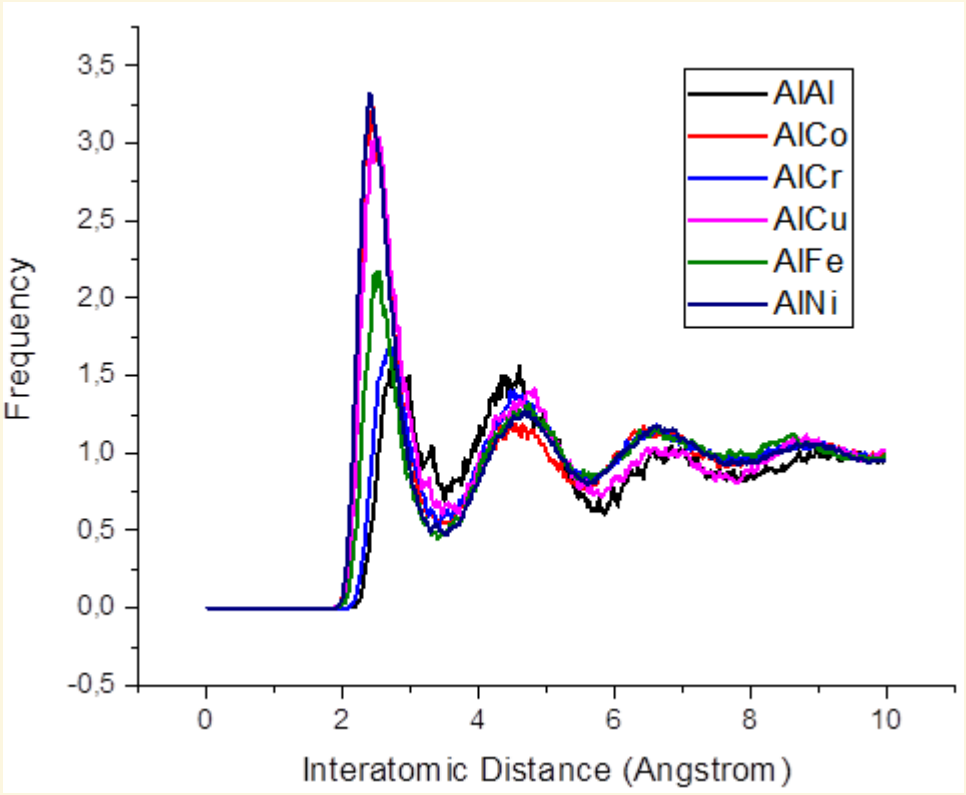


- Hardness of splats higher than hardness of bulk specimens
- Data scattering on splats higher than on bulk specimens
- Decrease in hardness at 850 °C with increasing annealing time

Two-hardening mechanisms

T > 900°C : short-range order in single phase region
T < 900°C : precipitation mechanism in γ/γ' phase region

Results: ab initio molecular dynamics



- Crystalline state not reached at 1000°C (still liquid state)
- Liquid state reveals pronounced Short-Range Order
- Al prefers Ni/Co/Cu as nearest neighbors

	Al	Cr	Fe	Co	Ni	Cu
R(Å)	1.43	1.25	1.24	1.25	1.25	1.28

Conclusions and outlook

Soft X-ray absorption spectroscopy:
Ni electronic structure seems to be different than the corresponding Ni pure metal

→ Further studies and measurements (e.g. at Al and Cr L-edges) needed

Extended X-ray absorption fine structure:
- 1st shell around Co and Cu atoms are the smaller and the bigger, respectively.
- 1st shell around Ni is the most ordered

Al-K edge spectrum still missing

→ Any relation to Ni-electronic structure?

Hardness
- Depends on temperature and annealing time
- Depends on specimen nature (bulk vs splat)

Two hardening mechanisms:
- SRO increase (single phase)
- Precipitation (γ/γ' region)

→ Splat vs bulk CCAs in XAS?

Ab initio molecular dynamics
Preferred nearest neighbors for Al (Ni, Co, Cu)

→ To be proved experimentally (e.g. XAS on Al-K edge)

Acknowledgements

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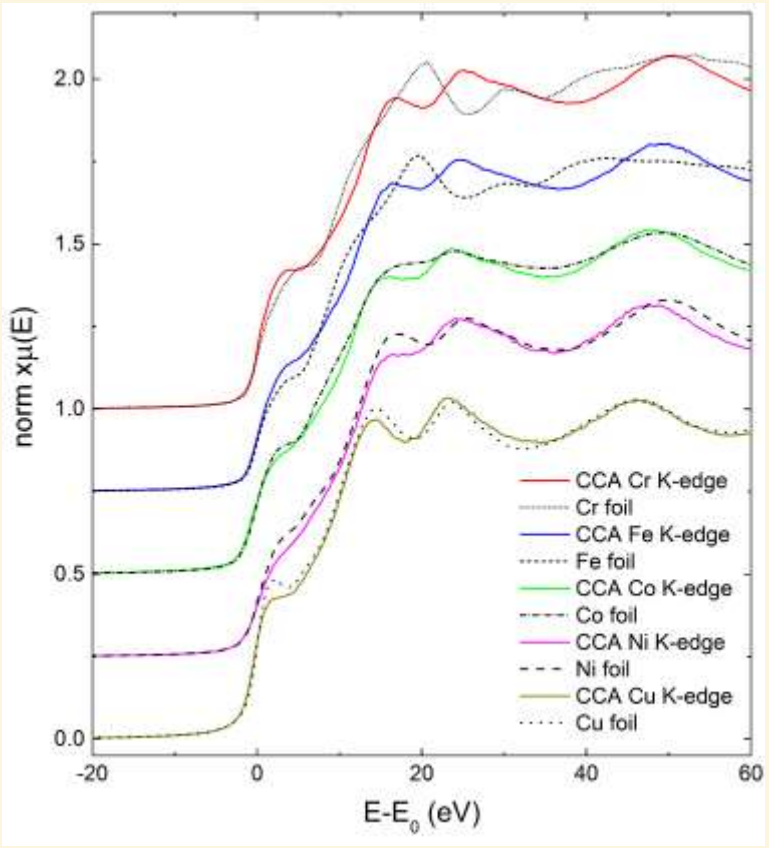
- A. Öner, C. T. Cakir, for the hardness measurements
- Dr. Y. Liu, for molecular dynamics simulations

Thank you for your attention!

Results: K-edge X-ray absorption near edge structure (XANES)



XANES spectra for Cr, Fe, Co, Ni and Cu K-edges at 20 K in the CCA. Black lines represent reference foils.

Pure metals and CCA:

K-edge split into two transitions

1s → mixed state (4s-4p-3d)
1s → 4p state

- Fe, Cr metals have bcc structure, Co metal hcp structure. Metals spectra not easily comparable with CCA spectra

Study of e.g. 2-component (FeNi) and 3-component (CoFeNi) alloys with fcc structure is necessary