Local Structure of High-Entropy Alloys: EXAFS *vs.* XRD analysis

Kirill Yusenko

Institute of Geology, Mineralogy and Geophysics, Faculty of Geosciences, Ruhr-University Bochum, Universitätsstr. 150, 44801 Bochum, Germany

kirill.yusenko@rub.de

High-entropy alloys have high complexity in their composition, but simple crystal structures typically limited by *fcc*, *bcc* and *hcp* structural types. Due to their high structural and chemical disorder, structural information about local ordering and local distortions obtained by X-ray diffraction and microscopy is limited and cannot be used to characterise each element with high level of precision. Element-specific data based on analysis of extended X-ray absorption fine structure spectra (EXAFS) can be used to characterise local environment in compositionally complex systems as a complementary tool. The probing of local ordering and inner relaxations in complex multicomponent systems at the atomic scale in an element-specific way opens a path to advance structural studies of compositionally complex materials.

Here, an extended study of the local atomic arrangements of constituent elements in several typical single-phase high-entropy alloys based on analysis of EXAFS K-edge spectra of 3*d* elements is reported. A reverse Monte Carlo simulation allows to perform a simultaneous fit of all available EXAFS spectra to reconstruct the local environment of *all* metals with high precision and also obtain element-specific pair distribution functions for each element. The approach is quite general and has been successfully used to study HEA's as nanoparticles, crystalline and amorphous thin films. A combination with *ex situ* and *in situ* high-temperature and low temperature studies gives a possibility to understand materials properties and performance in industry relevant processes. Quantitative information on interatomic distances, structural/thermal relaxations of each constituent and character of the local coordination for each element gives a deep inside into HEA's structure. This detailed information is further used to understand the role of individual components in macroscopic properties. The work demonstrates that even if all components of the equiatomic alloy are equally distributed, local distortions around specific atoms can play a key role in overall materials properties and can be associated with a presence of specific atom in the structure.

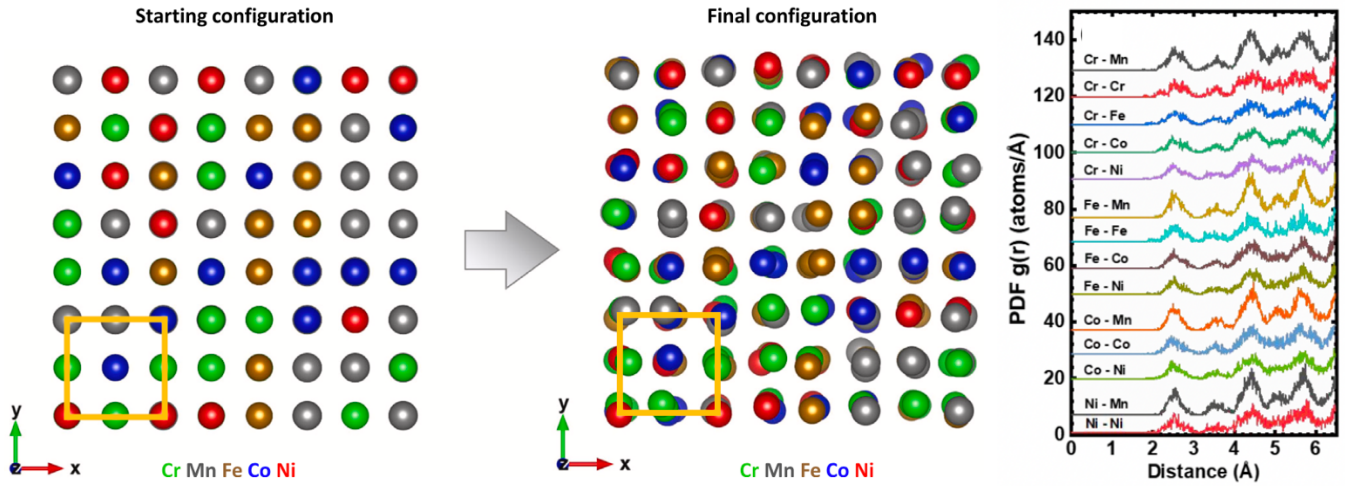


Figure 1. *Starting and final atomic configurations (5x5 supercells) obtained from the RMC simulation of EXAFS spectra of the fcc-CrMnFeCoNi HEA, corresponding partial pair distribution functions obtained from the RMC simulation [3].*

[1] A. Smekhova, K.V. Yusenko *et al.* Nano Research (2024). 17(6), 5336–5348.
[2] A. Smekhova, K.V. Yusenko *et al.* Nano Research (2023). 16(4), 5626–5639.
[3] A. Smekhova, K.V. Yusenko *et al.* J. Alloys and Compounds (2022). 920(5), 165999.
[4] A. Smekhova, K.V. Yusenko *et al.* Nano Research (2021). 15, 4845–4858.