High Entropy Alloys local structure study by Reversed Monte Carlo method

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Many of materials properties of high-entropy alloys (HEAs), including hardness, lowered thermal and electrical conductivity, as well as extremely high volumetric hydrogen density, seems to be bounded with the material crystal structure (observed on average and/or local scale). The HEAs are alloys composed of multiple elements (sometimes up to 5 different atom types) which can significantly differ in atomic radius. Nevertheless, HEAs properties are of a high interest, little is known about the exact structures of those materials.

From the average structure point of view, HEAs crystallizes in simple body centered-cubic structure and transforms into distorted CaF2-type upon deuteration. On the other hand, on a local scale HEAs show local distortions as well as short range order due to elements occupancy ordering.

Therefore, local structure investigations have been performed by using Reversed Monte Carlo method implemented in RMCProfile program. X-Ray and neutron Pair Distribution Function (PDF) data have been modelled. Our aim was to study different atom local environments and local short-range order. Due to the fact that HEAs studied here, were multielement systems (up to 5 elements) it seemed necessary to combine X-Ray and neutron PDF data due to significantly different X-Ray and neutron contrast for used metals and hydrogen/deuterium. This is only because of that, it was possible to model up to 15 partial contributions for relatively simple cubic structure where all partials are overlapped in r space.

Here, we demonstrate how Reversed Monte Carlo method implemented in RMCProfile program can give significant impact on local structure of complicated multielement systems (TiVNb, TiVZrNb, TiVZrNbHf and TiVCrNb) As a next step we performed local structure investigations of hydrated alloys such as TiVNbD5.7, TiVZrNbHfD10, TiVCrNbD2.2 and TiVCrNbD8) in which deuterium atoms occupy both tetrahedral and octahedral interstices with low occupancies. There is a significantly higher portion of occupied sites with nearest-neighbour metals with low valence-electron concentration. This finding, as well as inelastic neutron scattering, and density functional theory suggest higher mobility of hydrogen in between nearby interstitials.

The data has already been published in

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