Investigation of chemical interaction and electronic structure in $Al_8Co_{17}Cr_{17}Cu_8Fe_{17}Ni_{33}$ compositionally complex alloy by X-ray absorption spectroscopy and X-ray photoelectron spectroscopy

Topic Area: T6: Materials Characterization

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Changes in local electronic structure between pure Cr, Fe, Co, Ni and Cu and the corresponding elements in $Al_8Co_{17}Cr_{17}Cu_8Fe_{17}Ni_{33}$ compositionally complex alloy (CCA) have been studied by near-edge X-ray absorption fine structure (NEXAFS) spectroscopy and X-ray photoelectron spectroscopy (XPS). Analysis of redistribution and occupancy modification of transition metals' (TMs) 3*d* states was carried out on L-edge absorption spectra by NEXAFS, whilst charge transfer and energy distribution of occupied 3d states were investigated by means of XPS.

Occupancy of the 3*d* bands changes upon alloy formation: Cr and Co lose 3d electrons and Ni 3d occupancy increases while that of Fe is preserved. Moreover, maximum of Ni 3d empty states shifts away from Fermi level (E_f) by 0.5 eV, ascribed to the presence of Ni-Cr bonds. Ni-Cr bonding accounts for the decrease of electron density at E_f in the alloy, as well. Analysis of 2p XPS lines of the TMs showed negligible change in the net charge of the individual atoms. Variation of 3d states occupancies is therefore expected to be balanced by charge redistribution of delocalized 4s and 4p states.

Al contribution to the electronic structure transformation of the TMs is negligible, although covalent Al-TM bonds could be likely. This work determines that Cr assumes an important role in Ni local electronic structure and suggests formation of Ni-Cr bonds with covalent character. These findings could find application in tuning ductility[2] and phase stability[2] of CCAs due to the relation between valence electron concentration at E_f and Ni-Cr bonding.

1. S. Kasatikov et al., unpublished.
2. R. Chen, et al., Acta Materialia, 144, (2018) 129-137.