Experimental study of a new Heusler compound from chrome group - Ti2CrAl and Ti2MoAl

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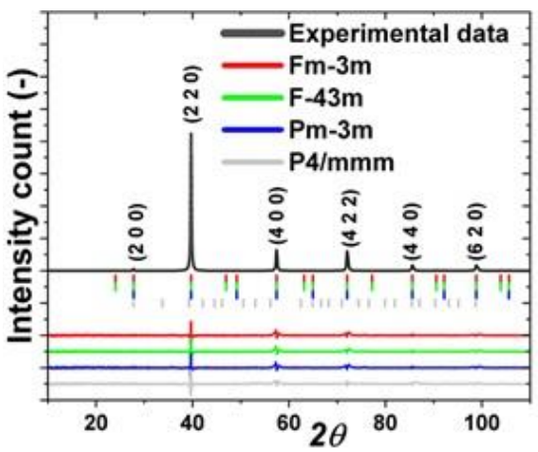
Heusler alloys were discovered in the early 20th century. With the beginning of the 21st century, interest of these materials increased due to their interesting properties and possible applications in spintronics and thermos-electric devices. Many Heusler compounds exhibit Half-Metallic Ferromagnetism (HMF) state. Ti_2CrAl was predicted by earlier ab-initio calculations [1,2] to be a Heusler compound which is near the HMF state. In our study we performed analysis of two prepared in our laboratory compounds: Ti_2CrAl and Ti_2MoAl. We successfully synthesized both samples and thoroughly investigated it with several experimental techniques.



We examined the X-ray diffraction pattern considering four structural models, most common one being simple Cu_2MnAl-type structure (space group: $Fm\bar{3}m$) and inverse Heusler structure of $CuHg_2$ Ti-type (space group: $F\bar{4}3m$). The Heusler alloys can also be viewed as a CsCl-type (space group: $Pm\bar{3}m$), superstructure when one lattice site exhibits a complete disorder or a tetragonal type structure (*P4 / mmm*). In Fig.1 we present our results for Ti_2MoAl compound.

Figure 1. XRD results for Ti_2MoAl compound

We also measured X-ray Absorption (XAS) and X-ray Photoelectron Spectroscopy (XPS) spectra and performed ab-initio DFT calculations. Heusler compound usually crystallizes in either simple or inverted structure - simple structure of Ti_2MoAl and Ti_2CrAl was confirmed by XRD and DFT studies. On the surface, a minor contribution from inverted Heusler structure can be deduced from comparison of XPS with DFT calculations.

References

1. J. Goraus, J. Grelska, at al., Surface Science 733 (2023) 122288.
2. J. Goraus, J. Czerniewski, at al., Alloys and Compounds 867 (2021) 159078.