A magnetic C36 Laves phase in Co-Fe-Ta system

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The computational tools at hand allow for an unprecedented prediction of new structures with desired physical properties. Yet, in many cases, no recipes are provided to synthesize them. In the case of a binary compound, we show a route to bring a theoretically predicted structure to a real material. In particular, we demonstrated the possibility to synthesize a C36 Laves phase ($hP24$ structure) with improved intrinsic magnetic properties in the Co-Fe-Ta system. Computational studies predict superior intrinsic magnetic properties for an experimentally not observed Fe_2Ta C36 Laves phase. This phase, however, occur in the Co-Ta system, which suggests the possibility of the existence of a stable compound along the $(Co_{1-x}Fe_x)_2Ta$ path. Following this route, we computationally predict a stable C36 Laves phase with improved intrinsic magnetic properties for large Fe content, and successfully synthesize it experimentally. This approach is general and can be applied to identify a synthesis path for a predicted material with desired properties.

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