"Artificial Multi-Elements" based on High Entropy Alloys as "building blocks" for novel magnetic alloys suitable for Permanent Magnets: Special cases ThMn₁₂ and SmFe₃CoNi

D. Niarchos^{1, 2}

¹Institute of Nanoscience and Nanotechnology, NCSR Demokritos, 15310 Athens, Greece ²AMEN New Technologies, Athens, Greece

Demand for rare earths or cobalt is set to soar the next decade boosted especially by demand for valuable NdPr or SmCo magnets used in electric motors (electric vehicles, wind turbines, consumer electronics, military & aerospace applications). The global permanent magnet market size is expected to reach \in 30 billion by 2030 from the current \in 20 billion. It is predicted that by 2030 a) Market for rare-earth oxides will increase 5-fold, b) annual NdFeB shortages of 48,000 tonnes expected by 2030, c) annual Dy oxide Shortages of 1850 tonnes is expected by 2030. Extending the forecasting of Dr. M.Sagawa , who has predicted that by 2050 every one on earth will be served by at least 2 robots each one having at least 10 magnets, the new market has to be served by novel groundbreaking approaches.

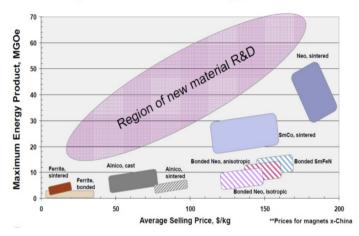
For centuries the design concepts of alloys has been based on only one or two principle elements, while minor fraction of other elements are added for property enhancement. This classical approach was broken in 2004 by Yeh et.al, who suggested of a new alloy design concept, which he called high entropy alloys. The original definition was "multiprincipal elements alloys composed of five or more elements in equal or near-atomic percentages". Most of the current dominant (PMs) are intermetallic compounds containing rare earth elements e.g. NdPr or Sm and Co, both expensive and originating mainly from either China or Congo. These natural elements from the periodic table have a fixed atomic radii, fixed valence electron configuration and specific electronegativity, parameters that are crucial for the formation of intermetallic compounds. By creating artificial multi-elements of the type of HEAs based on multicomponent rare-earth elements (RE-HEAs) and HEAs based on multicomponent transition metal elements (TM-HEAs), we have created a library of elements with tunable atomic radii, valence electron configuration and electronegativity. This approach enhances the opportunities for discovering novel permanent magnets.

The concept of using artificial elements based on either rare-earths or transition metals is depicted in Figure 2. for the case of SmCo_{5-} type alloys, an approach that we followed for the stabilization of the SmFe_3 CoNi magnetic phase. We have extended this substitutional approach to the class of $\text{RFe}_{12-x}\text{T}_x$ a and $\text{R}_2\text{Fe}_{14}\text{B}$ alloys and the results so far are given in Table 1.

Sample	Ms(emu/g)	$H_A(T)$	Tc (K)	Hc $_{(\text{expected})}$ (T)	$(BH)^{theor}_{max}$ (MGOe)
(RE-HEAs)-Co ₅	75-90	>10	> 800	>1	8-18
Sm-(TM-HEAs) ₅	65-80	> 8T	> 800	>1	8-15
(RE-HEAs)-Fe ₁₁ TiN $_x$	120-135	> 6T	570-600	>0.8	9-18
(RE-HEAs)2-Fe14B	125-145	3-6	550-600	>1	10-25

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We will present a general approach by unlocking the new possibilities of using artificial elements to create new magnetic alloys that can be processed towards (PMs) to address the opportunities that are shown in Figure 1.



Magnet Price versus Energy Product

Figure 1. Opportunities for novel magnet alloys, suitable for permanent magnets, as a function of $(BH)_{max}$ vs cost (Arnold Engineering).

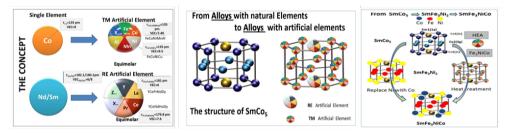


Figure 2. Three steps towards HEA-Magnetic Alloys. Step1 is the fabrication of the artificial elements RE-HEAs and TM-HEAs with variable atomic radii and valence electron concentration, Step2 use these artificial elements to synthesize model structures as counter-alloys of existing structures e.g. $SmCo_5$ and in Step3 with proper heat treatment stabilize through entropy optimization a phase e.g. $SmFe_3CoNi$, that otherwise is not possible because the formation energy is just slightly positive.

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