High entropy or big mistake? The new paradigm in materials design

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The development of human-kind is defined by materials which it had been using (i.e. Stone, Bronze, and Iron Age). In the XX century we have learned to analyze the structure of materials and therefore to study in-depth its influence on properties – namely physical and mechanical parameters. The next step was to learn to design materials based on needed properties – we would like to answer questions such as: How I need to produce a material that will have hardness higher than steel? This question can be restated as: What structure of material do I need to obtain such material? We learned to answer such questions for materials which structure and behavior were studied for years by many researchers and industrialists – monocrystals, polycrystals, and amorphous solids constituted by one element (or compound) as well as "traditional" alloys. By traditional, it is meant that we have only one dominant element (i.e. iron in steels, usually 90% and more) which is mixed with a small amount of other elements (I omit here yet another class of materials – composites). So at some point, the question arose: Can we exceed up-to-date classes of materials? The positive answer to that question was first proposed by Professor Ye Junwei in 2004 [1] and the final answer was given by Yeh et al. in publication [2]. The concept was called High Entropy Alloys (HEAs) and structural comparison between traditional and high entropy alloys is depicted in Fig. 1.

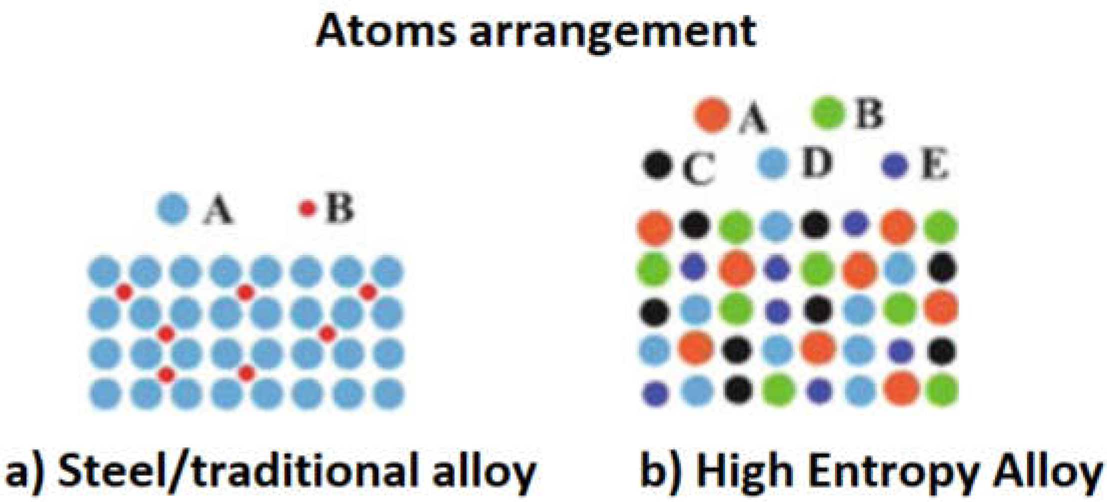

Fig. 1. Difference in atoms arrangement in traditional and high entropy alloy[1]

There are two main differences indicated by Fig. 1. – (1) in HEA all atoms are building the crystal structure whereas in the traditional alloy the crystal structure is built by element A and element B contributes as a defect of crystal structure, (2) in HEA all included elements are in the equimolar (or near equimolar) ratio – i.e. the whole alloy is made by 5 elements where each one constitutes 20% of all atoms. In our research [3] we used Cu (copper), Mo (molybdenum), Ta (tantalum), W (tungsten), and V (vanadium). Fig. 2a) shows the concentrations of the elements in the function of the depth of the HEA coating. It can be seen that the concentrations change and it is not perfectly equiatomic. However, none of the elements is in trace amounts. In Fig. 2 b) an etched nano-pillar of 500 nm of diameter before compression is visible, whereas in Fig. 2 c) the same pillar is pictured after compression. It was prepared by Focused Ion Beam (FIB) which uses high-energy ions to sputter atoms from the as-prepared surface. The etching is followed by nano-pillar compression where we used a nano-indenter with a flat tip to measure compressional strength.

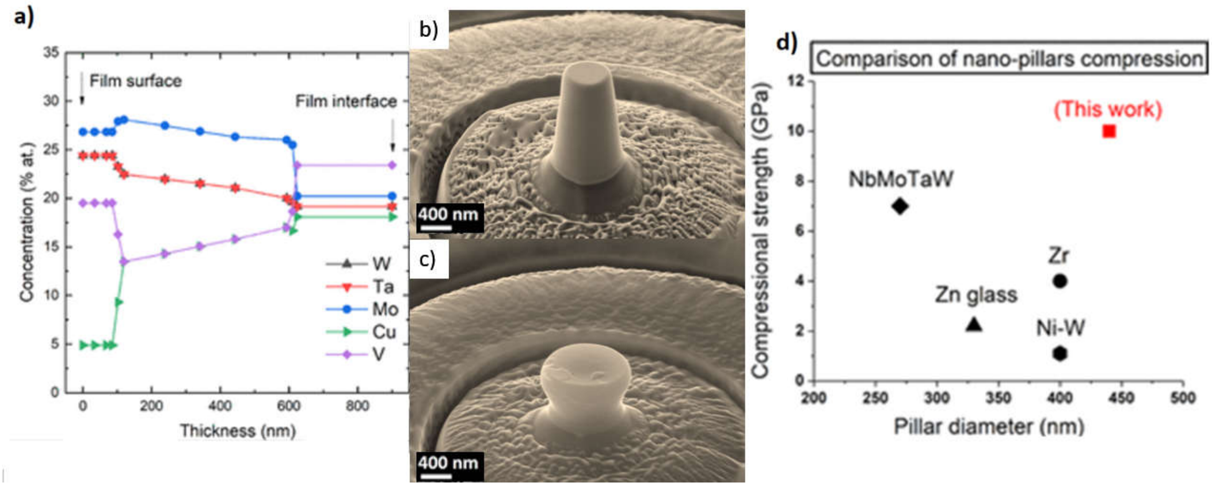

Fig. 2. a) Concentration of elements b) milled nano-pillar before compression c) milled nano-pillar after compression d) compressional strength results

As indicated in Fig. 2 d) it was possible to outperform other materials in terms of compressional strength. However, we all heard of graphene as the “next supermaterial” but it is rarely used in industrial applications so let’s hope that a lot of work that was put in High Entropy Alloys would not be a “next supermistake”.

Bibliography:

[1] Y. Zhang and Y. Zhang, *History of High-Entropy Materials*, no. 1. 2019.

[2] J. W. Yeh *et al.*, “Nanostructured high-entropy alloys with multiple principal elements: Novel alloy design concepts and outcomes,” *Adv. Eng. Mater.*, vol. 6, no. 5, pp. 299–303, 2004.

[3] S. Alvi *et al.*, “Synthesis and Mechanical Characterization of a CuMoTaWV High-Entropy Film by Magnetron Sputtering,” *ACS Appl. Mater. Interfaces*, vol. 12, no. 18, pp. 21070–21079, 2020.