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Study of the occupation sites in the lattice crystal by different elements composed of high-entropy alloys

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High Entropy Alloys (HEAs) are solid solutions of five or more elements, each contributing at least 5% atomic content. They typically crystalize in simple, ordered crystal structures (bcc or fcc) with high chemical disorder, leading to significant configurational entropy during solidification. HEAs are recognized for their outstanding mechanical properties, thermal stability, and corrosion resistance. Their unique composition gives rise to physical properties that cannot be predicted by the sum of their components, often resulting in surprising discoveries. Combining these properties with phenomena like magnetic order and superconductivity enhances their potential for advanced applications.

The discovery of the first superconducting high-entropy alloy (HEA), $Ta_{0.34}Nb_{0.33}Hf_{0.08}Zr_{0.14}Ti_{0.11}$, in 2014 was a significant milestone in the field [1]. This alloy, classified as a type-A HEA superconductor, is composed of transition metals, features a body- centered cubic (bcc) structure, and demonstrates superconducting transition temperatures (T_c) between 4.0 and 9.2 K, along with upper critical fields (μ_0H_{c2}) nearing 12 T. While studies have predominantly centered on Nb-Ta-rich HEAs, the exceptional superconducting performance of binary Nb-Ti systems indicates that NbTi-based HEAs could achieve even higher T_c and μ_0H_{c2} values, highlighting an exciting direction for future research.

The critical parameters strongly depend on the degree of crystallographic and chemical disorder, which is very difficult to study in detail using X-ray diffraction experiments (due to the averaged nature of their results). Therefore, an analysis of Absorption Fine Structure (XAFS) was proposed to support and extend the XRD study and the electronic structure theoretical calculation of HEA compounds. Due to the element selectivity, XAFS is extremely helpful in distinguishing between particular constituent elements in such studies. We studied: i) the titanium- and niobium-rich type-A HEA superconductors prepared by conventional arc melting method and ii) the high-entropy carbides powders synthesized by mechanical alloying. The Nb(18.98 keV), Ti(4.96keV), Zr(18keV) K- and Ta(9.88keV), Hf(9.56keV) L_3- absorption edge were measured in the fluorescence mode in the studied as well at the POLYX beamline. Detailed XAFS analysis provides thorough information that helps researchers understand these unique characteristics.

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