**METHOD**

**(FIRST PRINCIPLE STUDY)**

**To evaluate fermi energy (Ef), density states, coulomb pseudopotential(µ\*), electric specific heat per unit temperature per mole(Υ), and electron coupling constant(****𝛌) of the specimen sample [TaNb]0.31 (TiUHf]0.69, we have used basic physical quantities such as volume of unit cell of the specimen, No. of constituent atoms per unit volume(N) and electron density (n). To determine superconducting state transition temperature (Tc) of the specimen, we have used Mc. Millan formula as**



**Abstract**

The superconducting High entropy alloys (HEAs) have attracted attention of scientific world to their exciting properties as robustness of superconductivity against atomic disorder. An f-electron containing HEA, [TaNb]0.31 (TiUHf]0.69 which is the first to include an actinide element. This material is a body- centred cubic lattice with lattice constant a=3.41 A0. It exhibits superconductivity with a transition temperature Tc = 3.2 K experimentally observed. we have obtained fermi energy (EF), density of states, coulomb pseudo potential(µ\*), electronic specific heat per unit tempt per mole(Υ), electron- phonon coupling const(𝛌), Superconducting state transition temperature (Tc), Renormalization parameter (Z0), effective interaction strength [N(0)V] and isotope effect exponent (ẟ) of the sample [TaNb]0.31[TiUHf]0.69 by the first principles calculations based on the density functional theory (DFT).

**Superconducting Properties of Refractory Metal based Uranium Alloy**

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Specimen Sample: -

**Introduction**

[TaNb]0.31 (TiUHf]0.69

**The sample is actinide (Uranium) based high entropy alloy that exhibits phonon mediated superconductivity with transition temperature Tc≈ 3.2K as observed experimentally. This the first actinide based high entropy alloy as per our knowledge. Under the investigation of X-rays-diffraction, it was found that the material crystallizes in the cubic space group Im⁻m and in a body centered cubic lattice with lattice constant a= 3.41 Ao. Here after we have obtained fermi-energy (Ef), density of states, coulomb pseudopotential (µ\*), electronic specific heat per unit tempt per mole(Υ), electron phonon coupling constant(𝛌), Superconductivity state transition tempt (Tc), Renormalization parameter (Z0),effective interaction strength [N (0)V] and isotope effect exponent (ẟ) of the sample by first principle calculation**.

1.Gao, M.C; Yeh, Liaw; p.k.; Zhang, Y. High Entropy Alloys: Fundamental and Applications; Springer: Switzerland, 2015.

2. Zhang, X.; Winter, N; Witteveen, C.; Moehl, T.; Xiao, Y,; Krogh. F.; Schilling, A,; von Rohr. F.O. preparation and characterization of high entropy alloy (TaNb)1-x(TiUHf)x superconducting films. Phy. Rev.Res.2020,2,013375.

3. Nelson.; Chemey, A. T.;Hertz, M.; Choi,E; Graf,D.E.; Latturner,S,;Albrecht-Schmit, T.E.;Wei,K; Baumbach, R.E. Superconductivity in an Uranium containing high entropy alloys.Sci. Rep2020,10,4717

**REFERENCES**

**DISCUSSION**

HEA ⦋TaNb]0.31 (TiUHf]0.69 has small electron-phonon coupling constant(𝛌) which indicates that the superconducting state of the material can be described by BCS theory within the weak electron phonon coupling range. The experimental superconducting phase transition temperature of the material is 3.2K, while calculated TC is 2.3K, so it is appealing to consider the framework proposed by the authors. Zr- containing analogue HEA ⦋TaNb]0.31 (TiZrHf]0.69 has experimental TC =5.6K which is greater than that of U-containing HEA ⦋TaNb]0.31 (TiUHf]0.69 having experimental TC = 3.2K. This comparison indicates that the presence of U-ion suppressed the value of electron-phonon coupling and weakened the bond of cooper pairs. After all, actinide/ lanthanide containing HEA superconductors have become emerging class of HEA that will enable studies of the impact of natural radiation damage and long-term robustness of its superconducting properties.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Material** | **µ\*** | **𝛌** | **TC** | **Z0** | **N(0)V** | **ẟ** |
| ⦋TaNb⦌0.31(TiUHf)0.69 | 0.0869 | 0.4996 | 2.3K | 1.4541 | 0.3686 | 0.4484 |

The calculations of the following parameters listed in table are purely analytical.

**RESULTS**