Electron capture decay rate change and *Ab initio* calculation of electron density at the nucleus

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Introduction

Electron Capture (EC) decay rate is proportional to the density of electrons at the nucleus. So, it can be influenced by the electronic environment around the decaying nucleus, pointed by Segré and Daudel [1]. It was expected that low-Z nuclei would be most susceptible to the changes in the environment and thus the decay rate change of ^{7}Be in different media was studied by several groups as ^{7}Be is the lightest nuclei decaying by EC process [2, 3, 4]. However, the decay rate change of high-Z nuclei like ^{109}In and ^{110}Sn implanted in Au and Pb was measured recently and an enhancement of EC rate ~1% was observed in a compact medium like Au compared to that of Pb.

The nuclear matrix elements for EC process are generally determined from terrestrial measurements. We know that in all terrestrial EC decay rate measurements, the decaying nucleus is present in a media. So the medium effect should be incorporated correctly before extracting the nuclear matrix element for these EC decay process from the terrestrial measurement. These nuclear matrix elements thus determined are basic inputs for astrophysical processes and abundance calculations. Thus, it becomes important to understand observed decay rate changes of nuclei undergoing EC decay in different media in order to extract the nuclear matrix element of a EC decay process correctly.

Change of EC decay rate of ^{7}Be and LMTO method calculation

In order to understand the observed decay rate change of ^{7}Be in different environment, in our previous studies we performed first principle calculations based on density functional technique (DFT) using tight-binding linear muffin-tin orbital (TB-LMTO) method calculations [5]. In this method all relevant atomic physics calculations were done by solving the relativistic Dirac equation assuming a point nucleus. We determined the average number of 2s electrons of ^{7}Be in different host media and observed that it has an approximately linear relationship with the experimentally measured decay rate of ^{7}Be in different media. We estimated the electron density within ^{7}Be nucleus using Hartree's calculations [6] and found that the change in decay rate of ^{7}Be in different host thus calculated agrees reasonably with the available experimental measurements [2].

Calculated electron density within ^{7}Be nucleus using WIEN2K

With the availability of modern computational facility and technique, it is now possible to compute the electron density at every point within a solid material. So, we used one of these codes, WINE2K[7] and calculated electron density within ^{7}Be nucleus present in Au, Al and Pd. We used face centered cubic (fcc) crystal structured host materials for our calculations and observed that the change in decay rate can be qualitatively understood on the basis of lattice parameters and electron affinity of these hosts.

Table 1: Host Properties

Host	Lattice parameter (Å)	Electron affinity (eV)
Au	4.08	2.31
Al	4.05	0.44
Pd	3.89	0.56

We find in Table 1., Au has very high electron affinity compared to the others. As a result of higher electron affinity, it pulls electrons reducing the electron density at

implanted ^{7}Be nucleus and we find ^{7}Be decays (0.27±0.15) % faster in Al compared to that in Au. On the other hand, even though electron affinity of Pd is lower than that of Au, ^{7}Be in Pd probably experiences compression due to the smaller size of Pd lattice and hence ^{7}Be decays faster in Pd by (0.8±0.2) % compared to that in Au.

When ^{7}Be is implanted, it is expected that it would occupy empty interstitial positions at the end of its trajectory and we performed our calculations placing beryllium at octahedral and tetrahedral positions which are the empty interstitial positions in a fcc lattice. We first performed our calculation placing beryllium at every octahedral position Fig1(a). However, implanted ^{7}Be concentration in host lattice is essentially very low. So, we constructed supercells with one beryllium in a unit cell and also a much larger supercell having one beryllium in eight unit cells at octahedral position as shown in Fig1(b) and 1(c) respectively. We also performed similar supercell calculations placing Be at tetrahedral positions.

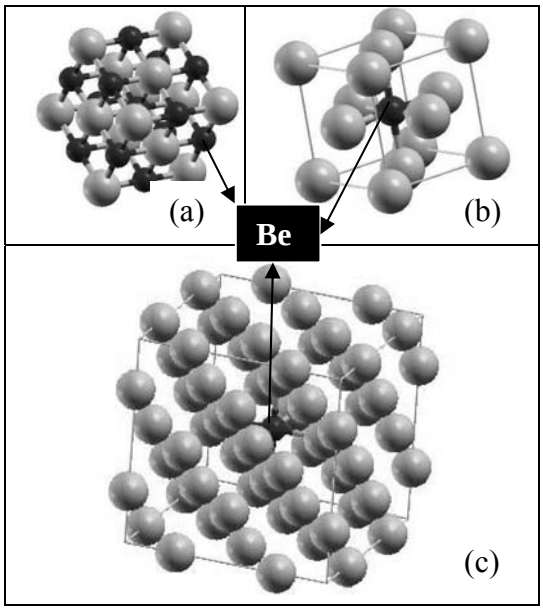

Figure 1:Different lattice configurations considered with Be occupying octahedral position in a fcc lattice

We calculated electron density at 2.6 fm, which is within ^{7}Be nuclear radius using WIEN2K code. All four electrons of the Be atom were considered to be valance electrons. We find that when beryllium occupies all octahedral positions, no supercell as shown in Fig 1(a), the electron density at beryllium nucleus computed using WIEN2K code can explain reasonably the observed change in ^{7}Be decay rate. However, electron density at beryllium nucleus in Au considering supercells or beryllium occupying tetrahedral positions is found to be considerably higher compared to that in Al or Pd. This result is in disagreement with the observations. We also tried shifting the host atoms and implanted atom positions but unable to explain experimental observations.

Conclusion

We find that the electron density computed using WIEN2K code cannot explain the observed change in decay rate when a realistic low density impurity configuration is considered. It might be the inner electron wave functions change under compression has not been properly taken care of and hence electron density computed using this code cannot explain the observed decay rate change of ^{7}Be in different host media.

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