Change in Electron Capture decay rate of ^{7}Be under compression: Experimental observation vs *ab-initio* calculations

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Introduction

The effect of the extra-nuclear environment on nuclear decay process has become a topic of current interest for its application in astrophysics and also in geophysics. About 8 TW of heat is produced inside the earth because of the electron capture decay of ^{40}K and this heat plays an important role in the tectonic plate movement. So it is important to study the change of electron capture decay rate under compression, because the decay rate of electron capturing nuclei is expected to change at high pressure deep inside earth. Change in electron capture nuclear decay rate due to pressure is attributed to the change in the electron density at the nucleus of the decaying atom. In this work we have performed *ab-initio* density functional calculations for determining the electron density at the nucleus in order to understand the observed change in decay rate of radioactive ^{7}Be in ^{7}BeO under compression. Hensley et al. [1] applied high pressure up to 270 kilobars to ^{7}BeO crystals and found that the decay rate of ^{7}Be increased by (0.59±0.1) %. We used density functional codes (a) TB-LMTO (Tight-Binding Linearized Muffin-Tin Orbital) [2] and (b) WIEN2K [3] to calculate the change in electron density under compression at beryllium nucleus in BeO lattice.

Method of calculation

We used two density functional codes (TB-LMTO and WIEN2K) to calculate the electron density at beryllium nucleus in compressed and uncompressed beryllium-oxide lattice. In density functional calculations, the total energy of electron-nucleus system (modeled with some approximations) is minimized self-consistently under periodic boundary condition using relativistic electronic wave functions. The required inputs are the lattice parameters of BeO and atomic structures of beryllium and oxygen atoms. There is no adjustable free parameter in these codes. Input lattice parameters of BeO, from x-ray data available in literature were used for un-compressed normal BeO lattice calculations. For electronic structure calculations under compression, reduced lattice parameters were estimated based on ~10% change in volume of BeO under 240 kilobar pressure [1] and given as input in the calculations.

Change in Decay rate calculated using TB-LMTO method

After the completion of self-consistent electronic structure calculation of a system TB-LMTO code provides a total wave function projected on different eigenstates of each constituent atom. Thus, $|\langle\psi_{total}|\psi_{Be2s}\rangle|^2$ calculated using the code represents the average number of 2s electrons of beryllium ion in BeO lattice. We found that the average number of 2s electrons of beryllium ion in BeO under compression (~10% volume reduction) and without compression was about the same indicating about the same electron density at the beryllium nucleus for both compressed and un-compressed beryllium ion. We estimate the electron capture decay in compressed and un-compressed beryllium ion would be the same within ~0.1%.

Change in decay rate calculated using WIEN2K

WIEN2K code directly calculates the electron density at the nucleus after energy minimization has been achieved by a self-consistent process. We performed WIEN2K code calculations in two different ways – by first considering that both 1s and 2s electrons are valence electrons and also by considering 1s as a core state and only 2s as valence state. The electron density calculated at the nucleus using this code and contributions from different orbitals are given in Table 1.

We find that the electron density at the nucleus increases by ~0.1% for the compressed beryllium ion (~10% volume reduction of BeO lattice) compared to the un-compressed case. Such a small increase (~0.1%) is not in agreement with the observed result of Hensley et al. [observed increase by (0.59±0.1) %] by about a factor of six. The result is independent of how we do the calculations i.e. whether 1s electrons are considered as core electrons or not. The results indicate that the electron capture should increase because of the compression of 1s state. WIEN2K code does not consider any such compression of the core and actually treats the core sates as those for a free atom (wave function becoming zero at infinity). Such assumptions of the density functional codes seem to be questionable.

Table 1: Electron density at ^{7}Be in BeO using WIEN2K code

configurations		Electron density at the ^{7}Be nucleus in BeO	
		compressed	uncompressed
1.	Total 1s+2s valance	35.32977	35.294175
2.	Core(1s)	34.52232	34.56204
	Valance (2s)	0.841507	0.765747
	Total	35.363738	35.327787

Conclusion

The state of the art density functional codes such as WIEN2K and TB-LMTO cannot explain the experimental results regarding the rather large increase of electron capture decay rate under compression. The probable reason for such disagreement seems to be the compression of inner electronic orbitals. The physics of such compression is not included in the density functional codes because they assume that the wave function for the inner core electrons of the constituent atoms becomes zero at infinity. Such effects should be included in the density functional codes to explain the electron capture decay rate data under compression.

References

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