# Atomic Structure Calculation of Sm Using the Method of Multi-Configuration Dirac-Fock

Angom Dilip , A. Fukumi, T. Kondo, M. Iinuma, I. endo and T. Takahashi

*Photon Physics Laboratory,*
*Hiroshima University, 1-3-1 Kagamiyama,*
*Higashi-Hiroshima, 739-8526, Japan*
*E-mail:angom@photon.hepl.hiroshima-u.ac.jp*

The closely spaced opposite parity levels in some of the rare earth atoms offers the unique possibility of carrying out atomic parity non - conservation(PNC) experiments. The advantages of using rare earth atoms are:

- The almost degenerate opposite parity levels can enhance the PNC effects significantly.
- Measurement on a string of isotopes can eliminate the inaccuracy from the theoretical calculations.

Among the rare earth atoms, the 15639.80cm$^{-1}$ and 15650.55cm$^{-1}$ levels of Sm are being investigated for PNC experiments in our group [1]. These levels have also been proposed as promising candidates for EDM measurement [2].

As a part of the experimental effort, it is desirable to have an estimate of the expected magnitude of the PNC effects. This can be carried out using the methods of atomic many-body theories. The existance of many configurations with the same shell occupation poses a great difficulty in the structure calculation of atomic Sm. A multiconfiguration based method would be an appropriate choice. For our calculations we have used GRASP92 [3], a relativistic multiconfiguration Dirac-Fock(MCDF) atomic structure code.

Table 1: The lowest multiplet of Sm in units of cm$^{-1}$

| Level | Expt | Porsev | Present work |
|---|---|---|---|
| $^7F_1$ | 292.58 | 285 | 276 |
| $^7F_2$ | 811.92 | 810 | 788 |
| $^7F_3$ | 1489.55 | 1523 | 1487 |
| $^7F_4$ | 2273.09 | 2376 | 2326 |
| $^7F_5$ | 3125.46 | 3331 | 3271 |
| $^7F_6$ | 4020.66 | 4361 | 4294 |

The structure calculations on the low-lying levels of Sm have been carried out in earlier works[4, 5]. But the levels of interest for the PNC experiments are both high-lying. The calculations involving higher levels are in general difficult due to the strong configuration mixing and more so with the rare earth atoms. As a starting point we have investigated the low-lying

levels using GRASP92 and our results for the ground state multiplets are given in the Table: 1. Only the ground state configuration $4f^6 6s^2$ was used for this calculation. For comparision, the results of Porsev [5] and experimental values [6] are also given.

The higher multiplet levels were also calculated with selected configurations and total angular momentum states. The selection was necessary as the number of configurations increases rapidly when the excitations to higher angular momentum shells like $5d$ are included. And orbitals till $4f$ shell were considered core. Results from the latest calculation with the orbital space of $(1-7)s$, $(2-7)p$, $(3-7)d$ and $4f$ are given in Table: 2. The configuration space consisted of all possible combinations of two electron fillings within the valence space $(6-7)s$, $(6-7)p$ and $(5-7)d$ orbitals. The total angular momentum was restricted to $J = 0, 1$ and 2. With this calculation we can estimate the correlation effects from the valence shells.

Table 2: Excitation energy of the low-lying levels in Sm

| Level | Expt | Porsev | Present work |
|---|---|---|---|
| $^7F_1$ | 292.58 | 285 | 276 |
| $^7F_2$ | 811.92 | 810 | 790 |
| $^9G_0$ | 13796.36 | 11339 | 11147 |
| $^9G_1$ | 13999.50 | 11533 | 11338 |
| $^9G_2$ | 14380.50 | 11906 | 11704 |
| $^9H_1$ | 10801.10 | 12739 | 13227 |
| $^9H_2$ | 11044.90 | 12693 | 13444 |

Compared to the single configuration calculation, there is an improvement in the fine-structure splitting of the ground state multiplet but level sequence of the higher levels is still not correct. This implies that the configurations added are more important for the correlation effects to the ground state multiplet. For the configurations $4f^6 6s^2$ and $4f^6 5d6s$, mixing through $4f$ excitations with configurations like $4f^5 5d6s6p$ and $4f^5 5d^2 6p$ will be important. These will be the next step in our study. Along with the energy levels we also calculated the HFS constants but in absence of the core excitations, the results shows very large deviations from the experimental values.


[1] A. Fukumi, I. Endo, T. Horiguchi, Y. Ishida, T. Kondo, T. Kuwamoto, H. Matsuzaki, T. Nakamura, T. Takahashi, Z. Phys. D **42**, 243-249(1997).

[2] S. Rochester, C. J. Brown, D. Budker, D. DeMille and M. Zolotorev, Phys. Rev. A **59**, 3840(1999).

[3] F. A. Parpia, C. Froese Fischer, I. P. Grant, Comput. Phys. Commun. **94**, 249-271.

[4] K. T. Cheng and W. J. Childs, Phys. Rev A **31** 2775(1985).

[5] S. G. Porsev Phys. Rev. A **56**, 3535(1997).

[6] C. Martin, R. Zalubas and L. Hagen, *Atomic Energy Levels–The Rare Earth Elements* Natl. Bur. Stand. U. S Ref. Data Ser. No. NSRDS-NBS 60 (U. S. GPO, Washington, DC, 1978).