Physica Scripta. Vol. T80, 446–447, 1999

M1-Transitions of Ti-like Highly Charged Ions

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Received September 13, 1998; accepted in revised form November 26, 1998

PACS Ref: numbers: 31.15.Ne, 31.30.Jv, 32.10.Fn, 32.30.Jc, 52.20.-j

Abstract

Ground-term fine-structure levels and their magnetic-dipole (M1) transition properties of Titanium-like ions are investigated theoretically through the atomic number Z=37-103. An anomalous stability in wavelength of J=3-2 M1-transition reported by Feldman [J. Opt. Soc. Am. B **8**, 3 (1991)] is explained in terms of a concept of the critical atomic number beyond which the relativistic nature dominates in the corresponding fine-structure. The Tokyo-EBIT facility [J. Phys. Soc. Jpn **65**, 3186 (1996)] enabled us to observe the corresponding line in the visible range for Xe^{+32} and Ba^{+34} ions. The measured wavelengths are consistent with measurements by the NIST group [Phys. Rev. Lett. **74**, 1716 (1995)], however there remains a considerable discrepancy from present calculations.

1. Introduction

A systematic investigation of atomic structures along an isoelectronic sequence is the best way to understand the role of relativistic effects on atomic structure. In general, the relativistic effects rapidly increase as the atomic number Z increases. In many-electron systems, however, the screening effect by surrounding electrons competes with the relativistic effects, so a more complicated analysis of the relativistic atomic structure is required. In the transition from the correlation region to the relativistic region, interesting phenomena in many-electron atomic structures can manifest themselves, *e. g.* level crossings.

Using an Electron-Beam-Ion-Trap (EBIT), precise measurements of atomic structures in highly charged ions are feasible. Understanding the relativistic atomic structure of highly charged ions is essential for diagnostics and modeling of high-temperature plasmas. Feldman [1] found that the magnetic-dipole line of the transition between two ground-term fine-structure levels, $(3d^4)_{J=3}$ and $(3d^4)_{J=2}$, for the Titanium-like sequence stays in the visible and the near-UV range over a wide atomic number range. This line is convenient for plasma diagnostics, since the visible and the near-UV transition usually can be measured more accurately. However, this finding is a puzzle from the point of view of relativistic atomic structure theory, since it seems to be inconsistent with the common knowledge that wavelengths of transitions in isoelectronic sequences rapidly fall to shorter wavelength as the atomic number increases. In the present work, we propose a possible mechanism for the stability in the wavelength in terms of the concept of the critical atomic number beyond which the relativistic nature dominates in atomic structures.

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2. Results and Discussions

Throughout the present work, calculations were performed using the GRASP92[2] program package. A set of subshell wavefunctions was obtained by a multi-configuration Dirac-Hartree-Fock calculation in the extended-average-level mode with a minimal electronic configuration, $3d^4$. The configuration interaction calculations were then performed with the minimal electronic configuration. In a systematic survey of the magnetic-dipole transition properties, the nuclear volume effect, the mass polarization effect and the QED effects were completely neglected for simplicity. As discussed in the last part of this paper, to make a comparison between the present calculations and experimental measurements, more elaborate and accurate calculations have also been performed.

The ground-term fine-structure of Titanium-like ions consists of $(3d^4)_{J=0,1,2,3,4}$ levels. Fig. 1 (a) shows wavelengths of the magnetic-dipole transition among the J=1,2,3,4 levels. As seen in the figure, it is a common feature for all transitions that at small atomic numbers the wavelength rapidly falls into a shorter wavelength (almost proportionally to Z^{-4}), whereas at large atomic numbers the wavelength gently decreases (almost proportionally to Z^{-1}). It is remarkable that the line for the J=3-2 transition stays within the visible and the near-UV region over a wide range of atomic number, while other transitions already decrease in wavelength. Particularly, for the range Z=60-70 the wavelength for the J=3-2 transition is almost constant. In subsequent discussions, we refer to this feature as the anomalous stability. A 'spike' in the wavelength of the J=4-3 transition corresponds to an intersection between the fine-structure levels of J=3 and J=4 at around Z=52. Fig. 1 (b) shows the magnetic-dipole matrix elements. The magnetic-dipole matrix elements along the Titanium-like sequence behave similarly for all the transitions. This suggests that there is no peculiarity in the wave functions of the J=2 and 3 levels.

To understand a mechanism for the anomalous stability in the wavelength of the J=3-2 transition, we introduce a concept of a critical atomic number. Fig. 2 shows the configuration interaction coefficient for $3d^3_{3/2}3d_{5/2}$ for the J=2 and J=3 levels. As Z increases, the coefficient of $3d^3_{3/2}3d_{5/2}$ approaches unity, since there the relativistic effect dominates over the electronic correlations. Although somewhat arbitrary, we define the critical atomic number as the atomic number beyond which the absolute value of the coefficient for the dominant contribution is larger than 0.9. A possible mechanism for the stability in the wavelength of the transition between the J=3 and J=2 levels is illustrated in Fig. 3. It is

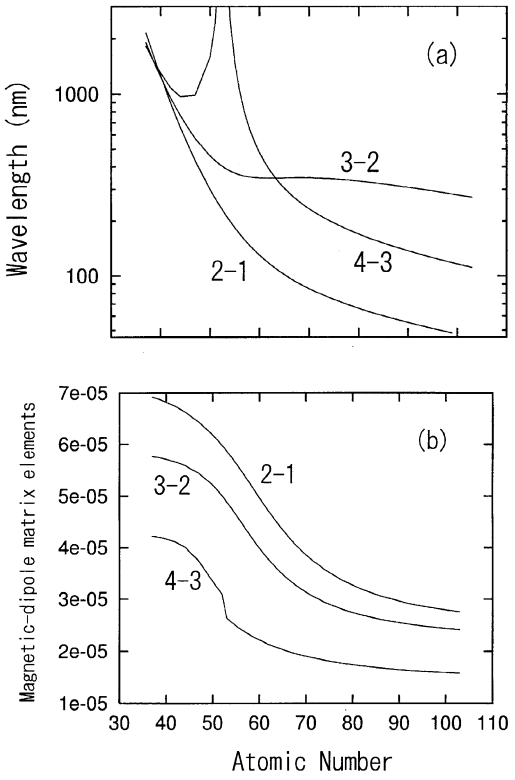

Fig. 1. (a) Wavelength of the magnetic-dipole transition among the ground-term fine-structure levels. (b) Magnetic-dipole matrix elements.

essential that the critical atomic number for the upper level is smaller than that for the lower level.

To compare with experimental wavelengths, more elaborate calculations were performed for Xe^{+32}, Cs^{+33}, Ba^{+34}, Nd^{+38} and Gd^{+42} ions. A set of subshell wavefunctions was prepared by performing term dependent multi-configuration Dirac-Hartree-Fock calculations in the extended-average-level mode with the minimal configuration, $3d^4$. The electronic correlation effect, the lowest order QED effects, the nuclear volume effect and the mass polarization effect were taken into account through the relativistic configuration interaction calculations. It is noted that we completely neglected contributions from subshells beyond the K, L and M shells. Table I shows a comparison between the present calculations and experimental measurements[3] for the wavelength of the J=3-2 M1-transition. The present calculations predict this wavelength to be about 10 nm shorter than the experimentally measured ones for all ions discussed here. The discrepancy seems to grow as the atomic number increases. Contributions to the electronic correlations from the outer subshells which are neglected in the present calculations may be sizable [4].

3. Summary

A systematic investigation of the magnetic-dipole transition among the ground-term fine-structures has been presented for the Titanium-like sequence. The anomalous stability in the wavelength of the J=3-2 transition is explained in terms of the critical atomic number. To have stability in the transition wavelength, it is essential that the critical atomic number for the upper level is smaller than that for the lower level. It is intriguing to investigate if a similar situation could occur in other atomic systems. A comparison between the present calculations and the experimental measurements shows that there remain considerable discrepancies. It is noted that the transition energy between two fine-structure levels discussed here is about 10^{-5} of their absolute energies. To obtain such a high precision in *ab initio* calculations is still difficult for many-electron atomic structure theories.

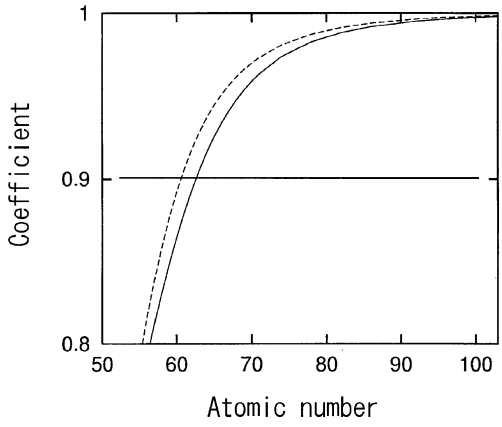

Fig. 2. Configuration interaction coefficient for the dominant configuration, $3d_{3/2}^3 3d_{5/2}$. Solid curve represent the coefficient for J=2 level, and broken curve for J=3 level.

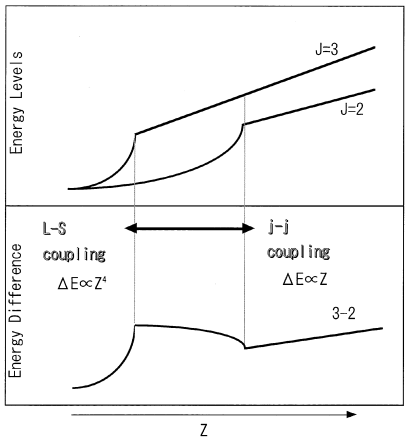

Fig. 3. Mechanism of the stability in the transition wavelength.

Table I *Wavelength of the magnetic-dipole transition between the ground-term fine-structures,* $(3d^4)_{J=3}$ *and* $(3d^4)_{J=2}$. *Experimental uncertainties in wavelengths measured with the Tokyo-EBIT[5] include only statistical error.*

Z	Present (Th.)	Tokyo-EBIT (Ex.)	NIST [3] (Ex.)
54	403.659	413±0.02	413±0.2
55	391.190	–	–
56	382.476	393±0.02	393.2±0.2
60	361.246	–	375.3±0.2
64	355.530	–	371.3±0.2

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