Measurement of the $3d$-$4f$ transition in Ni-like Er for use in a photopumped x-ray-laser scheme

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A measurement of the Ni-like Er $3d_{3/2}$-$4f_{5/2}$ transition energy is presented. The value differs from a previous prediction that was based on an interpolation of measurements of the transition in elements of nearby atomic numbers. This transition was previously thought to have an energy very near the H-like Al Ly-α_2 line, making the system a favorable candidate for resonant photopumping. The measured energy difference between the Er $3d$-$4f$ and Al Ly-α_2 transitions is 1.8 ± 0.3 eV or 1040 ppm indicating that the overlap is not as favorable as previously thought. The difficulties with the previous interpolation are discussed. Additional measurements of the $3d_{3/2}$-$4f_{5/2}$ transition energies in Ni-like Pr, Yb, and Pt are presented that achieve a precision better than 100 ppm. Together with the value for Er, these are used to derive a new interpolation with better predictive capabilities.

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INTRODUCTION

In addition to collisional excitation and recombination, photopumping has been considered as the pumping mechanism for an x-ray laser [1]. One such photopumping scheme proposed by Nilsen [2] would use the Ly-α_2 transition in H-like Al to pump the $3d_{3/2}$-$4f_{5/2}$ Ni-like Er. This excited state in Ni-like Er would then decay to the upper level of a lasing transition. (See Fig. 1 in Ref. [2].) The success of this scheme relies on how well the two line energies overlap. Reference [2] indicated that the two transitions differed by only 280 ppm at 7.176 Å (1728 eV). This 2 mÅ difference was considered encouraging for successful photopumping for this system since the Doppler width of the Al lines in a plasma with an ion temperature of 450 eV is 2.3 mÅ.

However, this suggestion of a good resonance was not based on a measurement of the Er line itself, but rather on an interpolation of the measurements of elements of nearby atomic numbers [2,3]. Furthermore, those measurements had an estimated uncertainty of 5 mÅ or greater. In this paper, we present measurements of four $3d_{3/2}$-$4f_{5/2}$ Ni-like lines including the Er transition with a much higher precision than previous measurements. We redo the interpolation using these four new data points and show that the previous interpolation incorrectly predicts a good photopumping resonance.

EXPERIMENT

The measurements were done on the electron-beam ion trap (EBIT) at Lawrence Livermore National Laboratory (LLNL). A monoenergetic electron beam ionizes, excites, and radially traps ions which are studied by their emitted x rays. An axial trap is formed by three cylindrical electrodes through which the beam passes. Relative voltages on these three electrodes restrain the ions. EBIT has been described in detail elsewhere [4].

The charge balance of the trapped ions is primarily determined by the beam energy. As such, EBIT has an advantage over laser-produced or tokamak plasmas for such experiments due to its ability to control the charge balance and the excitation process. By choosing the electron-beam energy, we can select a dominant charge state. In particular, by sequentially recording spectra at beam energies just below the respective ionization potentials, the line emission from different charge states can be unambiguously identified. Moreover, blends with satellite lines produced by dielectronic recombination can be avoided by proper choice of the beam energy [5].

The x-ray energies of the $3d_{3/2}$-$4f_{5/2}$ transition in four Ni-like ions (Pr, Er, Yb, and Pt) were measured and are listed in Table I along with previous measurements of that transition in various other ions. Also in Table I, are the theoretical predictions for the transition energies based on a multiconfiguration Dirac-Fock calculation using the Grant computer code [6] in the extended average level approximation. The x-ray wavelengths were analyzed in a flat-crystal vacuum spectrometer [7] and Fig. 1 shows sample spectra.

The Er measurements were done with a potassium acid phthalate (KAP) crystal ($2d=26.6$ Å) in second order. To determine the wavelength of the Er line, the H-like Al Ly-α lines were used for calibration. The H-like Al Ly-α_1 and Ly-α_2 are separated by 1.3 eV, which is just about equal to the full width at half maximum (FWHM) resolution of the measurement. For the wavelength standard, the values of Garcia and Mack [8] were used. The result for the Er line is 1725.9 ± 0.3 eV (7.1837 Å$\pm$1.3 mÅ). This is 6 mÅ from the interpolation prediction. The Ly-α_2 line at 1727.7 eV (7.1763 Å) is measured to a precision of 0.1 eV and therefore the Al-Er energy difference is 1.8 ± 0.3 eV or 1040 ppm.

The Pr line was measured using the theoretical energies for the He-like Ne $K\gamma$ and $K\delta$ transitions for calibration. The theoretical values were taken from Ref. [9] and adjusted for the ground-state energy calculated by Drake [10]. Because the value for the Ne $K\gamma$ transition was listed incorrectly in Ref. [9], an interpolation was made. The values used are 11.0008 Å and 10.7641 Å, respectively. This set of measurements was also done with a KAP crystal ($2d=26.6$ Å) in second order. The ener-

TABLE I. Measured, calculated, and fitted energies (in eV) of the $3d_{3/2}$-$4f_{5/2}$ transition in Ni-like ions. The theoretical values are from our present calculations. The fitted energies are based on the quadratic interpolation of all data, i.e., Eq. (2).

Ion	Theory (eV)	Experiments (eV)	Experimental reference	Quadratic fit (eV)
Pr^{31+}	1144.95	1144.06±0.08	Present work	1144.05
Sm^{34+}	1326.24	1324.6±2.8	[16]	1325.11
Gd^{36+}	1454.14	1452.8±3.4	[16]	1452.97
Dy^{38+}	1587.75	1585.5±4.0	[16]	1586.60
Er^{40+}	1727.11	1725.9±0.3	Present work	1726.05
Tm^{41+}	1798.96	1799.5±1.3	[13]	1797.97
Yb^{42+}	1872.28	1872.9±1.4	[13]	1871.35
Yb^{42+}	1872.28	1871.38±0.16	Present work	1871.35
Hf^{44+}	2023.33	2024.2±1.7	[3]	2022.55
Ta^{45+}	2101.08	2098.9±1.8	[3]	2100.37
W^{46+}	2180.32	2179.4±1.9	[3]	2179.68
W^{46+}	2180.32	2160±15	[16]	2179.68
Re^{47+}	2261.06	2260.8±2.1	[3]	2260.49
Pt^{50+}	2512.38	2511.9±0.5	Present work	2511.93

gy was determined to be 1144.06±0.08 eV.

The Yb line was measured using the He-like Al $K\beta$ and $K\gamma$ transitions for calibration. Again, we use the values calculated in Ref. [9] and adjusted for the ground-state energy calculated by Drake [10]. The values employed are 6.6347 Å and 6.3138 Å, respectively. A pentaerythritol (PET) crystal ($2d=8.742$ Å) was used in first order. The energy was determined to be 1871.38±0.16 eV.

The Pt measurement is described in Ref. [11] and was done with a Ge(111) crystal ($2d=6.532$ Å). H-like Si Ly-β and Ly-γ were used for calibration and the wavelength standards were taken from Ref. [8]. The energy was determined to be 2511.9±0.5 eV.

The one-standard-deviation uncertainties enumerated above result from contributions due to statistics and systematics. The statistical uncertainty results purely from the precision to which the line centroids can be determined. Systematic uncertainties vary from case to case. For all the measurements, possible electronic gain shift effects were checked for by alternating between the calibration and sample measurements. No gain shifts were observed and thus no uncertainty is assigned. In two cases (Al-Er and Al-Yb), the calibration spectrum possesses some contamination from the sample which partially blends with the calibration lines. The necessity of subtracting out the contamination introduced a systematic uncertainty for those two cases of roughly 0.1 eV. In the case of the Pt measurement, the line fell outside the calibration region. This introduced a systematic error due to gain nonlinearities (see Ref. [11]).

The precision of the calculation of the standard wavelengths used for calibration indicates that the uncertainty arising because of the use of theoretical values is small. This last uncertainty is estimated to be 0.003 eV for the H-like Al lines used to calibrate the Er and Pt points. This estimate arises from comparing the calculations of Erikson [12] and Garcia and Mack [8]. Based on the differences in the ground-state energies of Vainshtein and Safronova [9] and Drake [10], the uncertainties of the He-like calibration lines used for the Pr and Yb points is estimated to be 10 ppm or 0.010 eV and 0.015 eV, respectively. The interpolation procedure used for generating the Ne $K\gamma$ calibration line increases the uncertainty of the Pr datum to 0.04 eV. All systematic uncertainties were added linearly to the statistical uncertainties to arrive at the values quoted in this report.

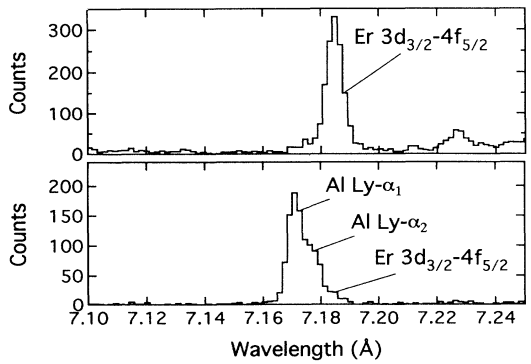

FIG. 1. The spectra of H-like Al Ly-α, and Ni-like Er.

THE INTERPOLATION

In Refs. [2] and [3], the measured energies (E) divided by atomic number (Z) were fit to a straight line of the form $a+bZ$. If we take the previous data from Table I for the $3d_{3/2}$-$4f_{5/2}$ transition and fit it by this procedure, we obtain

$$E_{\text{fit}}/Z = a + bZ \ . \tag{1}$$

Here, $a=-20.5\pm0.2$ and $b=0.675\pm0.003$ and energies are in eV. We can now define the residuals of the linear fit $\delta E/Z=(E_{\text{measured}}-E_{\text{fit}})/Z$. Figure 2 shows the residuals of the linear fit to the $3d_{3/2}$-$4f_{5/2}$ transition energies divided by the atomic number versus Z. The data used in this fit are only those points available prior to this work.

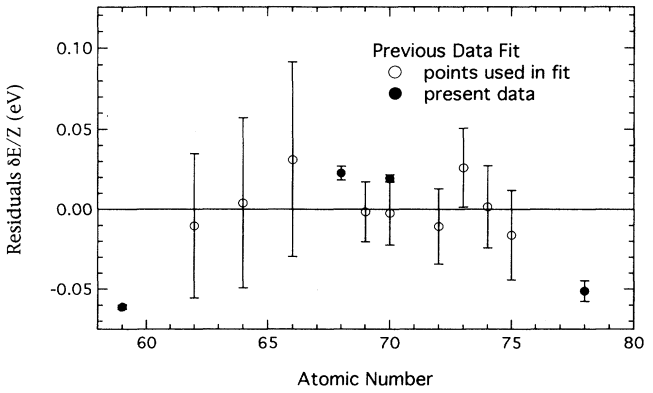

FIG. 2. The residuals of a linear fit of the reduced energy (E/Z) versus the atomic number (Z) for the data available prior to this work. Superimposed on this plot are the points measured here.

This is the fit that Nilsen [2] refers to in predicting the Er value to be at 7.178 Å(1727.3 eV). Also shown on this plot are the points that we have measured. There are two conclusions to draw from Fig. 2. Our data are much more precise than the previous laser-produced plasma data, and a linear fit will not accommodate our data.

If we now fit all the measured data for the $3d$-$4f$ transition given in Table I to a quadratic form using

$$E_{\text{fit}}/Z = a + bZ = cZ^2 , \tag{2}$$

then we obtain values for $a = -16.4 \pm 0.2$, $b = 0.557 \pm 0.006$, and $c = 8.6 \pm 0.5 \times 10^{-4}$. Figure 3 shows a similar residual plot using this fitting function. This latter fit is dominated by the recent measurements because of the smaller uncertainties but is a good representation of all the data. The energy values predicted by this interpolation are listed in Table I. Both the linear and quadratic fits weighted the data by the quoted total uncertainties.

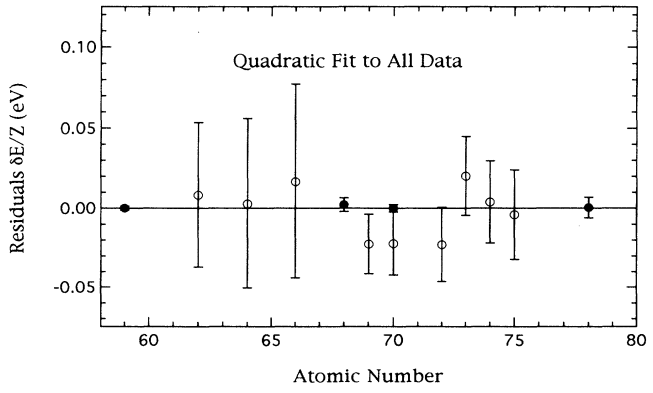

FIG. 3. The residuals of a quadratic fit of the reduced energy (E/Z) versus the atomic number (Z) for all the data presented in Table I. Solid points denote EBIT data while open circles are data from Refs. [3,13,16].

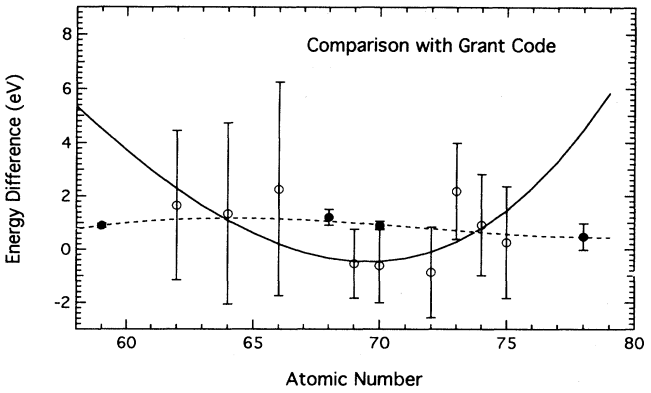

FIG. 4. The difference of the Grant computer code predictions and the values derived from the linear and quadratic fits. Superimposed are all the measured points. Solid points denote EBIT data. The solid line is the difference between the Grant computer code results and the linear fit described in the text. The dashed line is the difference between the Grant computer code results and the quadratic fit described in the text.

Figure 4 shows the difference between predictions for the transition energies and the two fits. The theoretical predictions for the transition energies are based on a multiconfiguration Dirac-Fock calculation using the Grant computer code [6] in the extended average level approximation. In the region of $Z = 68$, there is an obvious discrepancy between the predicted values for the two fitting functions. The linear fit predicts a value much too high because of the high values of the measurements at $Z = 69$ and 70 of Klapish *et al.* [13]. Though the linear fit was very useful for identification of lines [3], the experimental precision of the data (5 mÅ) was too poor to predict an Er value to sufficient accuracy for application to the photopumped x-ray-laser scheme.

In previous work [11,14,15], we have noted a constant offset between the measured values and the theoretical predictions. For these data, the Grant computer code predictions were typically 0.9 eV high.

CONCLUSIONS

The Doppler broadening in a plasma is relatively simple to predict. For a typical ion temperature of 450 eV, the broadening of the Al line is 2.3 mÅ. Thus, one could be assured of a good overlap for an Er-Al separation of 1.2 mÅ (170 ppm) or less. However, the measured difference between the Er and Al lines is 7.4 mÅ and one would need to rely on other processes such as opacity broadening or bulk Doppler shifts to provide the necessary linewidth. These effects are less well known and much more plasma dependent. As such they are difficult to predict and render the overlap candidate dubious.

Theory can only predict transition energies in these ions to approximately 1000 ppm whereas the overlap requirement is typically of the order of 100 ppm. Therefore, measurements are necessary to verify potential pho-

topump laser schemes. Interpolation techniques are very useful as an aid to improve the predictive power of the theory. For such interpolations to be successful to a required precision, they must be derived from data of comparable precision.

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