Atomic Database Development of Mid-to-High-Z Elements

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1 Introduction

Detailed atomic databases are needed for some applications, such as in hydrodynamics codes for plasma diagnostics and analysis of x-ray spectra. For plasma diagnostics requiring data for many ionization stages with many fine-structure levels, atomic models developed using very complex calculations have limitations. Again, for accurate diagnostics, a detailed level accounting cannot be simplified by an averaging process such as used in the average atom model, which will inhibit all the important and relevant radiation dynamics. To include a large number of states with a minimum of computational effort, we have developed atomic models where many of the multiplet levels are lumped into the configuration states, but the important low-lying states are kept at fine structure levels and they are connected by the relevant atomic processes to allow detailed analysis of diagnostically important emission processes.

This model for F-like and Ne-like stages has already been used for diagnosing[1] selenium plasmas. In the present work we use this model to calculate databases for all L- and M-shell ionization stages of titanium. Currently, z-pinch experiments are being performed using titanium wires producing x-ray emission with very high yields. Titanium is also an important element in tokamak discharges for fusion research. Our complete database will include both radiative and collisional data, including dielectronic recombination (DR) connecting all the levels for all the ion stages. However, we will present here only partial data for Ti XIX and Ti XX.

Effectiveness of this method will be evaluated by comparing our results with other published calculations, and these theoretical methods used to calculate the data for all important processes when properly benchmarked by measurements can provide adequate data.

2 Atomic Model

For the Ti XIX and TI XX ion stages we have kept all the n=2 and 3 fine structure levels while the higher lying excited levels are lumped in our model. The Ti XX model consists of 10 levels including the ground level, two Δn=0 $2p$ excited state, 5 fine structure levels of the n=3 manifold, one lumped n=4 level and one lumped level of n=5, 6, and 7 excited states. The Ti XIX model contains 25 levels including the ground state, fine structure levels of 9 n=2 and 10 n=3 excited states, 3 lumped inner-shell excited configurations of $2p3l$, one lumped n=4 level and one lumped level of n=5,6, and 7 states. All the excited levels are fully coupled to the ground states and among themselves for each ion. Table 1 lists the energy level designations and energies of these levels.

The atomic structure data such as the energies and radiative transition probabilities for the fine-structure levels are calculated using the DFW atomic code of Sampson *et al.*[2]. For the lumped n=3 states, these structure data are obtained using the HFR (Hartree-Fock with Relativistic corrections) method of Cowan[3]. These radiative transition rates from the excited levels to the ground states

for Ti XX and XIX are also included in Table 1. Our level energies and transition probabilities agree very well with other state-of-the-art calculations.

For dipole allowed transitions, collisional data are obtained using the Semiclassical Impact Parameter (SCIP) method[4] and for other transitions, the Coulomb Born Distorted Wave (CBDW) method[5] is used to calculate collisional data coupling the levels in our model. For diagnostically important transitions when either the SCIP or the CBDW methods are inadequate, collisional data are obtained using a suite of more sophisticated fully relativistic atomic structure and distorted wave (RDW) codes[2, 6]. Collision strengths for some of the transitions for Ti XX and Ti XIX are shown in Tables 2 and 3 and they are compared to those obtained using another DW calculation[7]. Our collisional excitation data will be updated by including resonance excitation in the future. Electron-impact ionization cross sections are calculated by the exchange classical impact-parameter method. Again, for important transitions the ionization cross sections are replaced by those calculated using the RDW ionization codes of Ref. [8].

The ground to ground DR rates can be approximated by the semi-empirical formulas derived by Burgess and modified by Merts, Cowan, and Magee (BM)[9]. However for ions of interest, more accurate and detailed state-specific DR data are obtained using the HFR method of Cowan[3]. DR data such as autoionization rates and DR branching ratios from the ground and $\Delta n = 0$ states of the recombining ion to each specific fine structure level of the recombined ions are calculated. For low lying doubly-excited states, DR branching ratios are explicitly calculated, while for higher Rydberg states, we used a $1/n^3$ falloff extrapolation of the DR branching ratios. The DR rates for Ti XX and TI XIX are shown in Table 4. Our total ground-to-ground DR rates for Ti XX agree very well with those obtained by Chen using a multi-configuration Dirac-Fock calculation[10].

References

[1] A. Dasgupta, K. G. Whitney, H. L. Zhang, and D. H. Sampson, *Phys. Rev. E* **55**, 3460 (1997)

[2] D. H. Sampson, H. L. Zhang, A. K. Mohanty, and R. E. H. Clark, *Phys. Rev. A* **40**, 604 (1989)

[3] *Atomic Structure Code of R. D. Cowan*, "The Theory of Atomic Structure and Spectra", University of California Press, Berkeley, CA 1981

[4] E. Oran and J. Davis, *J. Appl. Phys.* **45**, 2480 (1974)

[5] J. Davis, P. C. Kepple, and M. Blaha, *J. Quant. Spectrosc. Radiat. Transfer* **16**, 1043 (1977)

[6] H. L. Zhang, D. H. Sampson, and A. K. Mohanty, *Phys. Rev. A* **40**, 616 (1989); D. H. Sampson, H. L. Zhang, and C. J. Fontes, *At. Data Nucl. Data Tables* **48**, 25 (1991); H. L. Zhang and D. H. Sampson, *Phys. Rev. A* **47**, 208 (1993)

[7] R. E. H. Clark, J. Abdallah, Jr., G. Csanak, J. B. Mann, and R. D. Cowan, *Theoretical Atomic Physics Code Development I. ACE: Another Collisional Excitation Code*, Los Alamos National Laboratory manual (December 1988)

[8] H. L. Zhang and D. H. Sampson, *Phys. Rev. A* **42**, 5378 (1990); D. H. Sampson and H. L. Zhang, *Phys. Rev. A* **45**, 1657 (1992)

[9] A. Burgess, *Astrophys. J.* **141**, 1589 (1965); A. L. Merts, R. D. Cowan, and N. M. Magee, Jr., Los Alamos Scientific Laboratory Report No. LA-6220-MS, 1976 (unpublished)

[10] M. H. Chen, *Phys. Rev. A* **33**, 994 (1986)

Table 1: Level identifications, state designations, energies and radiative decay rates to the ground levels for Ti XX and Ti XIX.

Ti XX				Ti XIX			
level	state	Eng (eV)	A^r (s^{-1})	level	state	Eng (eV)	A^r (s^{-1})
1	$1s^2 2s\ ^2S_{1/2}$	0.0		1	$1s^2 2s^2\ ^1S_0$	0.0	
2	$1s^2 2p\ ^2P^o_{1/2}$	4.0287[1]	1.466[9]	2	$1s^2 2s2p\ ^3P^o_0$	3.5842[1]	
3	$1s^2 2p\ ^2P^o_{3/2}$	4.7966[1]	2.504[9]	3	$1s^2 2s2p\ ^3P^o_1$	3.7888[1]	1.274[7]
4	$1s^2 3s\ ^2S_{1/2}$	8.0163[2]		4	$1s^2 2s2p\ ^3P^o_2$	4.3145[1]	
5	$1s^2 3p\ ^2P^o_{1/2}$	8.1276[2]	3.558[12]	5	$1s^2 2s2p\ ^1P^o_1$	7.4791[1]	1.408[10]
6	$1s^2 3p\ ^2P^o_{3/2}$	8.1504[2]	3.473[12]	6	$1s^2 2p^2\ ^3P_0$	9.6645[1]	
7	$1s^2 3d\ ^2D_{3/2}$	8.1926[2]		7	$1s^2 2p^2\ ^3P_1$	1.0018[2]	
8	$1s^2 3d\ ^2D_{5/2}$	8.1998[2]		8	$1s^2 2p^2\ ^3P_2$	1.0370[2]	
9	$1s^2 4l$	1.0851[3]	2.923[11]	9	$1s^2 2p^2\ ^1D_2$	1.1509[2]	
10	$1s^2 5l - 7l$	1.2663[3]	4.298[10]	10	$1s^2 2p^2\ ^1S_0$	1.3894[2]	
				11	$1s^2 2s3s\ ^3S_1$	7.6600[2]	
				12	$1s^2 2s3s\ ^1S_0$	7.7404[2]	
				13	$1s^2 2s3p\ ^3P^o_0$	7.8239[2]	
				14	$1s^2 2s3p\ ^3P^o_1$	7.8279[2]	4.073[11]
				15	$1s^2 2s3p\ ^3P^o_2$	7.8447[2]	
				16	$1s^2 2s3p\ ^3P^o_1$	7.8683[2]	5.508[12]
				17	$1s^2 2s3d\ ^3D_1$	7.9349[2]	
				18	$1s^2 2s3d\ ^3D_2$	7.9369[2]	
				19	$1s^2 2s3d\ ^3D_3$	7.9407[2]	
				20	$1s^2 2s3d\ ^3D_2$	8.0075[2]	
				21	$1s^2 2p3s$	8.0981[2]	1.421[10]
				22	$1s^2 2p3p$	8.2513[2]	
				23	$1s^2 2p3d$	8.3612[2]	2.604[10]
				24	$1s^2 2s4l$	1.0312[3]	1.261[11]
				25	$1s^2 2s5l - 7l$	1.1967[3]	1.807[10]

Table 2: Collision strengths for some of the n=2-2 transitions in Ti XIX.

Transition	Transition Energy(eV)	E/E_{th}	This Work	Ref. [7]
$2s^2\ ^1S - 2s2p\ ^1P$	6.793[2]	1.05	4.27[-1]	4.28[-1]
		3.47	4.84[-1]	4.82[-1]
		6.38	5.46[-1]	5.22[-1]
		9.85	6.04[-1]	5.62[-1]
		14.0	6.55[-1]	6.06[-1]
$2s2p\ ^1P - 2p^2\ ^1D$	4.413[2]	1.05	8.47[-1]	9.55[-1]
		3.47	9.58[-1]	1.04
		6.38	1.08	1.10
		9.85	1.19	1.18
		14.0	1.29	1.27
$2s^2\ ^1S - 2s2p\ ^3P_0$	3.548[2]	1.04	1.83[-3]	2.07[-3]
		1.64	1.76[-3]	2.03[-3]
		4.04	1.63[-3]	1.88[-3]
		9.04	1.39[-3]	1.60[-3]

Table 3: Collision strengths for some of the n=2-2,3 transitions in Ti XX.

Transition	Transition Energy(eV)	E/E_{th}	This Work	Ref. [7]
$2s\ ^2S - 2p\ ^2P_{1/2}$	4.036[2]	1.05	1.93[-1]	2.16[-1]
		3.47	2.17[-1]	2.34[-1]
		6.38	2.42[-1]	2.46[-1]
		14.0	2.92[-1]	2.79[-1]
$2s\ ^2S - 2p\ ^2P_{3/2}$	4.793[2]	1.05	3.80[-1]	4.20[-1]
		3.47	4.28[-1]	4.57[-1]
		6.38	4.79[-1]	4.82[-1]
		14.0	5.76[-1]	5.50[-1]
$2s\ ^2S - 3d\ ^2D_{3/2}$	8.201[3]	1.30	1.98[-2]	2.43[-2]
		2.20	2.28[-2]	2.84[-2]
		4.00	2.59[-2]	3.37[-2]
		9.00	2.84[-2]	3.91[-2]

Table 4: Dielectronic recombination rate coefficients (in 10^{-11} cm^3/sec) from the ground state of Ti XXI and the ground and $\Delta n = 0$ levels of Ti XX.

	Ti XXI		Ti XX		
T	This calc.	Ref. [10]	$1s^2 2s\ ^2S$		$1s^2 2p\ ^2P$
(keV)			$\Delta n = 0$	$\Delta n = 1$	
0.02			14.9	1.44(-4)	9.91(-4)
0.04			8.26	1.72(-2)	5.00(-2)
0.06			5.33	6.79(-2)	1.49(-1)
0.08			3.79	1.28(-1)	2.47(-1)
0.10			2.87	1.92(-1)	3.42(-1)
0.20	3.79(-7)	3.57(-7)	1.14	5.22(-1)	7.91(-1)
0.30	5.50(-5)	5.25(-5)	6.43(-1)	7.11(-1)	1.01
0.50	2.50(-3)	2.41(-3)	3.08(-1)	7.43(-1)	9.95(-1)
1.00	3.26(-2)	3.20(-2)	1.12(-1)	4.99(-1)	6.41(-1)
2.00	7.61(-2)	7.40(-2)	3.99(-2)	2.46(-1)	3.09(-1)
3.00	7.88(-2)	7.71(-2)			
4.00	7.08(-2)	6.91(-2)	1.42(-2)	1.03(-1)	1.28(-1)
5.00	6.16(-2)	6.07(-2)			
6.00	5.34(-2)	5.15(-2)			
8.00	4.09(-2)	3.93(-2)			
10.00	3.22(-2)	3.11(-2)	3.61(-3)	2.88(-2)	3.55(-2)