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铜到钼的类钠离子能级结构及软X射线光谱理论计算

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提 要

本文采用 Hartree-Fock 自洽场方法，从理论上计算了铜到钼的类钠离子 $1s^22s^22p^6nl$($n=3\sim6$, $l=0\sim5$)各能级能量。给出了有可能实现软X射线激光的跃迁($5g-4f$, $5f-4d$, $6g-4f$, $6f-4d$)的光谱性质：跃迁波长、振子强度，并和实验值进行了比较，跃迁波长的相对误差不超过千分之二。从计算结果可知，Se 的 $6f-4d$ 跃迁，Br 的 $6g-4f$ 跃迁，Zr 的 $5f-4l$ 跃迁，Nb 的 $5g-4f$ 跃迁都已进入水窗波段。

关键词： 类钠离子结构，软X射线激光。

一、引 言

近年来，X射线激光研究取得了迅速的进展，许多泵浦机制都观察到了软X射线波段的自发发射放大(ASE)[1~8]，其中包括类Ne和类Ni离子的电子碰撞激发泵浦和类H、类He、类Li离子的复合泵浦。目前研究最成熟，性能最好的是类氖硒离子电子碰撞激发激光(20.6 nm, 20.9 nm)，但是类Ne离子要达到水窗波长(相应于 $Z=64$)所要求的驱动激光功率水平远远超出了现有高功率激光装置所能提供的[9,10]。

类Li离子的软X射线激光实验表明[7,8,11]，利用复合泵浦机制，在比较低的激光强度下，就能实现软X射线的自发发射放大。类钠离子和类Li离子一样，由于都具有封闭内壳层带单个价电子的结构。其电离能比类H、类He或类Ne离子的电离能低得多。还有附加的双电子复合过程：

$$1s^22s^22p^6+e\xrightarrow[\text{跃迁}]{\text{无辐射}}1s^22s^22p^53s6f \text{ 或 } 3s6g\xrightarrow{h\nu_{3s-2p}}1s^22s^22p^66f \text{ 或 } 6g$$

其中 $1s^22s^22p^53s6f$ 和 $1s^22s^22p^53s6g$ 是自电离态。使得三体复合泵浦的类钠离子同样具有低泵浦要求，高效率和易于推向更短波长等优点。

本文采用美国 Los Alamos 国家实验室提供的原子结构及光谱计算程序[12]，采用 Hartree-Fock 自洽场方法[13]进行了原子结构的纯理论计算，给出了铜到钼的类钠离子 $1s^22s^22p^6nl$($n=3\sim6$, $l=0\sim5$)各能级能量值。对有可能实现软X射线激光的跃迁 $5g-4f$, $5f-4d$, $6g-4f$, $4f-4d$，计算结果跃迁波长与实验值比较，相对误差小于千分之二。所提供的数据为今后进一步实验和理论分析提供了依据，对软X射线激光的实验研究也有着重要的指导意义。

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二、计算方法与结果

本文采用的 Los Alamos 的计算程序包括三个部分：RCN34, RCN2, RCG9。用 RCN34,考虑相对论修正和 Breit 修正等，得到各电子轨道的径向波函数，径向积分参量和轨道平均能量。RCN2 利用 RCN34 提供的数据计算组态之间的各种积分参量，RCG9 求解多组态的哈密顿矩阵，从而得到各组态的能级能量值，各跃迁波长，振子强度等。程序的详细情况见文献[12]和[13]。

在表 1 中给出了铜到钼的类钠离子有关能级的相对能量。由此数据可计算出各能级之间

Table I-1　Energy levels of Na-like ions from copper to molybdnum (in 1000 cm^{-1})

Term	J	Cu^{18+}	Zn^{19+}	Ga^{20+}	Ge^{21+}	As^{22+}	Se^{23+}	Br^{24+}
$3s\,^2S$	1/2	0.000	0.000	0.000	0.000	0.000	0.000	0.000
$3p^2\,^2P$	1/2	331.577	340.282	367.060	384.932	402.863	420.918	439.026
	3/2	366.768	391.035	416.249	442.519	469.892	498.518	528.418
$3d^2D$	3/2	814.768	861.502	909.576	958.752	1008.949	1060.432	1113.183
	5/2	820.717	869.315	918.992	970.003	1022.287	1076.132	1131.544
$4s\,^2S$	1/2	2537.613	2782.934	3039.606	3307.788	3587.420	3878.673	4181.574
$4p\,^2P$	1/2	2670.472	2923.278	3187.462	3463.197	3750.415	4049.306	4359.870
	3/2	2684.416	2939.864	3207.050	3486.197	3777.204	4080.362	4395.692
$4d\,^2D$	3/2	2849.613	3113.842	3389.794	3677.708	3977.509	4289.474	4613.583
	5/2	2852.369	3117.191	3393.826	3682.522	3983.211	4296.181	4621.422
$4f\,^2D$	5/2	2924.617	3194.687	3476.586	3770.559	4076.536	4394.797	4725.341
	7/2	2925.622	3195.922	3478.088	3772.369	4078.699	4397.363	4728.364
$4s\,^2S$	1/2	3629.715	3984.131	4355.071	4742.792	5147.167	5568.499	6006.738
$5p\,^2P$	1/2	3695.544	4053.770	4428.539	4820.106	5228.352	5653.559	6095.700
	3/2	3702.459	4062.004	4438.274	4831.534	5338.984	5770.671	6113.572
$5d\,^2D$	3/2	3782.422	4146.290	4526.897	4924.483	5338.984	5770.671	6219.555
	5/2	3783.842	4148.014	4258.971	4926.958	5341.916	5774.118	6223.582
$5f\,^2F$	5/2	3820.450	4187.212	4570.762	4971.350	5388.904	5823.710	6275.772
	7/2	3820.970	4187.850	4571.537	4972.283	5390.020	5825.033	6277.329
$5g\,^2G$	7/2	3824.897	4192.109	4576.137	4977.229	5395.316	5830.686	6283.341
	9/2	3825.203	4192.485	4576.593	4977.778	5396.972	5831.464	6284.257
$6s\,^2S$	1/2	4199.079	4611.342	5042.946	5494.138	5964.819	6455.287	6965.509
$6p\,^2P$	1/2	4236.340	4650.797	5084.605	5538.009	6010.922	6503.614	7016.084
	3/2	4240.262	4655.469	5090.134	5544.505	6018.504	6512.421	7026.259
$6d\,^2D$	3/2	4285.126	4702.789	5139.908	5596.737	6073.200	6569.583	7085.888
	5/2	4286.949	4703.788	5141.110	5598.171	6074.898	6571.580	7088.220
$6f\,^2F$	5/2	4306.905	4726.207	5164.906	5623.523	6101.716	6599.866	7117.972
	7/2	4307.207	4726.578	5165.447	5624.066	6102.366	6600.636	7118.879
$6g\,^2G$	7/2	4309.652	4729.242	5168.337	5627.185	6105.718	6604.225	7122.710
	9/2	4309.831	4729.462	5168.603	5627.506	6106.100	6604.678	7123.243
$6h\,^2H$	9/2	4310.383	4730.043	5169.213	5628.141	6106.764	6605.368	7123.956
	11/2	4310.504	4730.191	5169.392	5628.356	6107.020	6605.670	7124.311

跃迁波长的理论值。

表 2 和表 3 分别给出了有可能实现软 X 射线激光的跃迁 $5g—4f$, $5f—4d$, $6g—4f$, $6f—4d$ 谱线性质的理论值和实验值。比较表 2、表 3 可知，跃迁波长的相对误差不超过千分之二。从计算结果还可以看到 Se 的 $6f—4d$ 跃迁，Br 的 $6g—4f$ 跃迁，Zr 的 $5f—4d$ 跃迁，Nb 的 $5g—4f$ 跃迁都已进入水窗波段，在实验上可向此方向努力。

Table I-2 Energy levels of Na-like ions from copper to molybdnum (in 1000 cm^{-1})

Term	J	Kr^{25+}	Rb^{26+}	Sr^{27+}	Y^{28+}	Zr^{29+}	Nb^{30+}	Mo^{31+}
$3s\ ^2S$	1/2	0.000	0.000	0.000	0.000	0.000	0.000	0.000
$3p\ ^2P$	1/2	457.255	475.639	494.060	512.560	531.234	549.921	568.661
	3/2	559.729	592.578	626.977	663.161	701.249	741.212	783.222
$3d\ ^2D$	3/2	1167.286	1223.008	1280.197	1339.207	1400.063	1462.795	1527.560
	5/2	1188.631	1247.684	1308.577	1371.689	1437.084	1504.809	1575.057
$4s\ ^2S$	1/2	4496.127	4822.573	5160.763	5511.021	5873.274	6247.606	6634.091
$4p\ ^2P$	1/2	4682.106	5016.294	5362.250	5720.280	6090.398	6472.586	6866.985
	3/2	4723.251	5063.340	5415.819	5781.050	6159.085	6549.957	6953.865
$4d\ ^2D$	3/2	4949.951	5298.840	5660.113	6034.150	6720.971	6820.640	7233.330
	5/2	4959.059	5309.364	5672.212	6047.994	6436.750	6838.541	7253.559
$4f\ ^2F$	5/2	5068.275	5423.877	5792.024	6173.094	6567.136	6974.212	7394.504
	7/2	5071.811	5427.992	5796.786	6178.574	6573.423	6981.380	7402.644
$5s\ ^2S$	1/2	6461.967	6934.472	7424.092	7931.162	8455.725	8997.813	9557.577
$5p\ ^2P$	1/2	6554.852	7031.285	7524.845	8035.887	8564.427	9110.513	9674.289
		6575.393	7054.789	7551.625	8066.283	8598.810	9149.262	9717.818
$5d\ ^2D$	3/2	6685.719	7169.463	7670.649	8189.655	8726.520	9281.316	9854.218
	5/2	6690.396	7174.866	7676.860	8196.761	8734.627	9290.513	9864.611
$5f\ ^2F$	5/2	6745.189	7232.257	7736.850	8259.342	8799.783	9361.968	9934.934
	7/2	6747.013	7234.377	7739.303	8262.166	8803.040	9361.968	9939.151
$5g\ ^2G$	7/2	6753.392	7241.125	7746.420	8269.658	8810.882	9370.188	9947.748
	9/2	6754.462	7242.371	7747.862	8271.317	8812.814	9372.388	9950.241
$6s\ ^2S$	1/2	7495.593	8045.818	8616.026	9206.608	9817.587	10449.019	11101.070
$6p\ ^2P$	1/2	7548.422	8100.900	8673.385	9266.243	9879.511	10513.236	11167.594
	3/2	7560.122	8114.293	8688.651	9283.576	9899.122	10535.344	11192.437
$6d\ ^2D$	3/2	7622.212	8178.854	8755.677	9353.069	9971.078	10609.768	11269.320
	5/2	7624.922	8181.983	8759.274	9357.184	9975.771	10615.091	11275.336
$6f\ ^2F$	5/2	7656.144	8214.671	8793.429	9392.804	10012.847	10653.628	11315.334
	7/2	7657.205	8215.904	8794.856	9394.446	10014.736	10655.781	11317.778
$6g\ ^2G$	7/2	7661.278	8220.224	8799.423	9399.258	10019.793	10661.089	11323.337
	9/2	7661.901	8220.949	8800.260	9400.222	10020.905	10662.356	11324.776
$6h\ ^2H$	9/2	7662.642	8221.713	8801.047	9401.033	10021.716	10663.188	11325.628
	11/2	7663.057	8222.195	8801.605	9401.674	10022.483	10664.060	11326.615

Table II The calculated wavelengths of interest in soft X-ray laser study of the Na-like ions from copper to Molybdenum

Z	$5g-4f$	$5f-4d$(nm)	$6g-4f$	$6f-4d$
29 CuXIX	111.077	103.004	72.200	68.620
	111.163	103.242	72.243	68.736
30 ZnXX	100.259	93.164	65.166	62.021
	100.345	93.400	65.209	62.136
31 GaXXI	90.946	84.676	59.110	56.332
	91.033	84.910	59.154	56.446
32 GeXXII	82.873	77.301	53.861	51.392
	82.959	77.534	53.904	51.505
33 AsXXIII	75.828	70.851	49.281	47.076
	75.914	71.083	49.324	47.189
34 SeXXIV	69.643	65.179	45.261	43.283
	69.730	65.409	45.304	43.394
35 BrXXV	64.184	60.162	41.712	39.930
	64.272	60.390	41.765	40.041
36 KrXXVI	59.341	55.703	38.565	36.952
	59.430	55.930	38.609	37.062
37 RbXXVII	55.028	51.722	35.761	34.296
	55.115	51.948	35.804	34.405
38 SrXXVIII	51.167	48.152	33.251	31.915
	51.254	48.377	33.295	32.024
39 YXXIX	47.697	44.940	30.997	29.775
	47.784	45.164	31.040	29.882
40 ZrXXX	44.568	42.038	28.963	27.841
	44.655	42.260	29.007	27.949
41 NbXXXI	41.737	39.407	27.123	26.089
	41.823	39.629	27.167	26.197
42 MoXXXII	39.166	37.015	25.453	24.498
	39.253	37.263	25.496	24.605
Oscillator stength gf	8.05	2.97	1.11	0.72
	10.43	4.23	1.43	1.23

Table III The measured wavelengths of interest in soft X-ray laser study of the Na-like ions from copper to Molybdenum

Z	$5g-4f$	$5f-4d$(nm)	$6g-4f$	$6f-4d$
29 CuXIX	111.274	102.960	72.22	68.65
	111.353	103.179	72.22	68.74
30 ZnXX	100.410	93.122		
	100.487	93.351		
31 GaXXI	91.071	84.649		
	91.149	84.867		
32 GeXXII	82.975	77.287		
	83.058	77.510		
33 AsXXIII	75.916	70.845		
	76.003	71.050		
34 SeXXIV	69.731#	65.188#		
	69.818#	65.406#		
35 BrXXV	64.242			
	64.331			
36 KrXXVI				
37 RbXXVII				
38 SrXXVIII				
39 YXXIX	47.736*	44.954*		
	47.820*	45.175*		
40 ZrXXX	44.395*			
	44.679	42.282*		
41 NbXXXI	41.767*	39.438*		
	41.853*	39.646*		
42 MoXXXIII	39.183*	87.012*		
	39.272*	37.239*		

Experimetal wavelength data adopted from Kononov 1979

#—from Brown 1986　*—from Reader 1990

参 考 文 献

[1] D. L. Matthew *et al.*; *Phys. Rew. Lett.*, 1985, **54**, No. 2 (Jan), 110.
[2] T. N. Lee *et al.*, *ibid*, 1987, **59**, No 11 (Sep), 1185.
[3] B. J. MacGowan *et al.*, *ibid*, 1987, **59**, No. 19 (Nov), 2157.
[4] S. Suckewer *et al.*; *ibid*, 1986, **55**, No. 17 (Oct), 1753.
[5] C. Chenais-Popovics *et al.*; *ibid*, **59**, No. 19 (Nov), 2161.
[6] G. P. Kiehn *et al.*; *SPIE* **831**, 1987, 270.
[7] P. Jaegle *et al.*; *J. Opt. Soc. Am*(*B*), 1987, **B4**, No. 4, 563.
[8] Zhi-zhan Xu *et al.*; *Appl. Phys.* (*B*), 1990, **B50**, No. 3, 147.
[9] M. D. Rosen *et al.*; *Phys. Flnids*, 1988, **31**, No. 3, 666.
[10] B. L. Whitten *et al.*; *J. Opt. Soc. Am.* (*B*), 1988, **B5**, No. 12, 2537.
[11] T. Hara *et al.*; *Jappanese J. Appl. Phys.*, 1989, **28**, No. 6, L1010,
[12] R. D. Cowan; *Los Alamos National Laboratory*, August 1986.
[13] R. D. Cowan; *The Theory of Atomic Structure and Spectra* (Berkely: University of California Press, 1981).
[14] E. Ya. Kononov *et al.*; *Physica Scripta*, 1979, **19**, No. 4, 328.
[15] C. M. Brown *et al.*; *J. Opt. Soc. Am.* (*B*), 1986, **B2**, No. 5, 701.
[16] J. Reader *et al.*; *J. Opt. Soc. Am.* (*B*), 1990, **B7**, No. 7, 1176.

Theoretical Calculation of Energy Levels and Soft X-ray Spectra for Na-like ions from Copper to molybdenum

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Abstract

The energy levels of Na-like ions from Copper to Molybdenum are reported. The transition wavelengths of $5g$—$4f$, $5f$—$4d$, $6g$—$4f$, $6f$—$4d$ are given as well as the oscillator strengths. These transitions are of potential interest for X-ray laser. The results indicate that the $6f$—$4d$ transition of Se ions, the $6g$—$4f$ transition of Br ions, the $5f$—$4d$ transition of Zr ions, the $5g$—$4f$ transition of Nb ions are all in the range of the "Water Window".

Key words: Na-like ions, Soft X-ray laser.