Division of Atomic, Molecular & Optical Physics
DAMOP

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ENHANCEMENT OF DATABASE NORAD-ATOMIC-DATA FOR ATOMIC PROCESSES IN PLASMA

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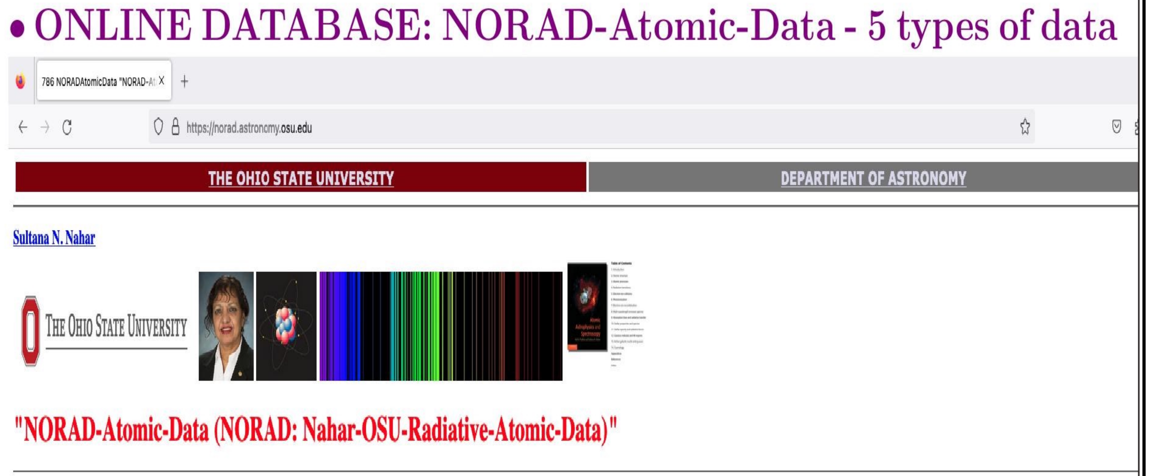
NORAD data and Atomic processes

• ONLINE DATABASE: NORAD-Atomic-Data - 5 types of data



Introduction	Accuracy & Benchmarking	Atomic Radiative Data 1 (Z upto 28)	Atomic Radiative Data 2 (Z > 28)	EIE Collision Data 3
Measured Lines & Energies Data 5	Measured Photoionization Data 6	Program Codes	PUBLICATIONS, NEWS	Line Ratios

• - NORAD-Atomic-Data Access metric charts

Introduction:

• Brief Description of NORAD-Atomic-Data database:

• The on-line NORAD-Atomic-Data based at the Ohio State University contains large amount calculated atomic data relevant to various radiative and collisional atomic processes, such as, excitation of energies, photoionization, electron-ion recombination, radiative transitions, lifetimes, etc relevant to astrophysical and laboratory plasmas. They are obtained mainly from large scale R-MATRIX calculations and some from atomic structure program SUPERSTRUCTURE carried at the Ohio Supercomputer Center (OSC) by Nahar et al

• Atomic Data files contents:
- i) Energies,
- ii) Oscillator Strengths, transition probabilities for allowed and forbidden transitions,
- iii) Photoionization cross sections,
- iv) Electron-Ion Recombination cross sections and rate coefficients,
- v) Lifetimes,

Following additional data are in process to be added

DATABASE FOR ATOMIC PROCESSES: NORAD-ATOMIC-DATA

• It contains high accuracy data for radiative atomic processes, obtained using the R-matrix (RM) codes and/or atomic structure code SUPERSTRUCTURE (SS)

• Data for atomic species: About 200 atomic species of elements H, He, C, N, O, F, Ne, ..., U

Data: - Energy levels ($n \leq 10$ with RM, $n \leq 6$ with SS)

1. Photoexcitation & De-excitation :

$$X^{+Z} + h\nu \rightleftharpoons X^{+Z*}$$

Data:-Oscillator Strength (f), Radiative Decay Rate (A), Line strength (S), Lifetime. New: Spectral points

2. Photoionization (PI) directly

$$X^{+Z} + h\nu \rightleftharpoons X^{+Z+1} + e$$

or through an intermediate autoionizing state

$$X^{+Z} + h\nu \rightleftharpoons X^{+Z**} \rightleftharpoons X^{+Z+1} + e$$

Data: - Photoionization cross sections, total and partial

3. Electron-ion recombination: radiative recombination (RR)

$$X^{+Z+1} + e \rightleftharpoons X^{+Z} + h\nu$$

& dielectronic recombination (DR) when an intermediate autoionizing state is formed

$$X^{+Z+1} + e \rightleftharpoons X^{+Z**} \rightleftharpoons X^{+Z} + h\nu$$

Data: - Recombination cross sections, and recombination rate coefficients

4. Electron-impact excitation (EIE):

$$e + X^{+Z} \rightarrow e' + X^{+Z*} \rightarrow e' + X^{+Z} + h\nu$$

New: • *Data: - Collision Strength (Ω), Effective Collision Strengths (Υ), Excitation rate Coefficients (q)*

• The results are mainly from the R-matrix calculations by Nahar et al. - New or updates of TOPbase, TIPbase

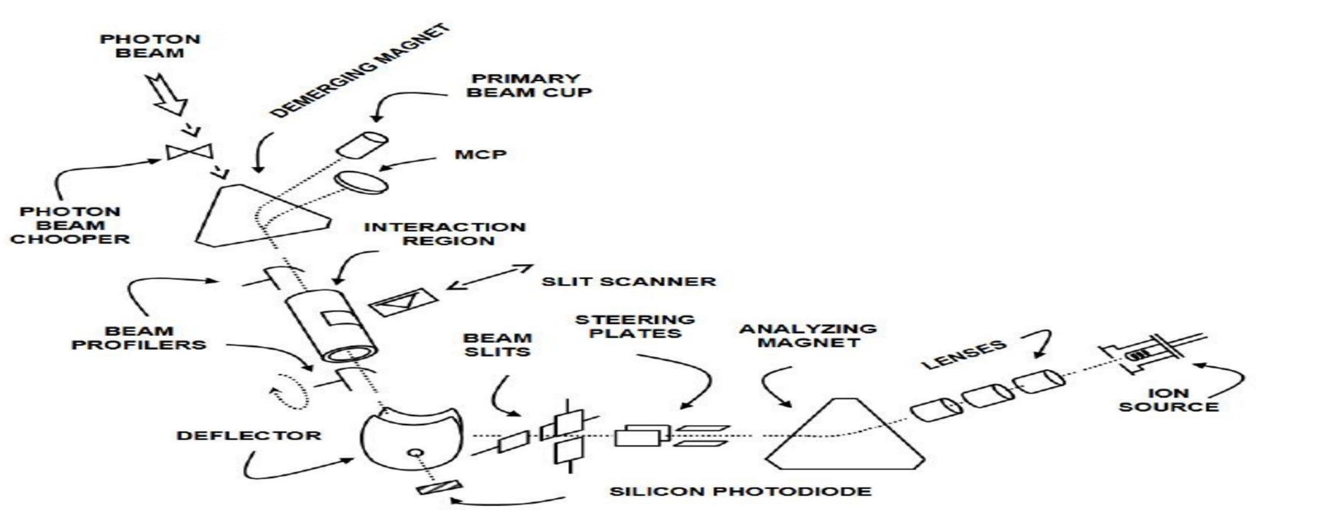
New: • Experimental data: Energies, Oscillator strengths, Photoionization cross sections

New: • Line ratios of two transitions via web interaction

Methods: ALS (experiment), R-matrix (theory)

New: - The x-ray K_α transition of elements for various astronomical, biomedical, fusion plasma application

• NORAD-Atomic-Data can be accessed from databases, ex - CfA-Harvard, International Atomic Energy Agency



• ALS station for measurement of photoionization cross sections

THEORETICAL CALCULATIONS: R-MATRIX CODES

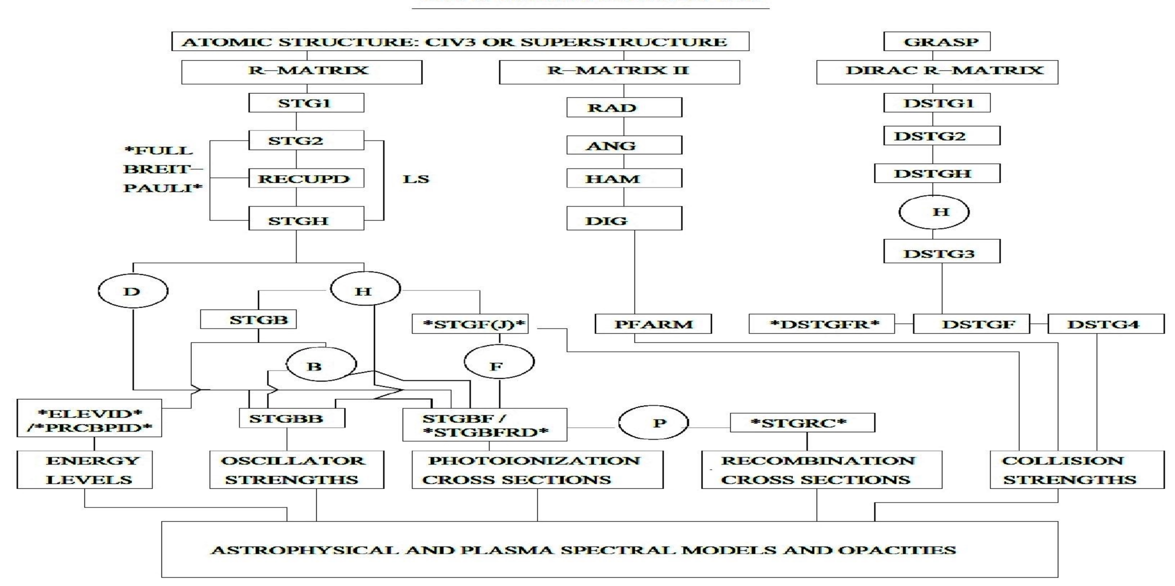
Large-Scale Atomic Calculations (Ohio Supercomputer Center)

VARIOUS COMPUTATIONAL STAGES AND RESULTS

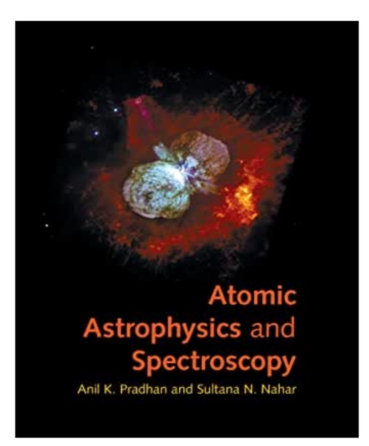
• R-matrix calculations can proceed in 3 branches - 1) LS coupling & relativistic Breit-Pauli, 2) LS coupling R-matrix II for Large configuration interaction, 3) DARC for Full Dirac relativistic

• Results - 1) Energy Levels, 2) Oscillator Strengths, 3) Photoionization Cross sections, 4) Recombination Rate Coefficients, 5) Collision Strengths; - Astrophysical Models

THE R–MATRIX CODES AT OSU

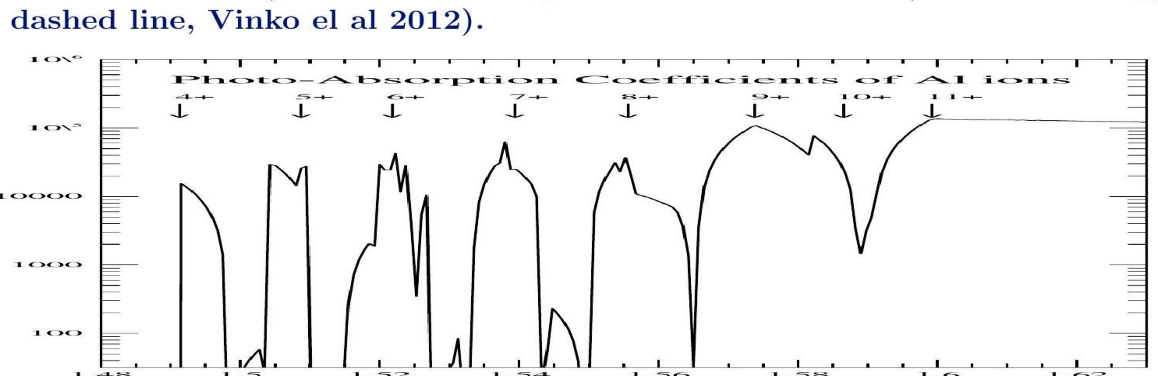


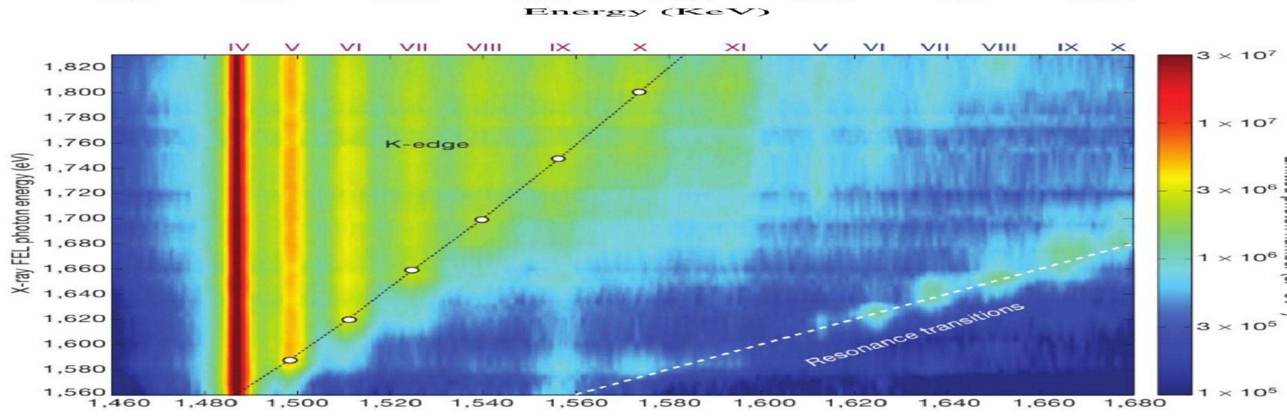
Theory is explained in the book:



BENCHMARKING OF THEORETICAL AND EXPERIMENTAL K_α RESONANT FLUORESCENCE OF Al

K_α resonant fluorescence in Al plasma in the x-ray region: TOP: Theory (Nahar & Pradhan 2015). BOTTOM: Experiment LCLS-XFEL (emissions along the white dashed line, Vinko el al 2012).





NORAD Data Tables

• Atomic Data Table 1: Each row gives files for various atomic processes of the ion on the left

ATOMIC DATA TABLE (Heavier to Lighter Elements)

Ion	ENERGIES	OSCILLATOR STRENGTHS	PHOTOIONIZATION	ELECTRON-ION RECOMBINATION	OTHER: Lifetime, Collision Strength
	E(LS, FS)	f, S, A (LS, FS, FORBID)	CROSS SECTIONS PX (LS, FS)	RATES (RRC), CROSS SECTIONS	
Ni II	E-LS	,	PX-Gd, PX-Total, PX-Partial	State-Specific & Total,	
Ni XXVI	E-FS	f-FS,	PX-Gd, PX-Total, PX-Partial	Level-Specific & Total, OMRX	
Ni XXVII	E-FS	,	PX-Gd-K, PX-Total, PX-Partial	Level-Specific & Total, OMRX	
Ni 27+	E-LS, E-FS	f-LS, f-FS, f-forbid	PX-Gd, PX-Total	Total RRC	
Fe I	E-LS	f-LS,	PX-Gd, PX-Total, PX-Partial	State-Specific & Total,	
Fe II	E-LS	f-LS, f-FS.1,f-FS.2,	PX-Gd, PX-Total, PX-Partial	State-Specific & Total,	lifetime-LS
Fe III	E-LS	f-LS, f-FS,,	PX-Gd, PX-Total, PX-Partial	State-Specific & Total,	lifetime-LS
Fe IV	E-LS	f-LS,, f-FS, f-FORBID	PX-Gd, PX-Total, PX-Partial	State-Specific & Total,	lifetime-LS
Fe V	E-LS	, ,	PX-Gd, PX-total, PX-Partial	State-Specific & Total,	
Fe XIII	E-LS	f-LS, f-FS,	PX-Gd, PX-Total, PX-Partial	State-Specific & Total,	lifetime-LS
Fe XV	E-FS	f-FS, f-exp, f-FORBID	,	,	lifetime-FS
Fe XVI	E-FS	f-FS, f-exp, f-FORBID	,	,	
Fe XVII	E-FS	f-FS, f-EXP, f-FORBID	PX-Gd-3cc, PX-Partial-3cc,	level-Specific & Total , OMRX	lifetime-FS

Tables are given in energy order for each symmetry & in LS multiplet form

Table 1: Sample set of fine structure energy levels of Fe XIV, grouped as components of LS terms.

$C_t(S_tL_t\pi_t)$		J_t	nl	$2J$	E(Ry)	ν	$SL\pi$
Nlv= 2, $^2L^o$: P (3 1)/2							
2p63s2	(1Se)	0	3p	1	-2.88230E+01	2.64	2P o
2p63s2	(1Se)	0	3p	3	-2.86520E+01	2.62	2P o
Nlv(c)= 2 : set complete							
Eqv electron/unidentified levels, parity: e							
3s3p2				1	-2.68030E+01	2.70	4P e
3s3p2				3	-2.67330E+01	2.71	4P e
3s3p2				5	-2.66410E+01	2.71	4P e
Nlv(c)= 3 : set complete							
Nlv= 9, $^2L^e$: S (1)/2 P (3 1)/2 D (5 3)/2 F (7 5)/2 G (9 7)/2							
3p2	(1De)	2	3d	5	-1.96549E+01	2.84	2DF e
3p2	(1De)	2	3d	7	-1.95955E+01	2.83	2FG e
3p2	(1De)	2	3d	7	-1.94588E+01	2.85	2FG e
3p2	(1De)	2	3d	9	-1.94215E+01	2.84	2G e
3p2	(1De)	2	3d	3	-1.94120E+01	2.83	2D e
3p2	(1De)	2	3d	5	-1.93740E+01	2.85	2D e
3p2	(1De)	2	3d	1	-1.88526E+01	2.85	2SP e
3p2	(1De)	2	3d	1	-1.87559E+01	2.86	2SP e
3p2	(1De)	2	3d	3	-1.87283E+01	2.88	2PD e
Nlv(c)= 9 : set complete							
Eqv electron/unidentified levels, parity: e							
3s3p2				1	-2.68030E+01	2.70	4P e
3s3p2				3	-2.67330E+01	2.71	4P e

Trsnsition levels are identified in energy table

Table 2: Sample set of f-, S and A-values for allowed E1 transitions in Fe XIV

26 13

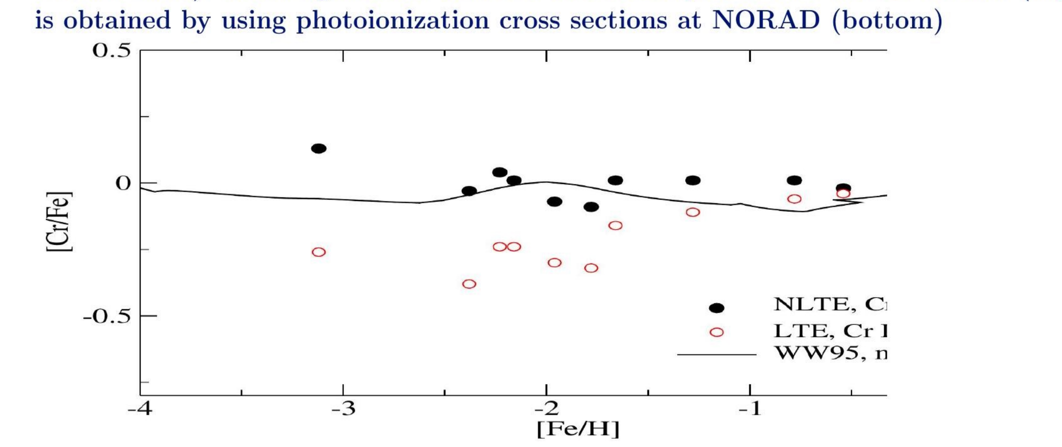
2 0 2 1 79 82 6478= gi Pi gk Pk Ni Nk NN

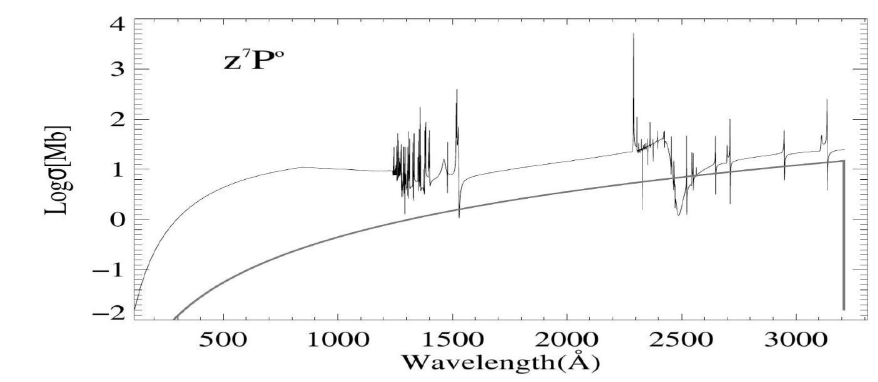
I_i	I_k	$\lambda(\AA)$	E_i(Ry)	E_k(Ry)	f	S	$A_{ki}(s^{-1})$
1	1	451.12	-2.6803E+01	-2.8823E+01	5.777E-04	1.716E-03	1.893E+07
1	2	237.74	-2.6803E+01	-2.2970E+01	-1.231E-04	1.927E-04	1.453E+07
1	3	211.68	-2.6803E+01	-2.2498E+01	-2.819E-01	3.929E-01	4.197E+10
1	4	207.44	-2.6803E+01	-2.2410E+01	-1.458E-03	1.991E-03	2.259E+08
1	5	161.86	-2.6803E+01	-2.1173E+01	-4.713E-04	5.023E-04	1.200E+08
1	6	19.07	-2.6803E+01	-2.0978E+01	-4.846E-07	6.086E-08	8.890E+06
1	7	82.85	-2.6803E+01	-1.5804E+01	-5.076E-05	2.769E-05	4.931E+07
1	8	82.65	-2.6803E+01	-1.5777E+01	-1.231E-05	6.699E-06	1.202E+07
1	9	81.13	-2.6803E+01	-1.5571E+01	-1.757E-05	9.386E-06	1.780E+07
1	10	79.57	-2.6803E+01	-1.5351E+01	-1.716E-05	8.989E-06	1.807E+07
1	11	78.44	-2.6803E+01	-1.5186E+01	-1.225E-06	6.329E-07	1.328E+06
1	12	74.23	-2.6803E+01	-1.4527E+01	-6.461E-06	3.158E-06	7.822E+06
1	13	75.68	-2.6803E+01	-1.4762E+01	-1.112E-06	5.542E-07	1.295E+06
1	14	70.74	-2.6803E+01	-1.3921E+01	-1.723E-06	8.026E-07	2.298E+06
1	15	69.09	-2.6803E+01	-1.3614E+01	-2.564E-02	1.166E-02	3.583E+10
1	16	67.70	-2.6803E+01	-1.3342E+01	-1.240E-05	5.528E-06	1.805E+07
1	17	63.45	-2.6803E+01	-1.2442E+01	-1.421E-05	5.937E-06	2.353E+07
1	18	58.22	-2.6803E+01	-1.1150E+01	-2.259E-01	8.658E-02	4.444E+11
1	19	57.12	-2.6803E+01	-1.0849E+01	-8.661E-03	3.257E-03	1.770E+10
1	20	56.89	-2.6803E+01	-1.0784E+01	-2.413E-03	9.037E-04	4.974E+09
1	21	54.05	-2.6803E+01	-9.9426E+00	-8.763E-06	3.119E-06	2.001E+07
1	22	53.17	-2.6803E+01	-9.6630E+00	-5.801E-03	2.031E-03	1.369E+10
1	23	52.92	-2.6803E+01	-9.5847E+00	-1.959E-02	6.826E-03	4.664E+10
1	24	52.46	-2.6803E+01	-9.4336E+00	-5.121E-03	1.769E-03	1.242E+10
1	25	52.11	-2.6803E+01	-9.3158E+00	-1.833E-05	6.290E-06	4.502E+07

APPLICATIONS

ASTROPHYSICAL APPLICATION

• Cr-to-Re ratio as probe of chemical evolution (Bergemann 2010, Woosley & Weaver 1995). Good agreement between NLTE analysis of Cr I and Cr II lines (top) is obtained by using photoionization cross sections at NORAD (bottom)





ENGINEERING APPLICATION

Study of thermodynamics and radiative properties of electrical discharge machining (EDM) plasma for temperature up to 10,000 K and pressure range 01.-1 MPa, with different amounts of iron in nitrogen from NORAD, Adineh et al (2012) find increase in net emission coefficient (NEC) with iron and contamination of iron strongly cools down the plasma.

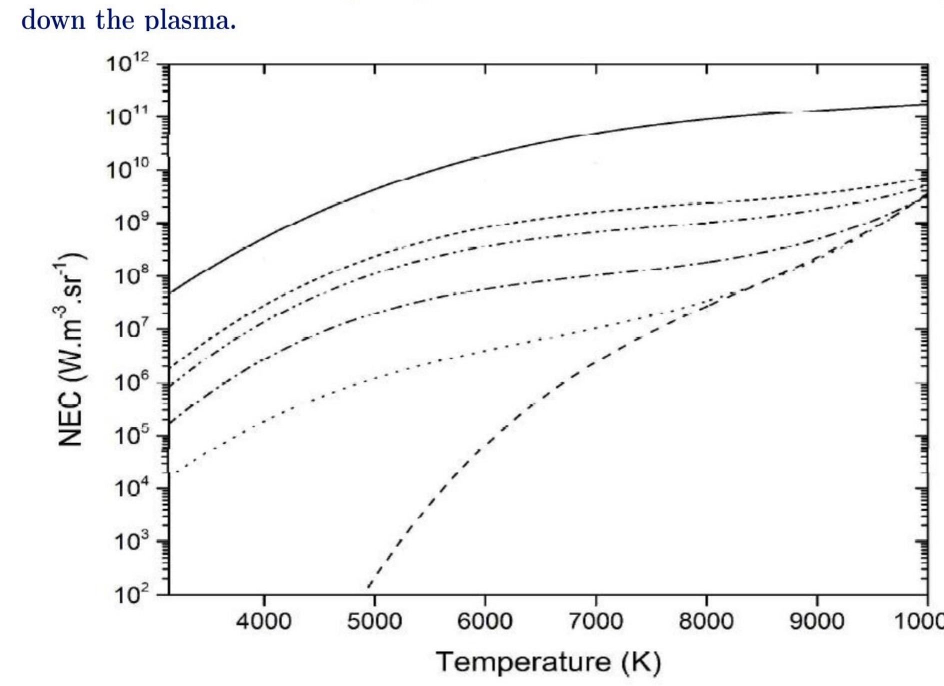


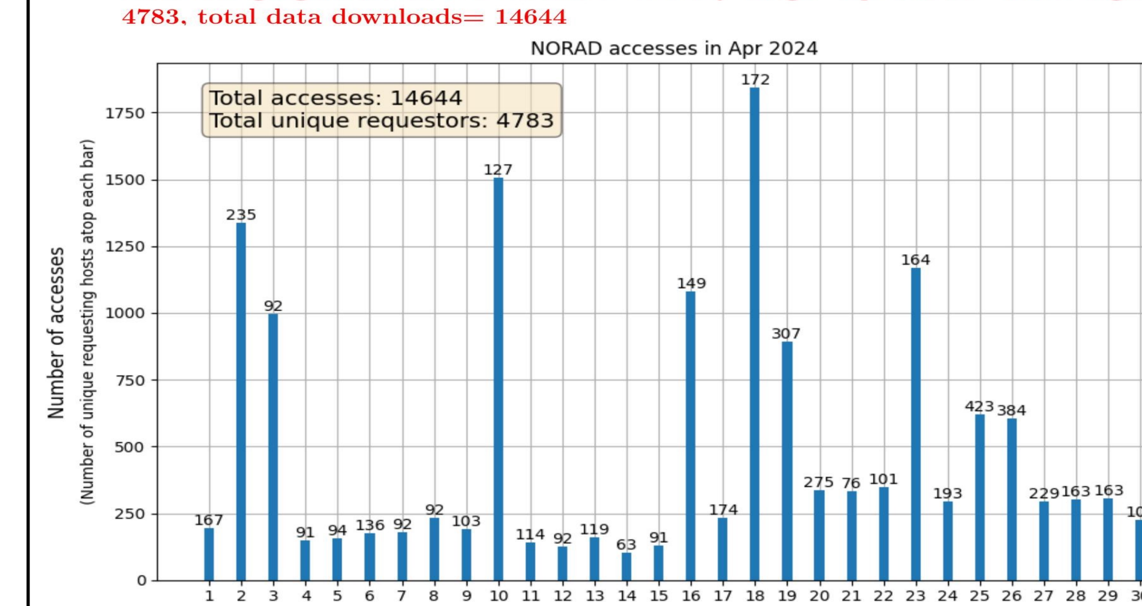
Fig. 6. NEC of nitrogen-iron arc plasma for various iron mole fractions at 0.1 MPa pressure and R_p=0. Dash line (100%N_2-0% Fe), dotted line (99.9%N_2-0.1% Fe), dash dot line (99%N_2-1% Fe), dash dot dot line (95%N_2-5% Fe), short dash line (90%N_2-10% Fe), straight line (0%N_2-100% Fe).

CONCLUSION

• NORAD-Atomic-Data was created in 2007. Most users: Astronomers. Physicists, Engineers, Chemists, atmospheric modelers etc.

• The amount of accessible is expected to considerably

• Following figure shows the metric of monthly usage: April 2024. Total llogin = 4783, total data downloads= 14644



Partially supported by Ohio Supercomputer Center