Non-LTE line formation of Fe (and other elements) and application to large-scale stellar surveys

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Stellar Atmospheres in the Gaia Era: Quantitative Spectroscopy and Comparative Spectrum Modelling

Spectroscopy of cool FGK stars

- gives the **largest** number of constraints to the models of formation and evolution of the Galaxy, stellar evolution, nucleosynthesis, and physical processes in stellar atmospheres and interior.

  Low-mass stars: old, $-6 <$ [Fe/H] $< +0.5$, spectra rich in atomic and molecular features → many chemical elements, "*well-understood*" *(Sun as a reference)*

- UVES VLT, HIRES Keck,…: huge archives of high-resolution spectra (Galactic halo, disk, bulge, clusters…)

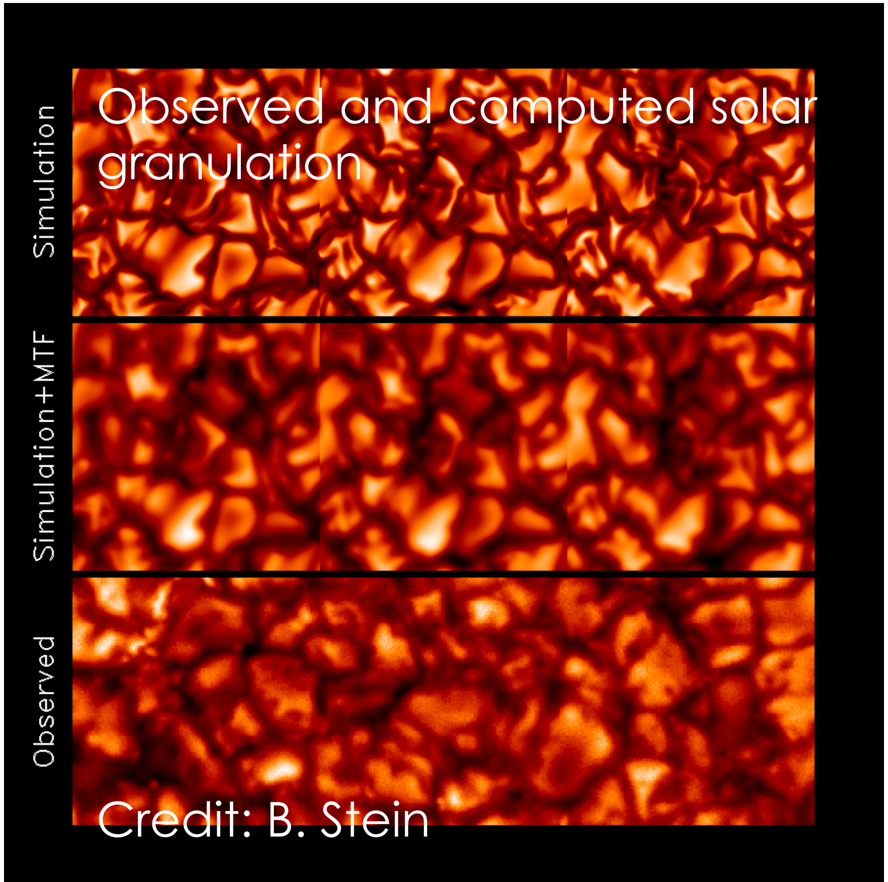
  More to come: → ~ $10^{[?]}$ objects with Gaia-ESO survey!

- **need physically-realistic models, which give accurate interpretation to these observed data**

Diagnostics of stellar atmospheres

non-trivial: demands model atmospheres and synthetic spectra to compare with observations

I. Convective envelopes:
overshoot into photosphere → 3D radiative hydrodynamics



Observed and computed solar granulation

Credit: B. Stein

Diagnostics of stellar atmospheres

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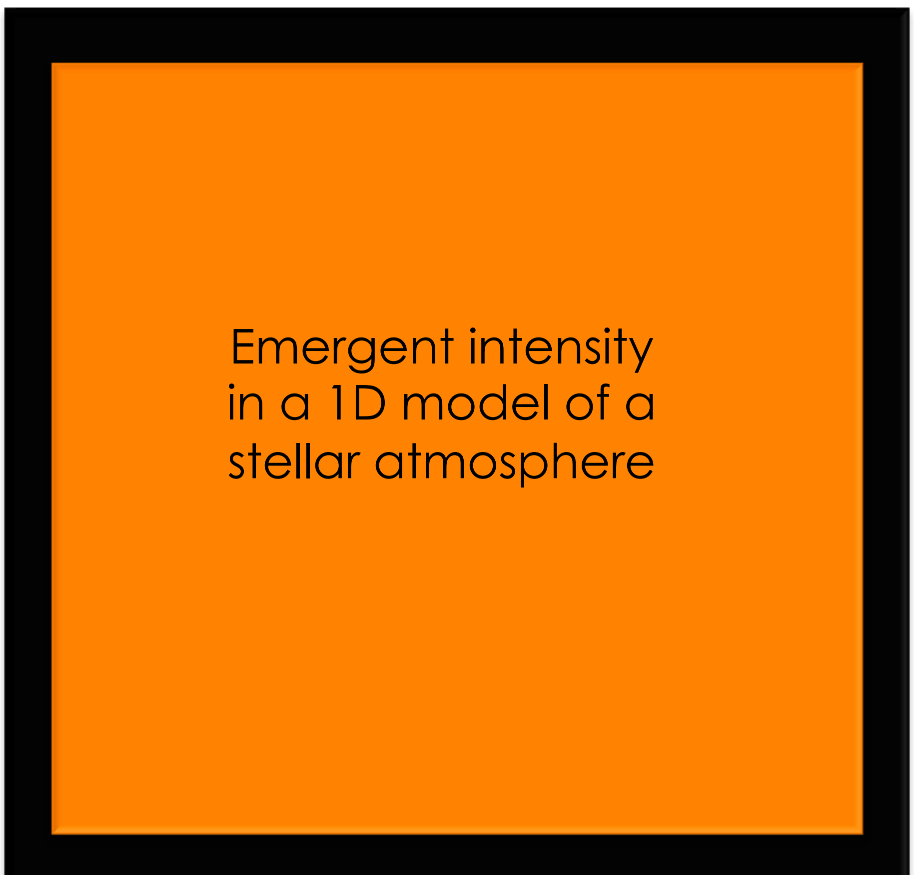
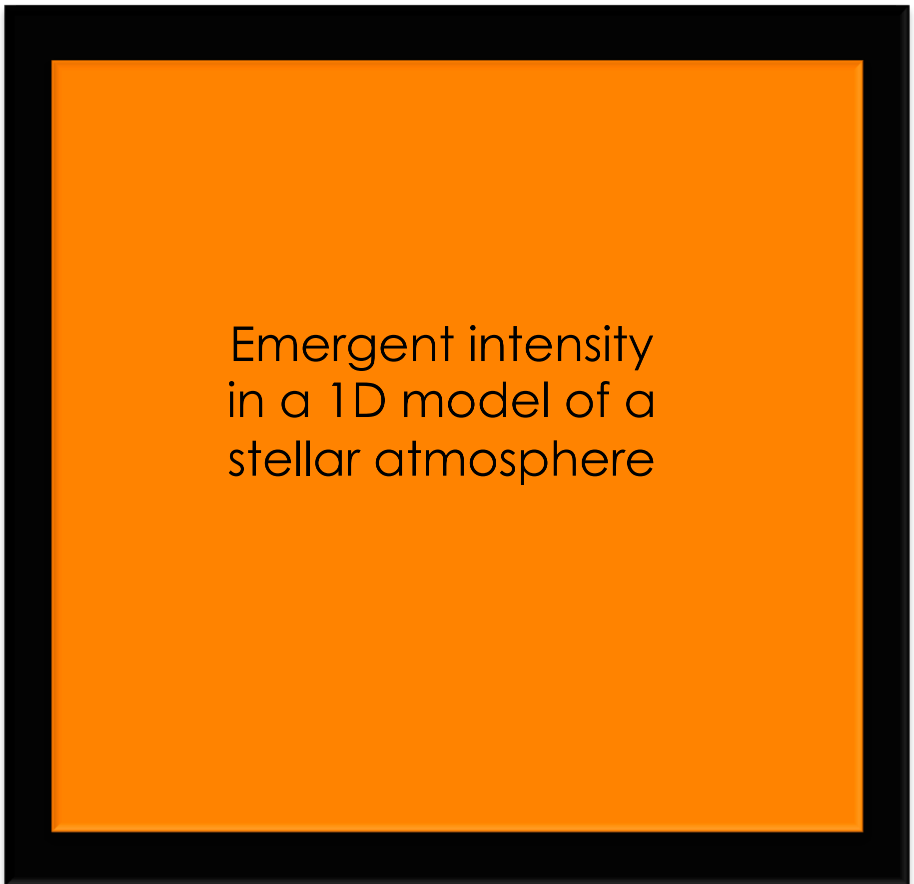


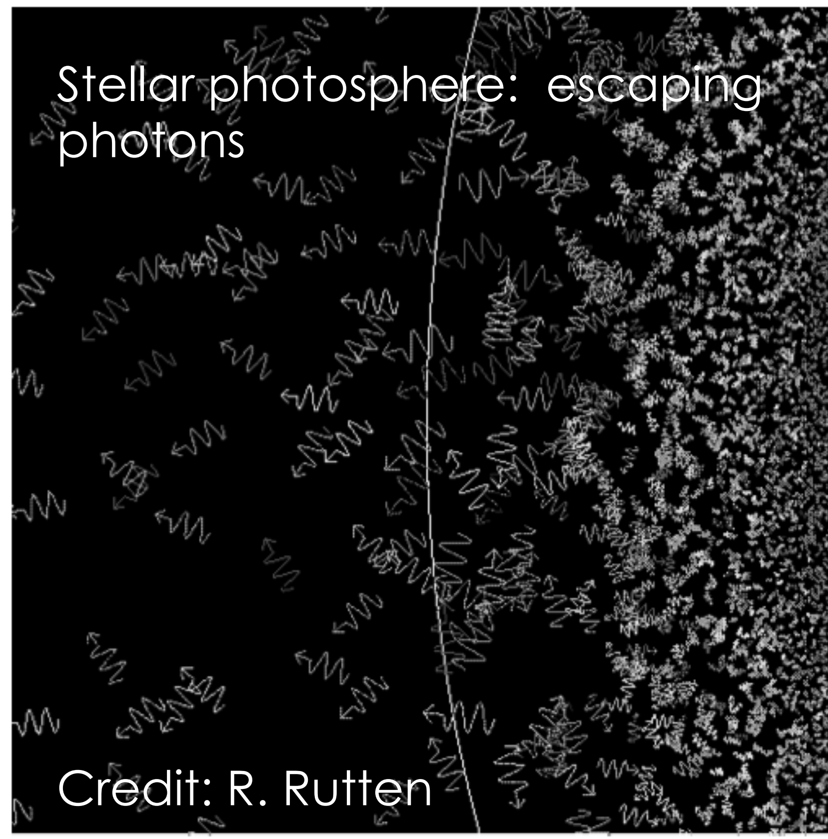
Diagnostics of stellar atmospheres

non-trivial: demands model atmospheres and synthetic spectra to compare with observations

I. Convective envelopes: overshoot into photosphere → 3D radiative hydrodynamics

II. Photosphere: Interaction of radiation field of non-local origin with gas particles → non-local thermodynamic equilibrium (NLTE)





Diagnostics of stellar atmospheres

- Solution of full 3D NLTE radiative transfer is absolutely necessary, albeit extremely computationally challenging
- **Most studies of FGK stars** are still restricted to **1D LTE**, which introduces severe systematic errors in stellar parameters and biases their interpretation

Our main project at MPA

explore NLTE and 3D line formation for various elements for a wide range of stellar parameters → construct a <3D> NLTE database for spectroscopic analysis of FGK stars

This talk: Fe

- a proxy of stellar metallicity [Fe/H]
- used to derive T_{eff} and log g
- Fe I and Fe II have, by far, the largest number of lines in a spectrum of a typical F-type star, thus enabling rigorous tests of the models

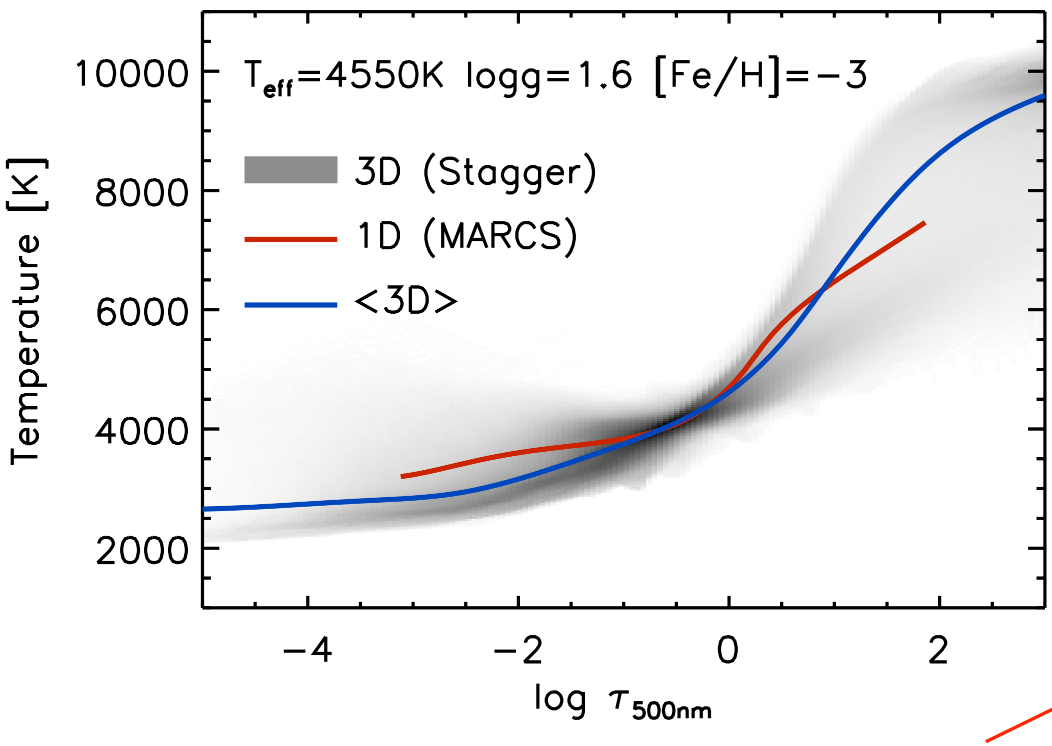
Methods

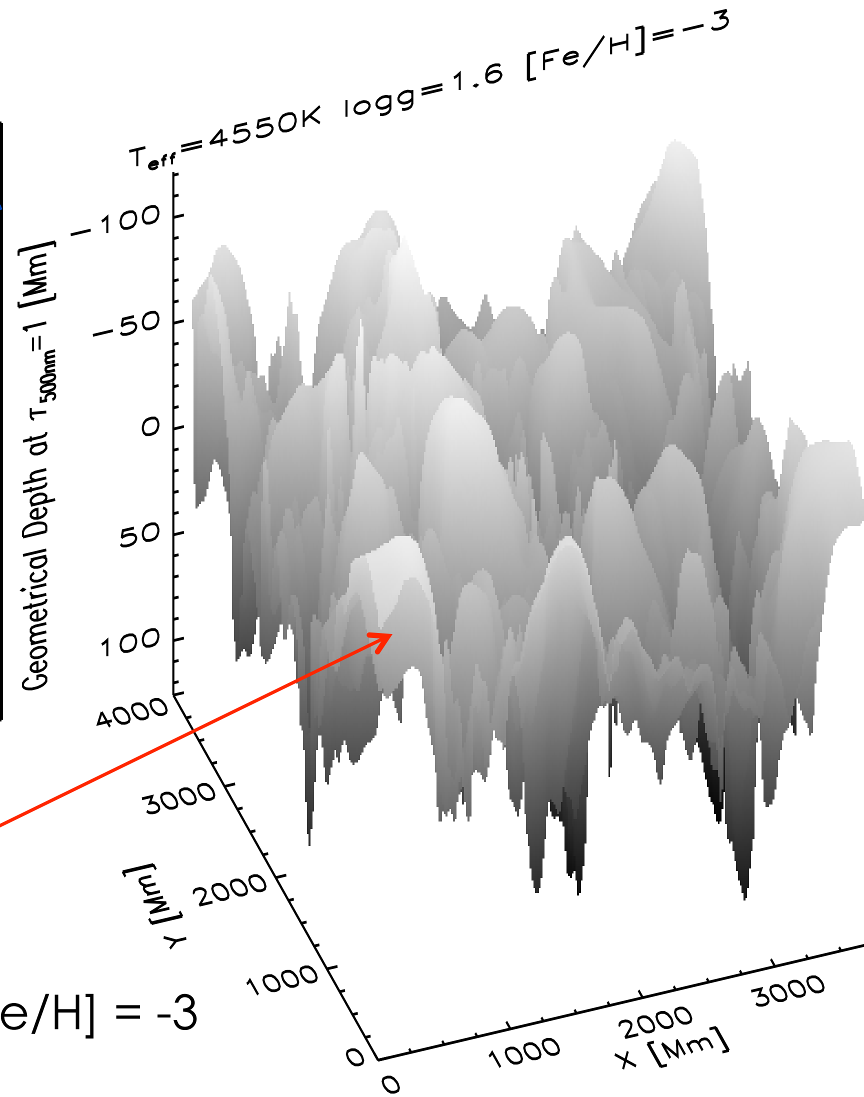
7 different program packages:

- 1D/3D LTE model atmospheres
- SE with multi-level NLTE RT codes
- Abundances with NLTE spectrum synthesis code

Model atmospheres

- 1D flux-constant LTE models: MAFAGS-OS, MARCS-OS
- 1D-averages of 3D radiation-hydrodynamic models of stellar convection (talk by Remo Collet)

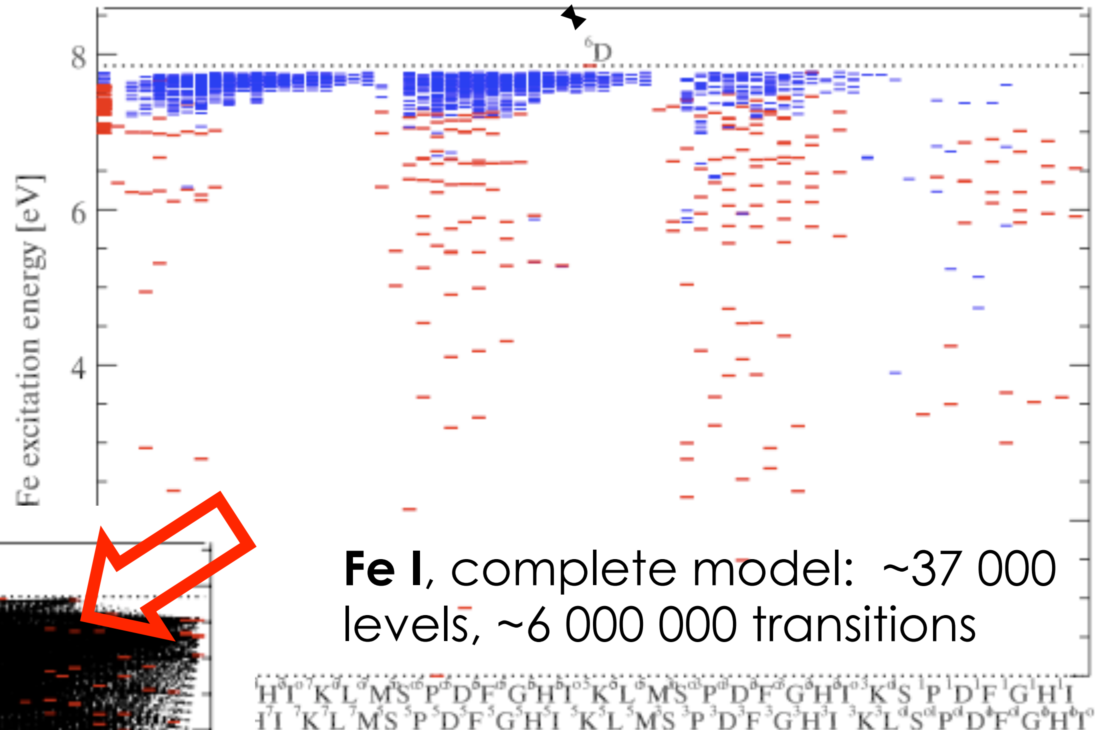




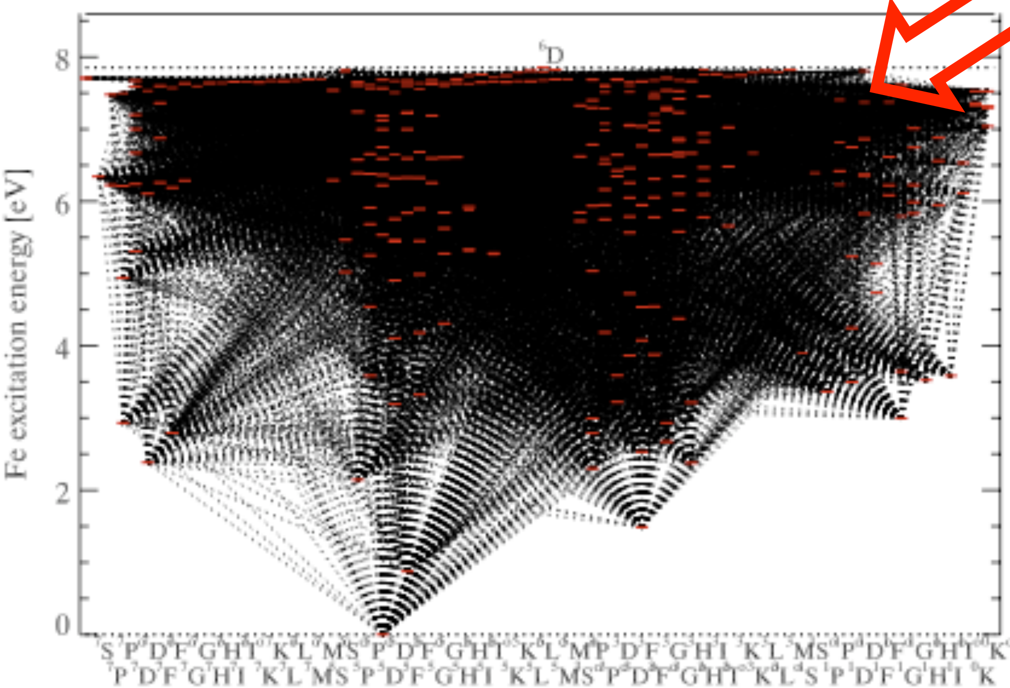
Surface of log τ (500 nm) = 1
in a 3D hydro model of a
metal-poor giant HD 122563, [Fe/H] = -3

NLTE model

Kurucz 2011: Levels, f-values
Bautista 2011: Quantum-mechanical photoionization
Classical recipes: H I and e impact excitation and ionization



Fe I, complete model: ~37 000 levels, ~6 000 000 transitions



Fe I, reduced model: 300 levels, 13 000 b-b transitions

NLTE RT codes (ALI):

- Detail
- MULTI2.3

complete redistribution in line transitions

Test stars

5 late-type stars with well-known parameters + EMP stars:

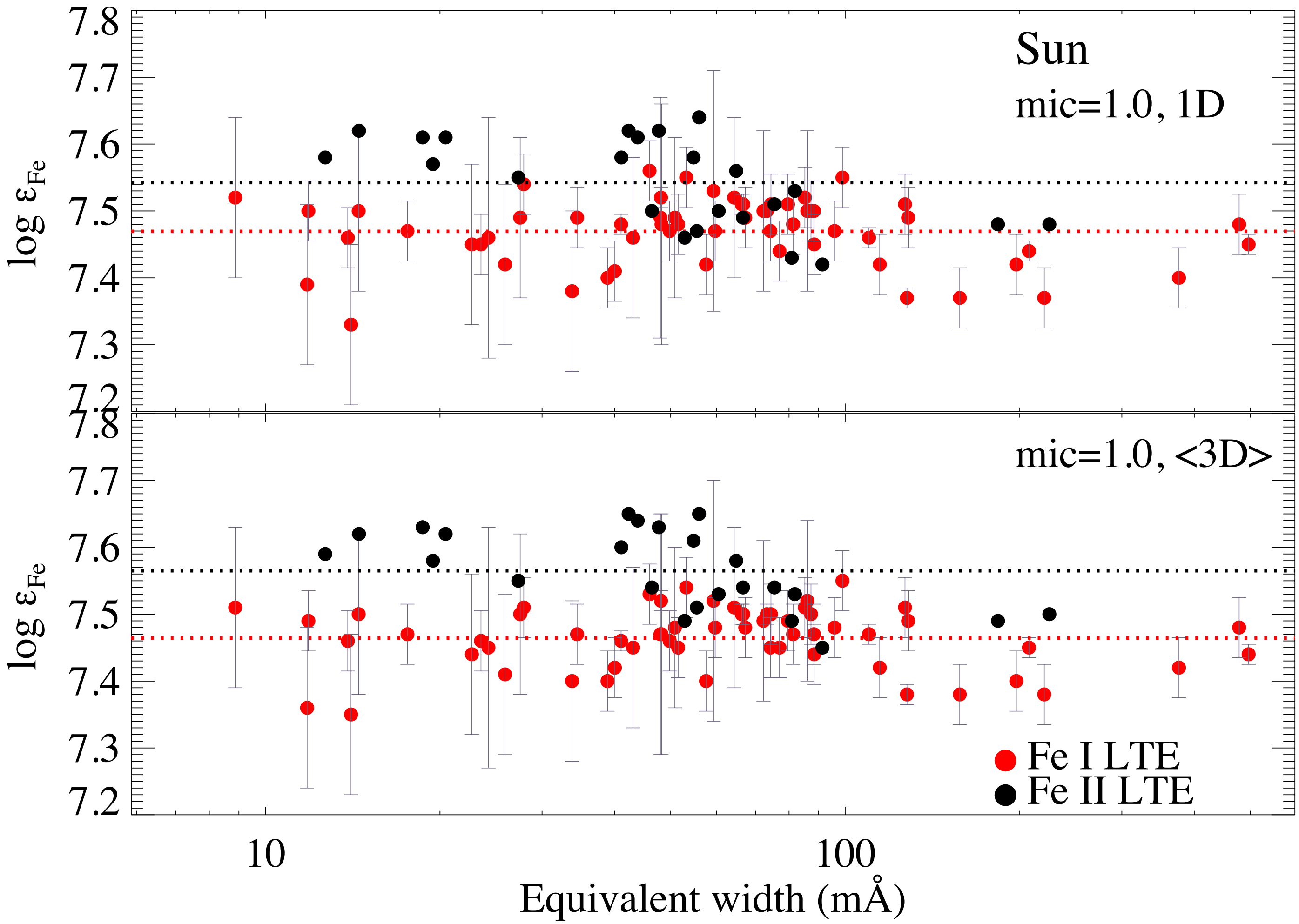
- Procyon: Mass + Radius (interferometry, astrometry)
- T_{eff}: Infra-Red Flux method and Balmer lines
- log g: Hipparcos parallaxes and Mg b lines
- metallicities and "micro-turbulence": excitation equilibrium of Fe II

Abundance analysis by visual profile fitting (full spectrum synthesis with blends), 20– 70 Fe lines per star

Stars	T_{eff}	log g	[Fe/H]	mic
Sun	5777	4.44	0	1
Procyon	6500	4.0	0	2
HD 122563	4600	1.6	-2.5	1.9
HD 84937	6350	4.0	-2.15	1.8
HD 140283	5780	3.6	-2.5	1.5
HE 1327-2326	6180	3.7	-5.9	1.0
HE 0107-5240	5110	2.2	-5.3	2.2

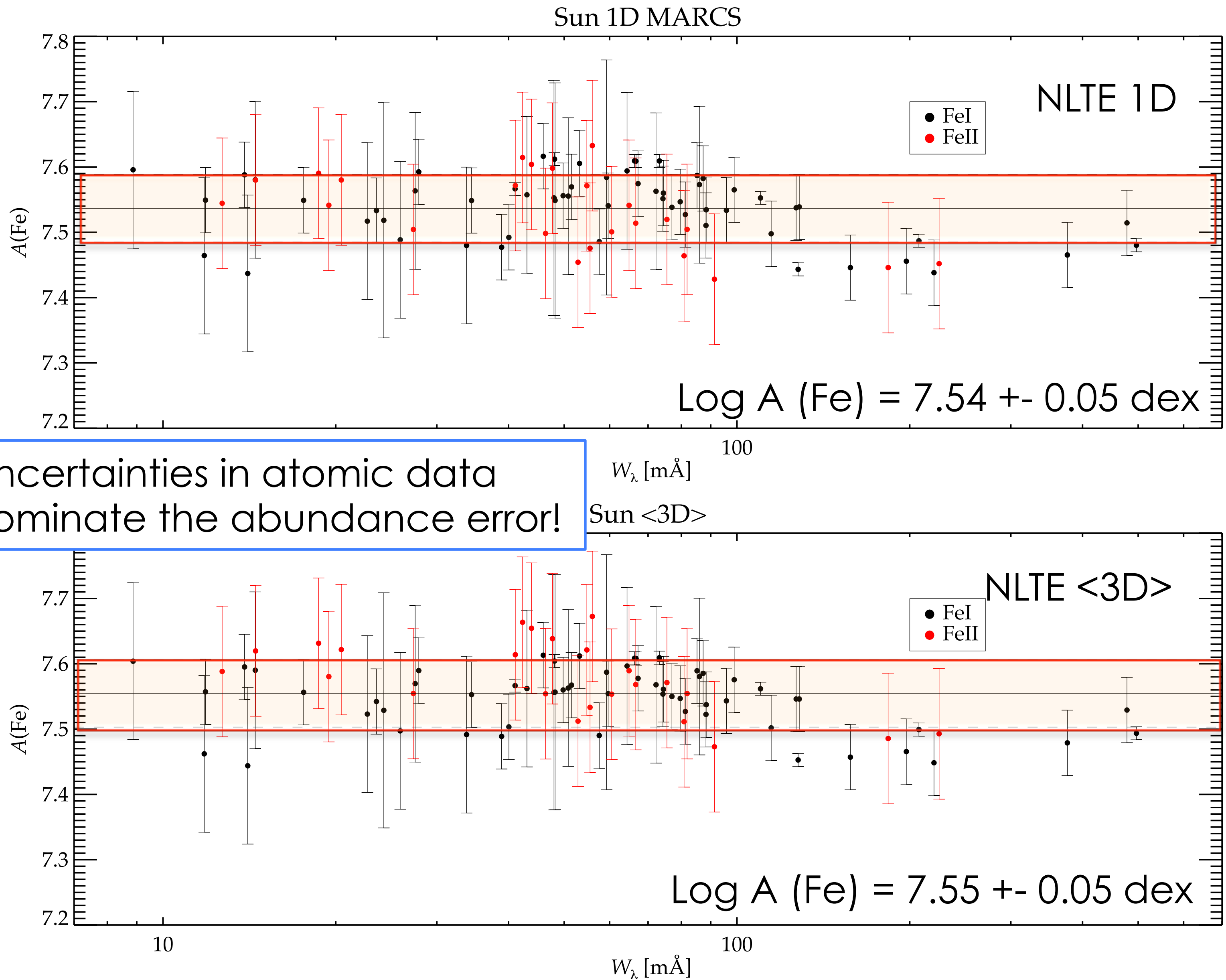
Results: Sun LTE

Huge line-to-line scatter in 1D and <3D>: 7.35 … log A(Fe) … 7.65 dex
(meteorites: log A(Fe) = 7.48 dex)



Results: Sun NLTE

Solar Fe abundance: <3D> - **7.55** dex, 1D - **7.54** dex

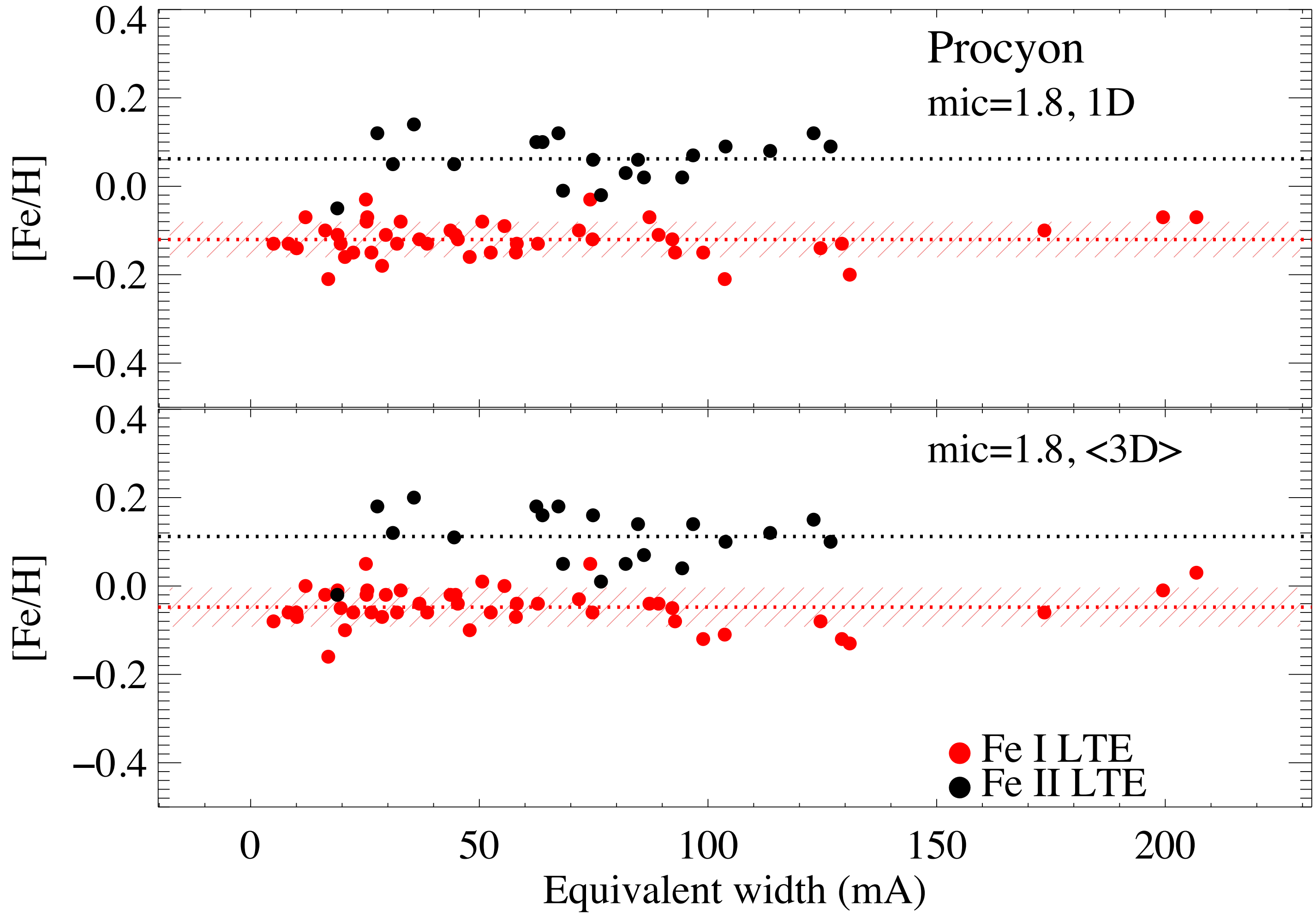


Sun: uncertainties in atomic data fully dominate the abundance error!

Results: Procyon LTE

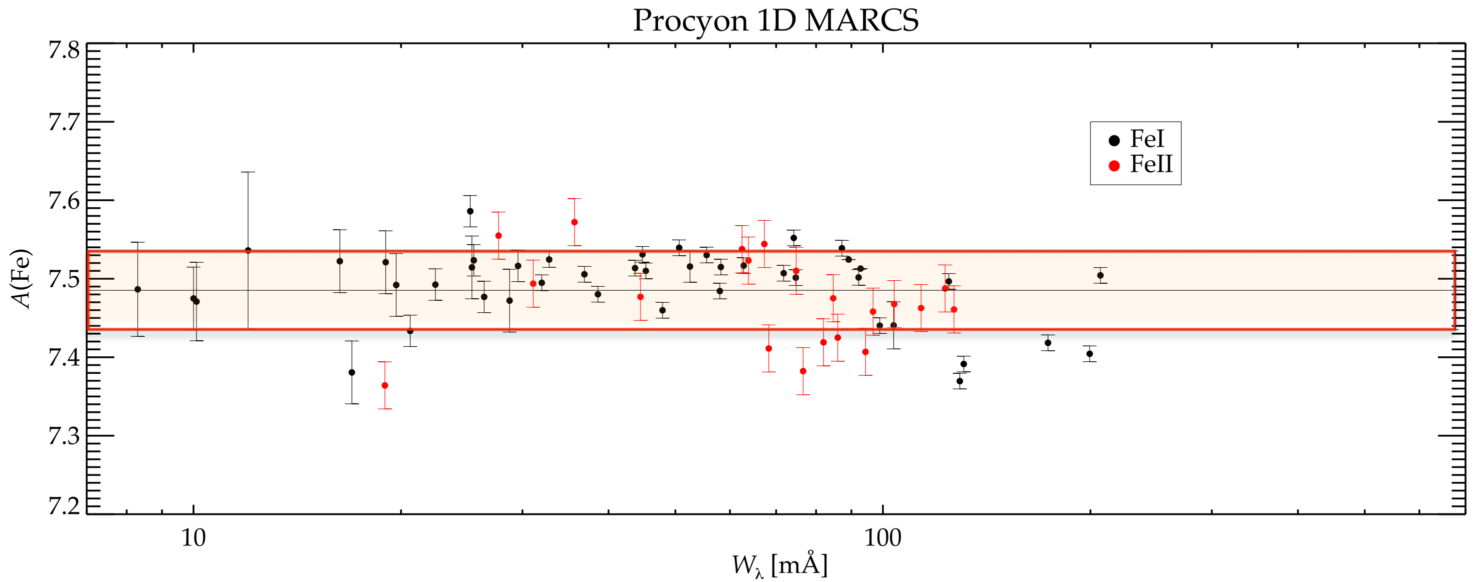
Visual binary: astrometric mass + interferometric ang. diameter

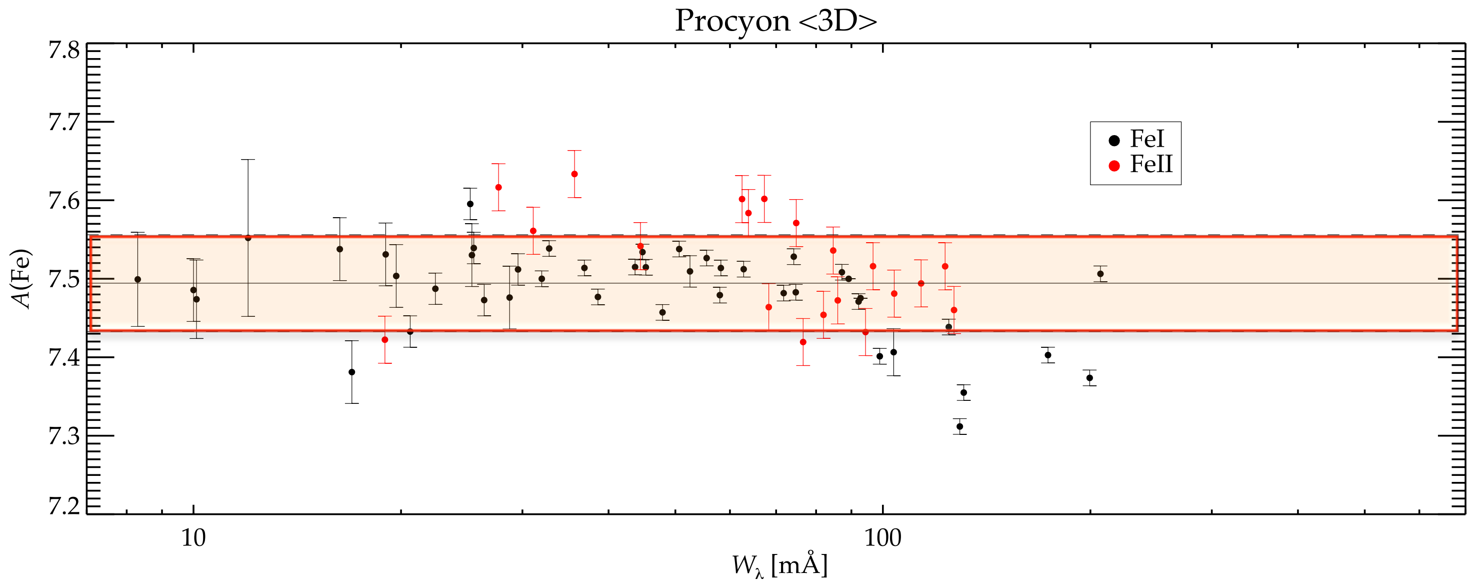
- super-solar metallicity (if LTE & Fe II) [Fe/H] = + 0.08 … + 0.12
- sub-solar metallicity (if LTE & Fe I) [Fe/H] = − 0.12 … − 0.03



Results: Procyon NLTE

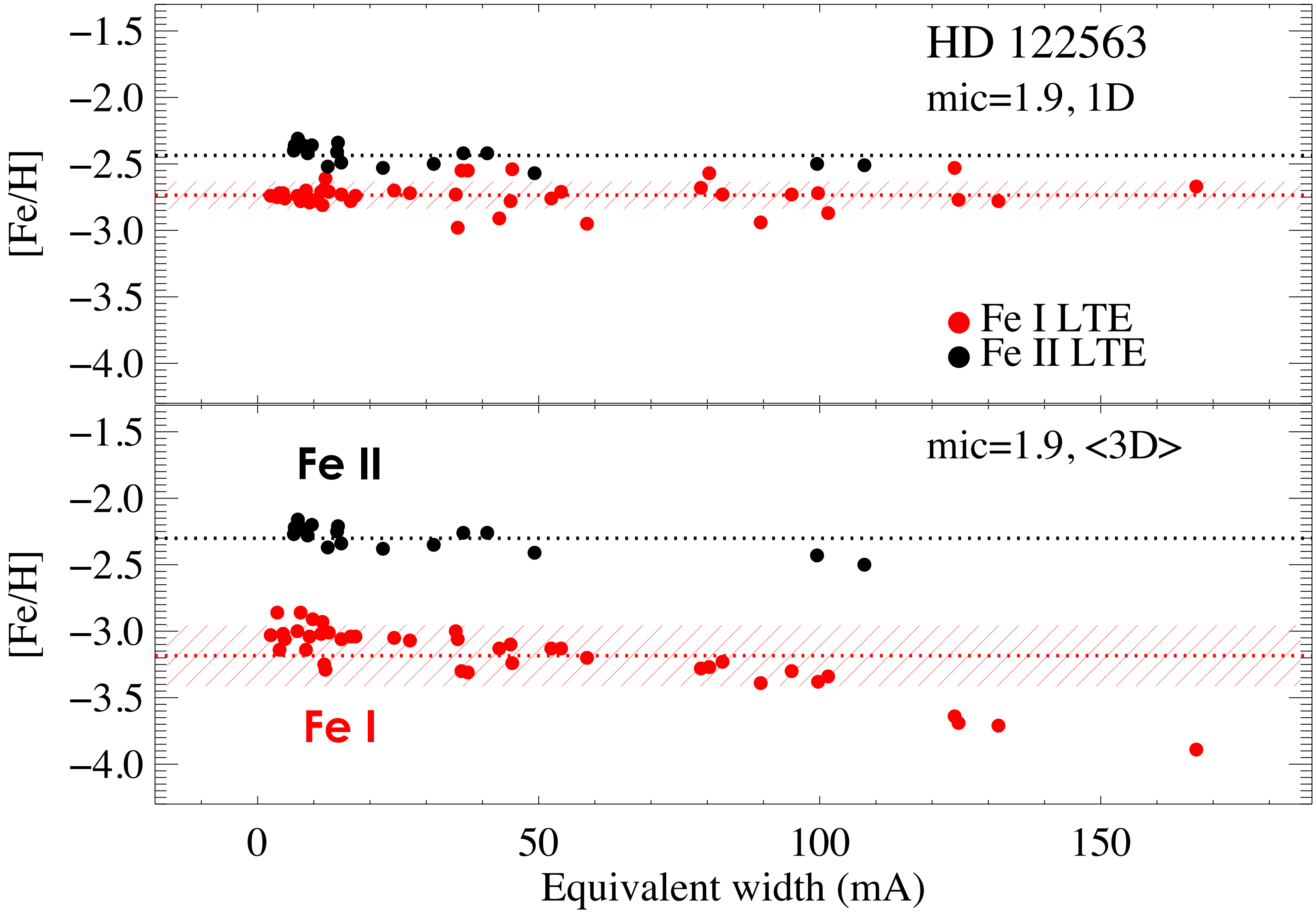
Metallicity from Fe I and Fe II lines: [Fe/H] = − 0.03 (albeit larger scatter in <3D>)



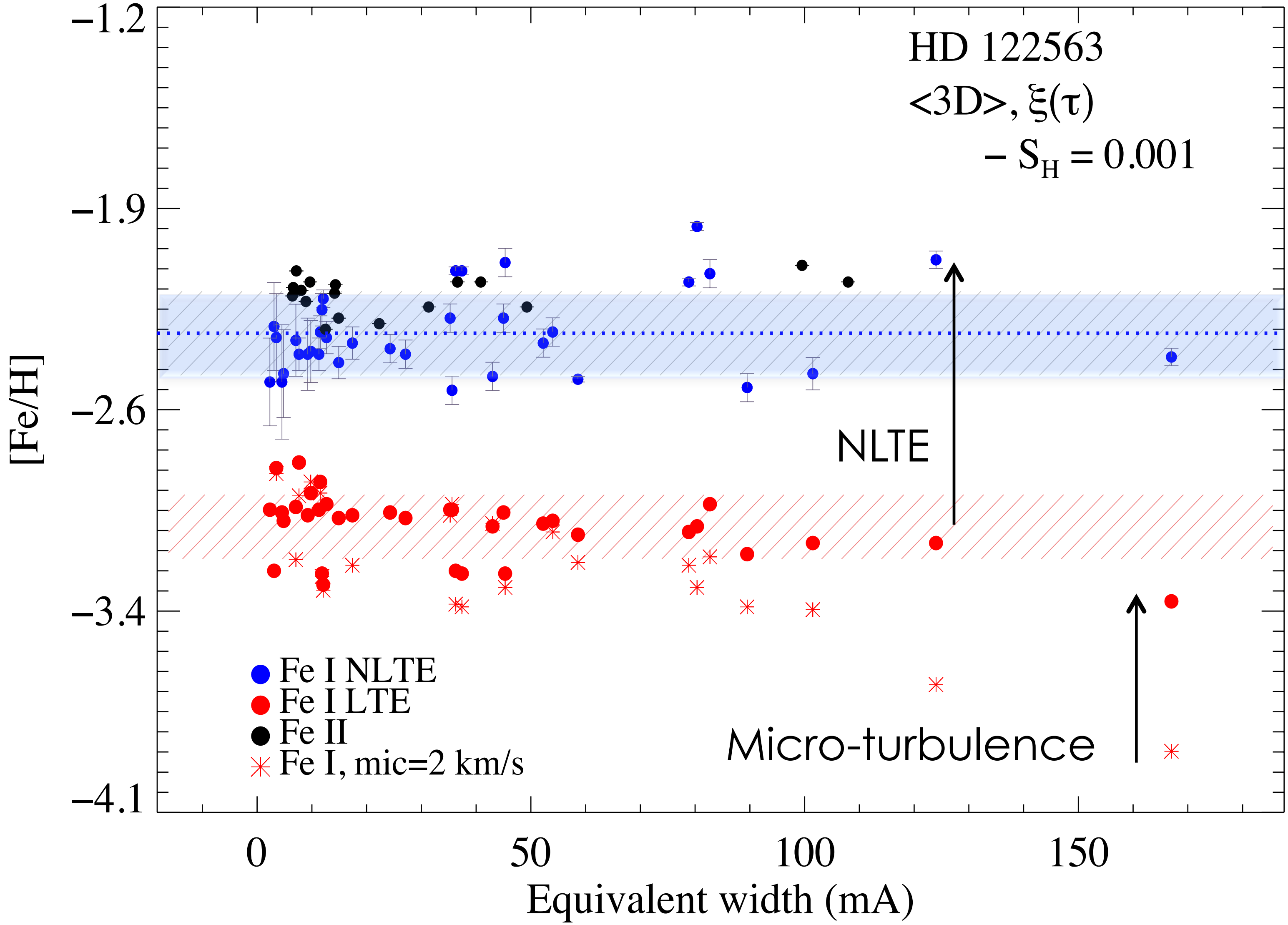


Best-studied halo field giant

HD 122563: T_{eff} = 4600, log g = 1.6 , [Fe/H] = − 2.3 … − 3.2 (LTE)

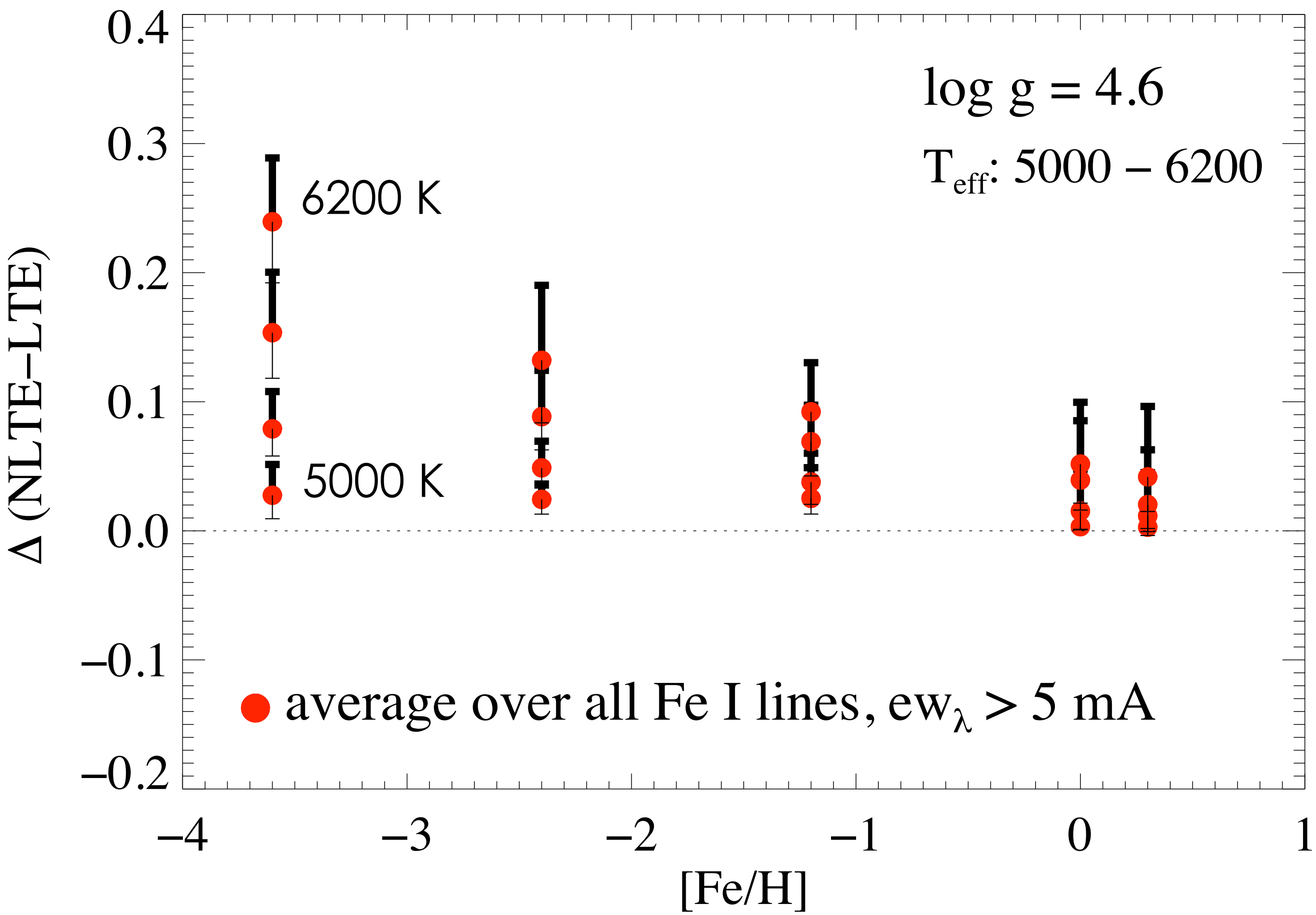


HD 122563: T_{eff} = 4600, log g = 1.6 , [Fe/H] = −2.3 +/− 0.1 (NLTE)



Grid of models: NLTE abundance corrections

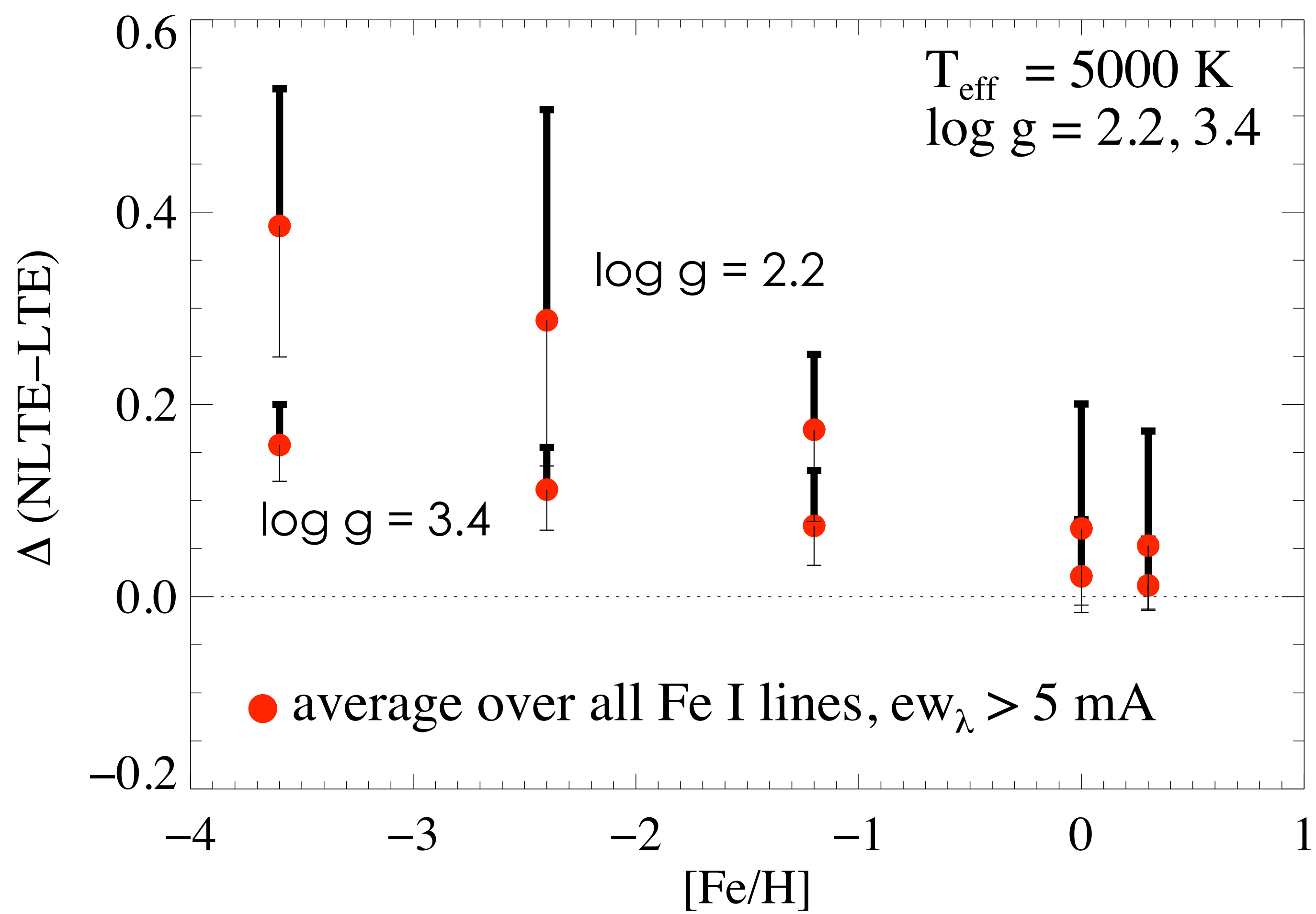
$A(Fe)_{NLTE} - A(Fe)_{LTE}$: ↑ with ↑ T_{eff}



Grid of models

↑ with ↓ [Fe/H], log g

Ionization balance achieved assuming LTE leads to progressively *underestimated* gravities (up to **1 dex @ [Fe/H] = -3**) and metallicities (up to **0.6 dex @ [Fe/H] = -3**).



MPA: NLTE abundance database for FGK stars

initially, results will be available for 1D and <3D> model atmospheres

1 H																	2 He
3 Li	4 Be											5 B	6 C	7 N	8 O	9 F	10 Ne
11 Na	12 Mg											13 Al	14 Si	15 P	16 S	17 Cl	18 Ar
19 K	20 Ca	21 Sc	22 Ti	23 V	24 Cr	25 Mn	26 Fe	27 Co	28 Ni	29 Cu	30 Zn	31 Ga	32 Ge	33 As	34 Se	35 Br	36 Kr
37 Rb	38 Sr	39 Y	40 Zr	41 Nb	42 Mo	43 Tc	44 Ru	45 Rh	46 Pd	47 Ag	48 Cd	49 In	50 Sn	51 Sb	52 Te	53 I	54 Xe
55 Cs	56 Ba	57 La	72 Hf	73 Ta	74 W	75 Re	76 Os	77 Ir	78 Pt	79 Au	80 Hg	81 Tl	82 Pb	83 Bi	84 Po	85 At	86 Rn
87 Fr	88 Ra	89 Ac	104 Rf	105 Db	106 Sg	107 Bh	108 Hs	109 Mt	110 Ds	111 Rg	112 Cn	113 Uut	114 Uuq	115 Uup	116 Uuh	117 Uus	118 Uuo

<< PERIODIC TABLE | Selected: Na | Interpolate (equivalent width) / Interpolate (LTE abundance) / Plot

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Logarithm of equivalent width [pm]:		[-1,2]
Temperature [K]:		[4000.0,8000.0]
Logarithm of surface gravity [cgs]:		[1.0,5.0]
Metallicity [Fe/H]:		[-5.0,0.5]
Microturbulence [km/s]:		[1.0,5.0]
Line wavelength [nm]:		

OK

<< PERIODIC TABLE | Selected: Na | Interpolate (equivalent width) / Interpolate (LTE abundance) / Plot

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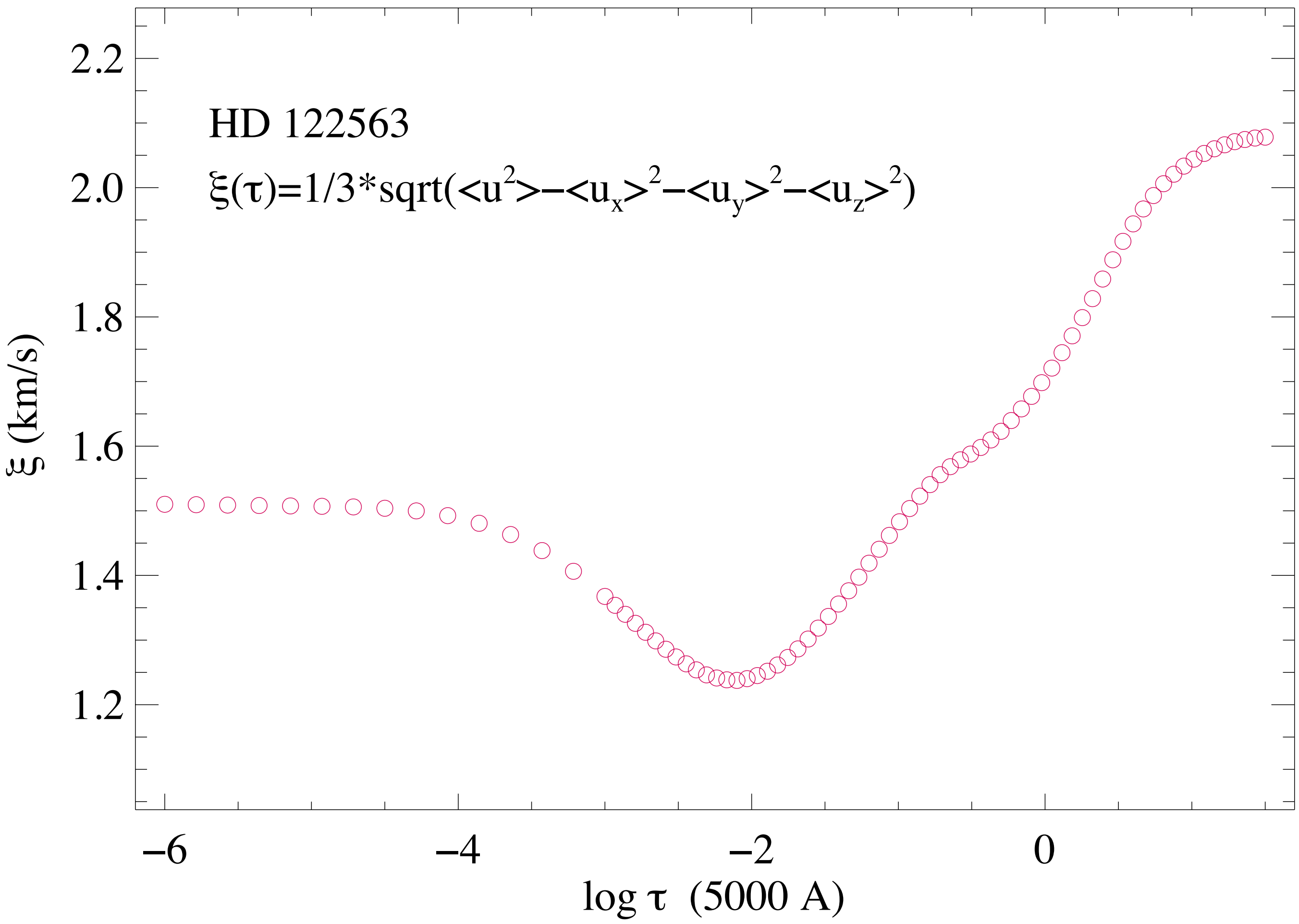
Logarithm of equivalent width [pm]:	1	[-1,2]
Temperature [K]:	6000	[4000.0,8000.0]
Logarithm of surface gravity [cgs]:	4	[1.0,5.0]
Metallicity [Fe/H]:	-2	[-5.0,0.5]
Microturbulence [km/s]:	1	[1.0,5.0]
Line wavelength [nm]:	568.8	

OK

EW [pm]	A(Na) LTE	A(Na) NLTE	Delta
10.00	5.97	5.78	-0.19

Conclusions

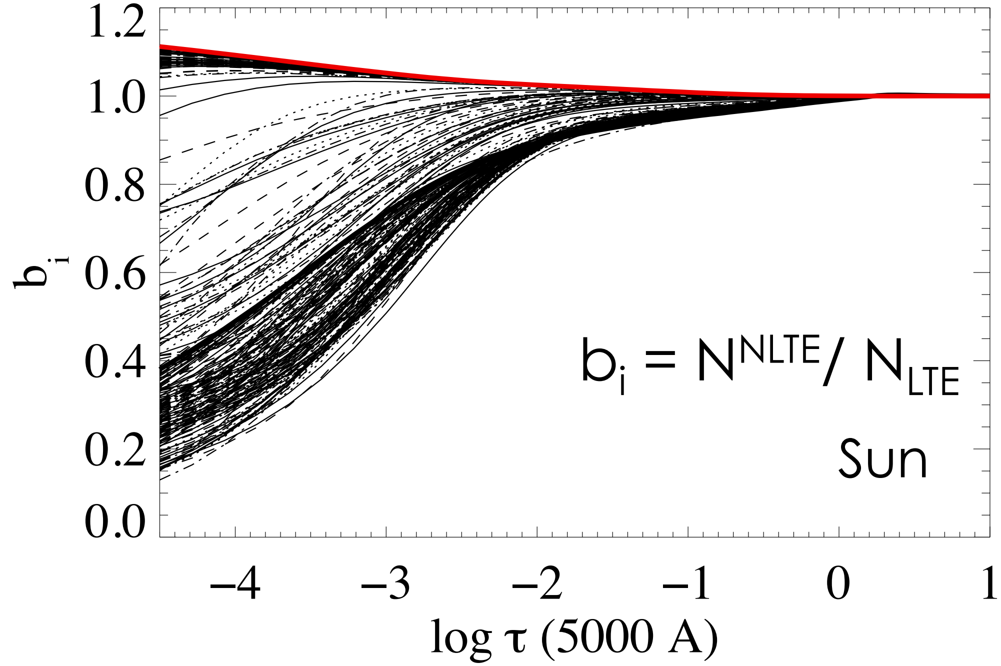
- FGK stars: photospheres are non-equilibrium systems and sub-photospheric convection strongly affects emergent radiation
- Classical1D LTE approach in the determination of basic stellar parameters (T_{eff}, log g, [Fe/H], abundances) from observed spectra is not valid.
- All minority species (Fe I, Ca I, Si I, Ti I,…) are affected by NLTE and 3D, particularly their abundance variations with metallicity. Dominant species (e.g., Fe II) are less affected, but hardly observed in stars with [Fe/H] < -1.
- That leads to **systematic errors** in stellar parameters that introduces strong biases in their interpretation in astrophysical context.

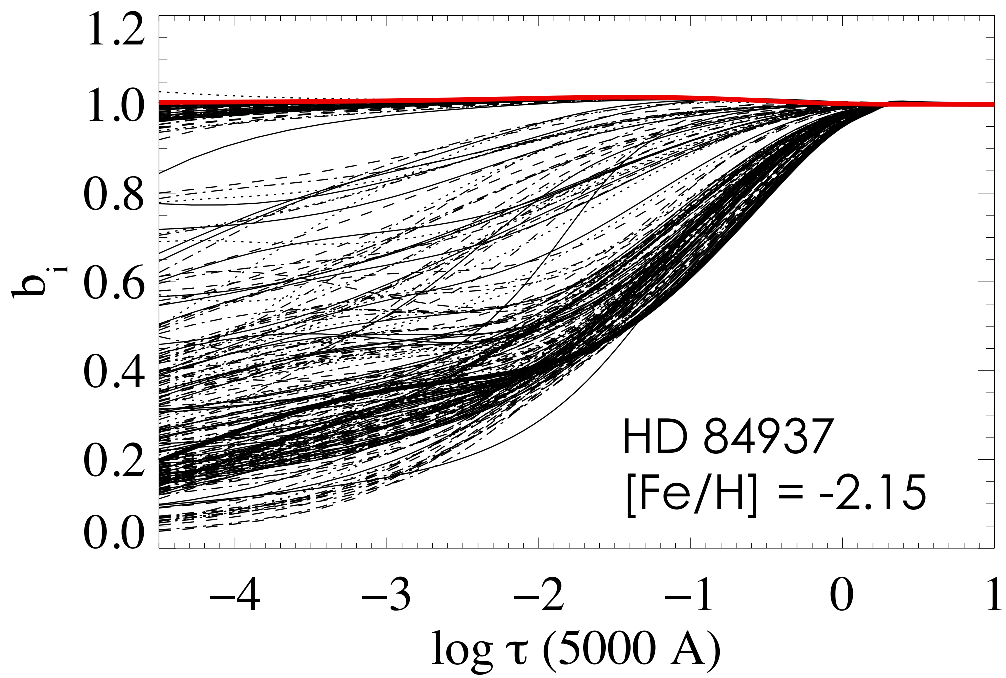

HD 122563
ξ(τ)=1/3*sqrt(<u^2>−<u_x>^2−<u_y>^2−<u_z>^2)
ξ (km/s)
2.2
2.0
1.8
1.6
1.4
1.2
−6
−4
−2
0
log τ (5000 A)

NLTE effects

Fe I is extremely sensitive to NLTE effects in FGK atmospheres:

- overionization due to strong non-local UV radiation field
- IR over-recombination
- non-equilibrium processes in numerous line transitions



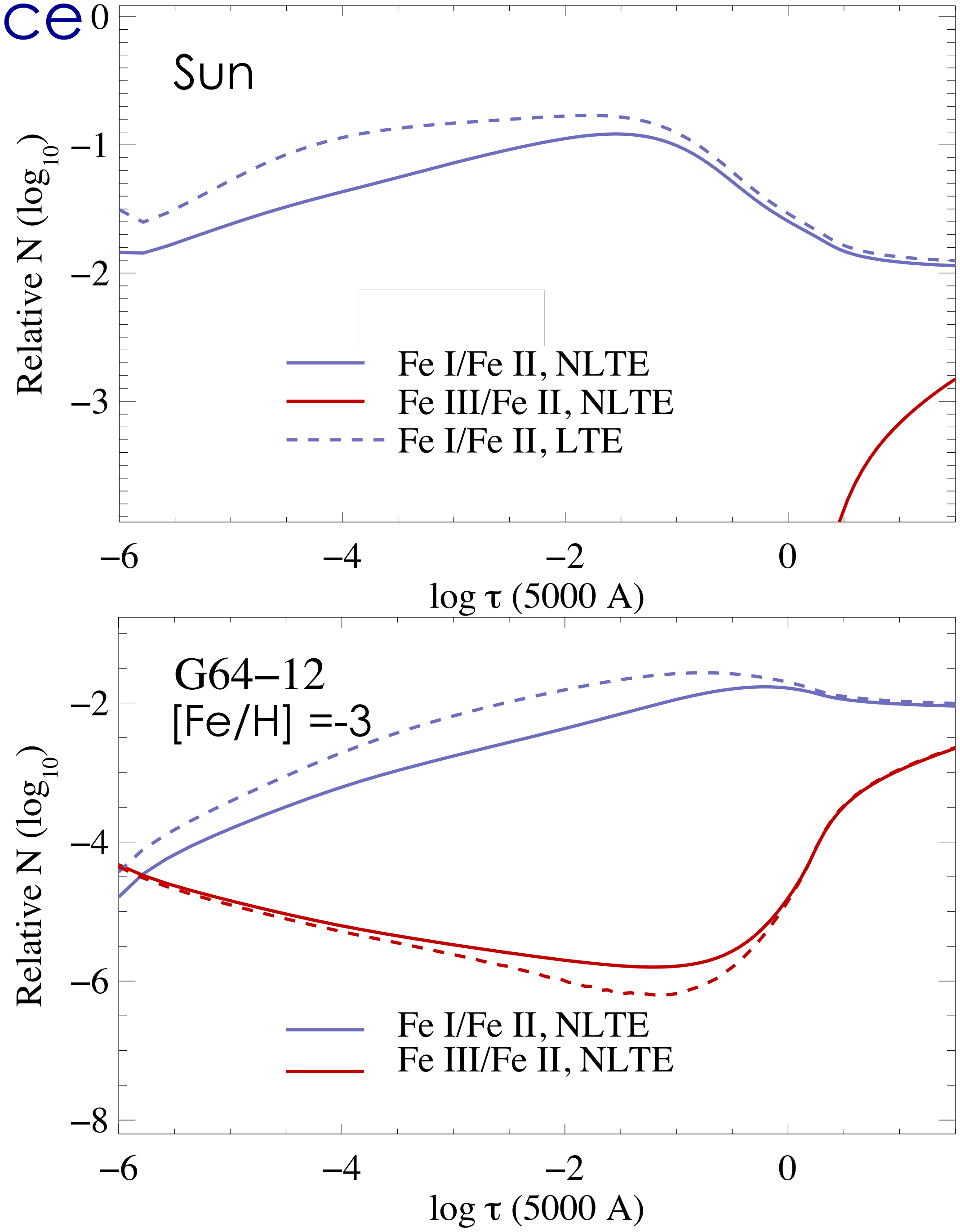


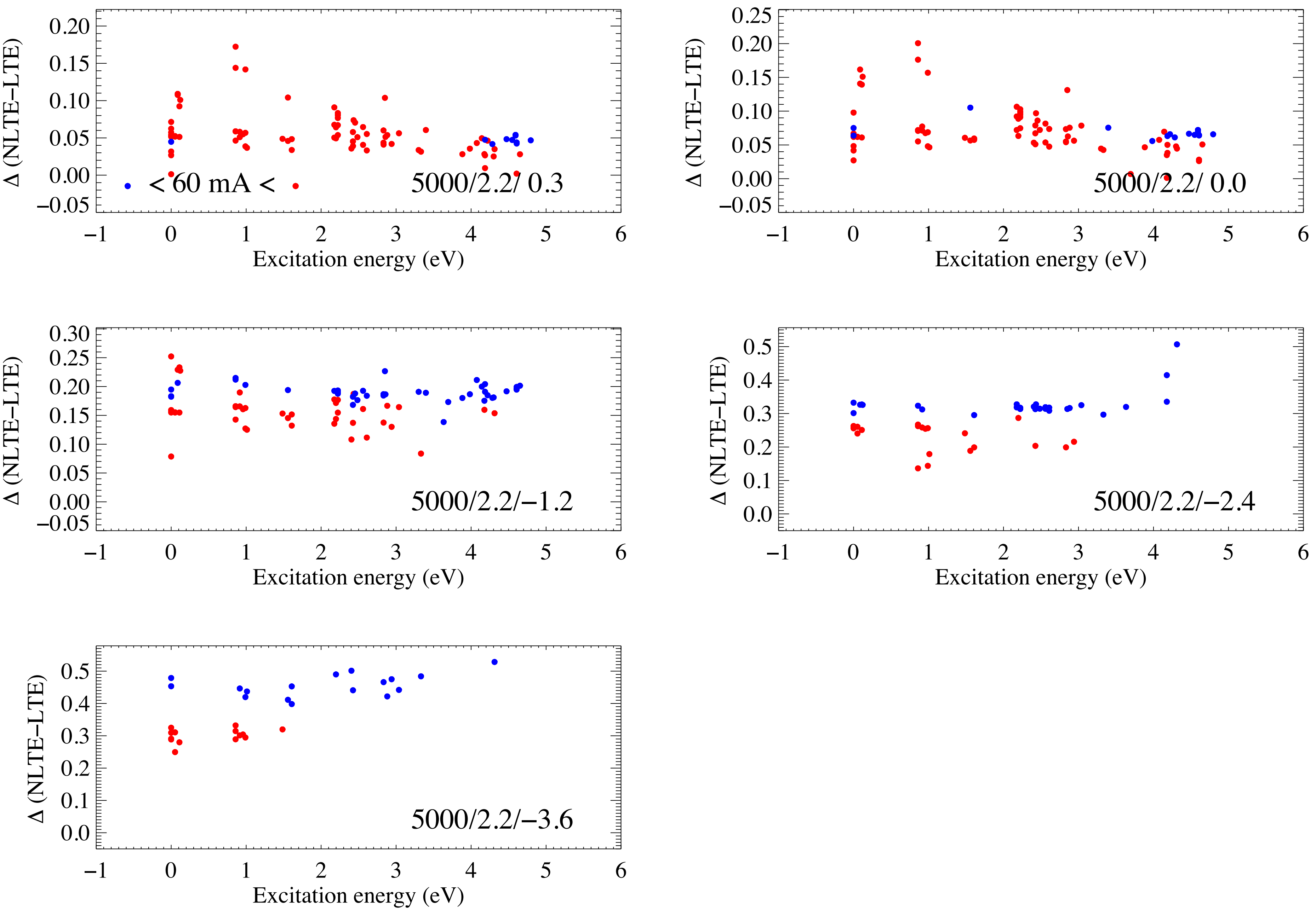
NLTE: Ionization balance

LTE overestimates ionization fraction of Fe I/Fe II by a factor of 2-5 → serious errors in:

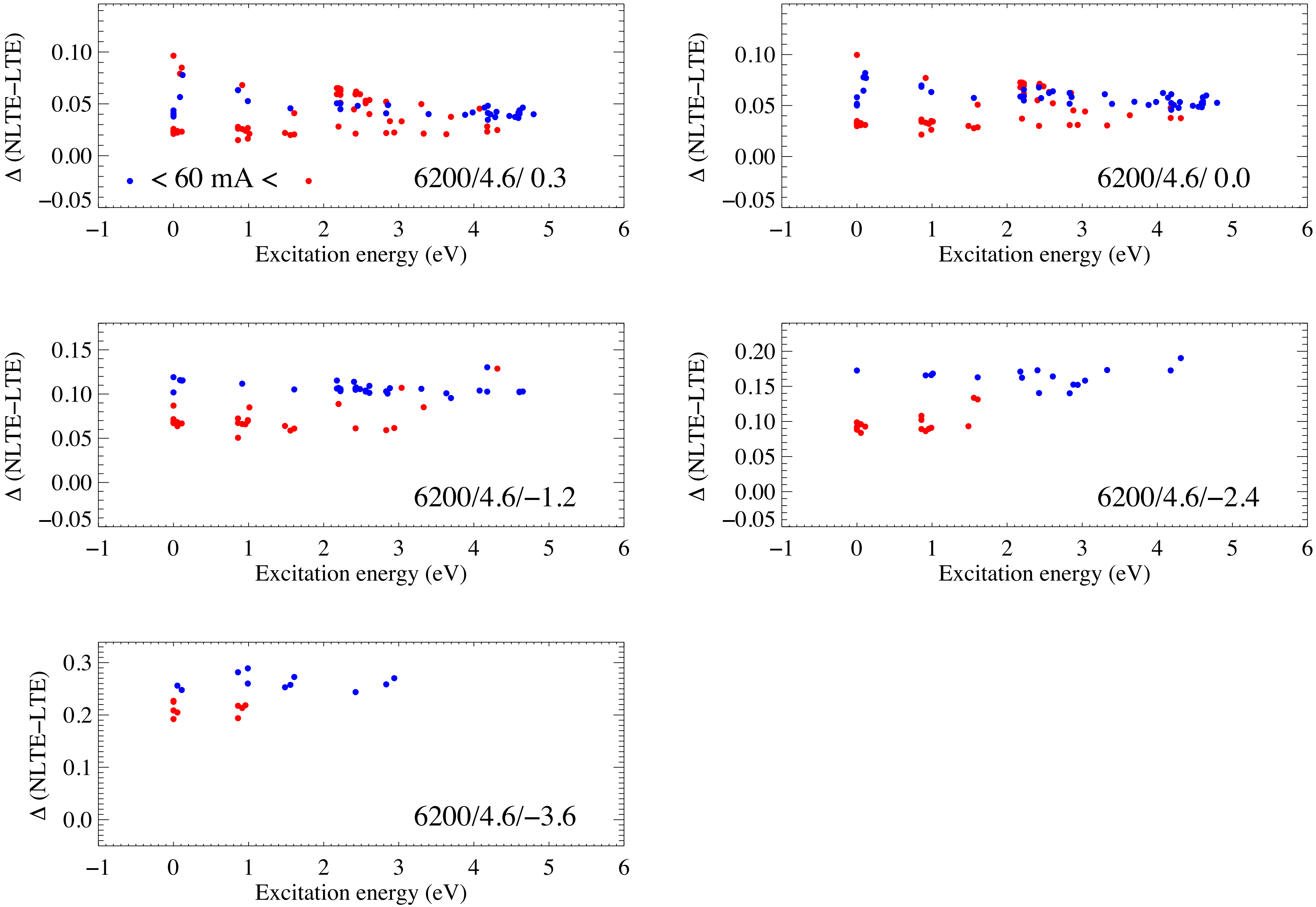
- **[Fe/H]**, determined either from Fe I

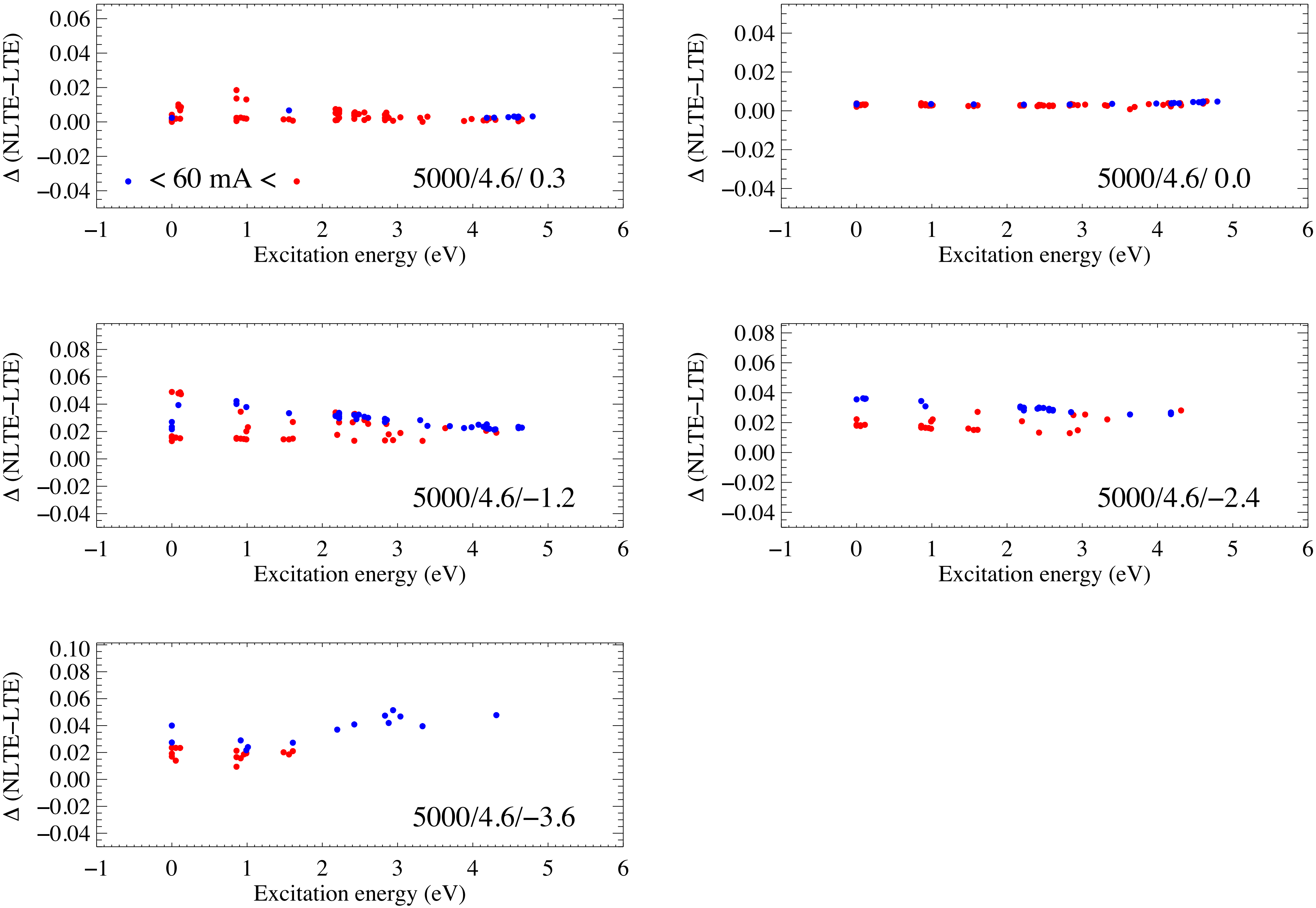
- **log g**, since
Fe II/Fe I – indicator of surface gravity





Δ (NLTE−LTE)
Excitation energy (eV)
< 60 mA <
5000/2.2/ 0.3
5000/2.2/ 0.0
5000/2.2/−1.2
5000/2.2/−2.4
5000/2.2/−3.6


Δ (NLTE−LTE)
Excitation energy (eV)
< 60 mA <
6200/4.6/ 0.3
6200/4.6/ 0.0
6200/4.6/−1.2
6200/4.6/−2.4
6200/4.6/−3.6


Δ (NLTE−LTE)
Excitation energy (eV)
< 60 mA <
5000/4.6/ 0.3
5000/4.6/ 0.0
5000/4.6/−1.2
5000/4.6/−2.4
5000/4.6/−3.6

$$dn_i/dt = \sum_{j \neq i} n_j P_{ji} - n_i \sum_{j \neq i} P_{ij}$$

assuming steady state and LTE, this requires:

$$\sum_{j \neq i} (n_i{}^* R_{ij} - n_j{}^* R_{ji}) = 0$$

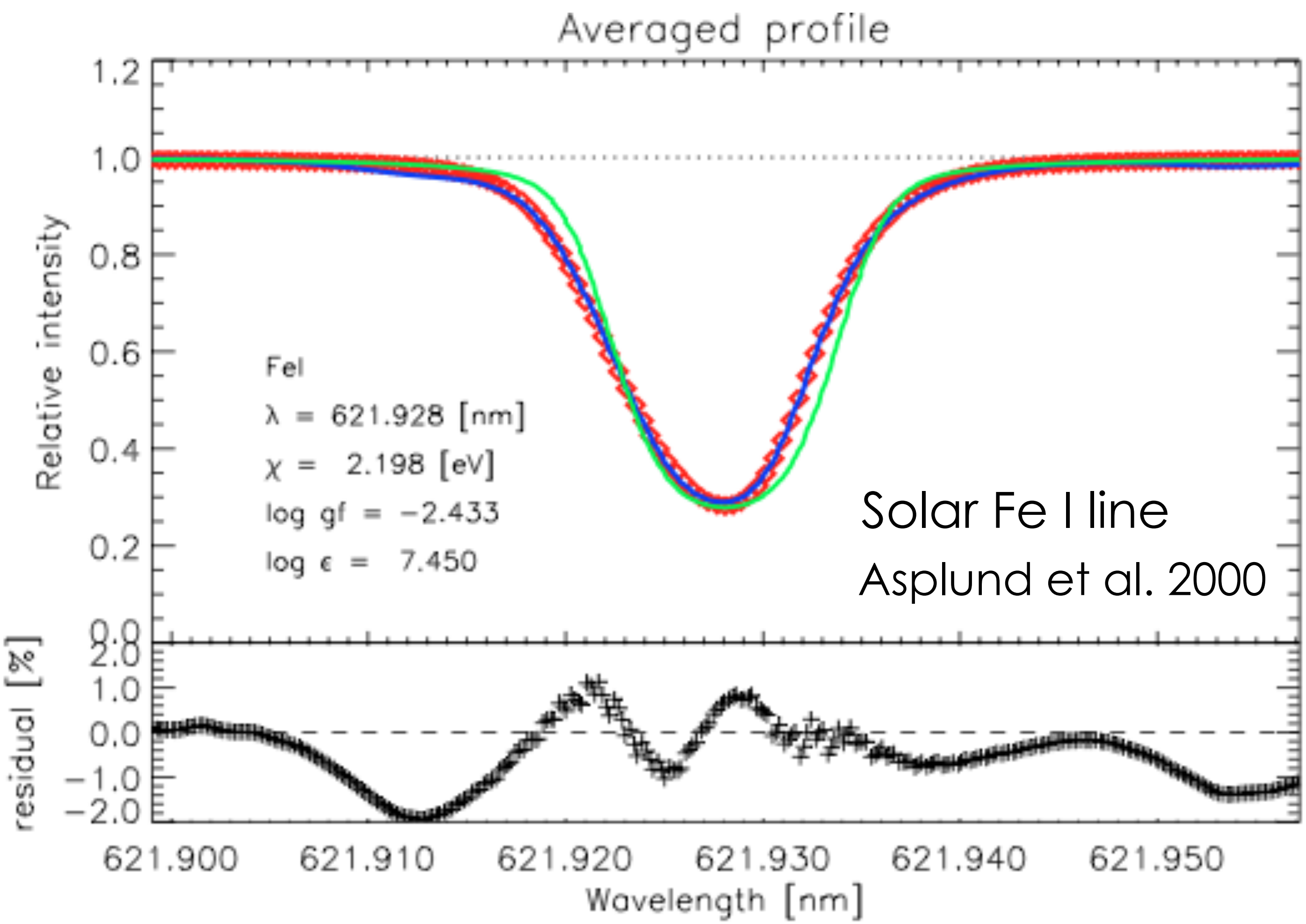
BUT, even for a 2-level atom:

$$n_1{}^* R_{12} - n_2{}^* R_{21} = -\tfrac{1}{2} n_1{}^* B_{12} \overline{B} [1 - \exp(-h\nu/kT)] \neq 0$$

Question: why do we still think that LTE is good, if it suffers from fatal physical inconsistency?

Line profiles with 3D models

The shapes of strong Fe lines can not be described by static 1D models.
C-shapes due to convective V fields!



Example: 'abundance' ratios as a function of [Fe/H]