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NLTE ionization equilibrium of Nd II and Nd III in cool A and Ap stars

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Abstract. The kinetic equilibrium of Nd II -Nd III in the atmospheres of A-type stars is investigated for the first time with a model atom containing 1651 levels of Nd II, 607 levels of Nd III, and the ground state of Nd IV. NLTE leads to an overionization of Nd II resulting in weakening the Nd II lines at mild neodymium overabundances relative to the solar Nd abundance ([Nd/H] < 2.5) and produces the opposite effect at the higher [Nd/H] values. NLTE abundance corrections grow with effective temperature and reach ~0.6 dex at $T_{\rm eff} = 9500$ K. The Nd III lines are strengthened compared with LTE. NLTE abundance corrections range between -0.3 dex and -0.2 dex for $T_{\rm eff}$ between 7500 K and 9500 K. Therefore NLTE effects may explain ionization discrepancies up to 0.8 – 0.9 dex, derived with the LTE approach.

NLTE effects are even larger for a stratified Nd abundance distribution compared with a homogeneous one resulting in positive NLTE abundance corrections up to 1.4 dex for the Nd II lines and negative ones as small as to -0.5 dex for the Nd III lines. The influence of uncertainty in the photoionization cross-sections on NLTE results is investigated. NLTE calculations were applied to Nd analyses in the atmospheres of roAp stars γ Equ and HD 24712.

Keywords. Atomic data, line: formation, stars: chemically peculiar, stars: abundances

1. Introduction

Abundance analyses of cool Ap stars revealed huge ionization discrepancies in Nd II–Nd III, which may reach 2 dex in the atmospheres of rapidly oscillating (roAp) stars (Ryabchikova *et al.* 2001). In a newer LTE analysis of one of them, γ Equ, Ryabchikova *et al.* (2002) interpreted the observed discrepancy using a stratified Nd distribution with the accumulation of the element above $\log \tau_{5000} = -8$. In upper atmospheric layers departures from LTE are expected. Thus non-local thermodynamical equilibrium (NLTE) line formation is used to obtain theoretical Nd II and Nd III line profiles and equivalent widths for a range of effective temperatures and Nd overabundances typical of the cool Ap stars.

2. NLTE calculations for Nd II - III

NLTE calculations were made with the DETAIL code using accelerated lambda iteration following the method described by Rybicki & Hummer (1991, 1992). DETAIL originally was created at Munich University by Butler & Giddings (1985) and modified later. In our NLTE calculations we use plane-parallel homogeneous model atmospheres computed with the MAFAGS code (Fuhrmann *et al.* 1997).

2.1. *Model atom*

The model atom includes 658 energy levels of Nd II from laboratory measurements (Martin *et al.* 1978, Blaise *et al.* 1984) and 993 levels of Nd II and 607 levels of Nd III predicted in this work. The predicted levels belong to quartet and sixtet terms of the $4f^4$ np (n = 7 - 11) and the $4f^3$5d 6p electronic configuration for Nd II and to triplet and quintet terms of the $4f^3$nl (nl = 4f, 5d, 6s) and $4f^25d^2$ electronic configuration for Nd III. The Nd II and Nd III spectra were calculated by using the RCN-RCG-RCE software package (Cowan 1981). The RCN subroutine determines the wave functions of the configurations by the Hartree-Fock single-configuration method with relativistic corrections. These wave functions are used to compute the average configuration energies, the Slater integrals of intra-configuration electrostatic interactions, the integrals of electric dipole transitions and inter-configuration electrostatic interactions, as well as spin-orbit interaction parameters. Using these quantities, the RCG subroutine computes the wavelengths and transition probabilities. By fitting the computed and experimental energy levels from (Blaise *et al.* 1984), the ab initio energy matrix parameters are modified and these parameters are again used by the RCG subroutine to compute a semiempirically adjusted spectrum. Calculated energy levels of the Nd II $4f^4$6p configuration agree with experimental values within several hundreds of cm^{-1}. Calculated gf values for the Nd II $4f^4$6s ^{6}I - $4f^4$6p transitions are greater by about 50% compared with new experimental data of Den Hartog *et al.* (2003). Similar accuracy is expected for the predictions of related values to the unknown $4f^4$np configurations.

Levels of the same parity with small energy differences were combined into single level. The final model atom includes 247 levels of Nd II, 68 levels of Nd III and the ground state of Nd IV.

For transitions between the measured Nd II energy levels, oscillator strengths f_{ij} are available in the Vienna Atomic Line Data Base (Kupka *et al.* 1999). Within 0.1 - 0.15 dex they are consistent with the new experimental data by Den Hartog *et al.* (2003). The remaining transitions f_{ij} have been calculated in this paper. No data on photoionization cross-sections for both Nd II and Nd III levels are available in the literature and we use hydrogenic cross-sections. For electron impact excitation we use the formula of van Regemorter (1962) for allowed transitions and that of Allen (1973) with $\Omega = 1$ for forbidden ones. Electron impact ionization cross-sections are computed according to Drawin (1961).

2.2. *Kinetic equilibrium calculations and NLTE effects*

NLTE calculations show that in the atmospheres of dwarfs with $T_{\rm eff}$ between 7500 K and 9500 K the ionization equilibrium of Nd II/Nd III deviates from the thermodynamical value. In line formation layers all the Nd II levels are underpopulated compared with the LTE populations while the Nd III levels are overpopulated at $T_{\rm eff} \leqslant 8000$ K (see Fig. 1, left panel for the LTE and NLTE total number densities of Nd II and Nd III in the model atmosphere with $T_{\rm eff} = 7700$ K) and keep their thermodynamical values for the higher effective temperatures. NLTE effects for the Nd II and Nd III lines are of opposite sign, and they are, therefore, important for the comparison of neodymium abundances deduced from these lines. In Fig. 1 right panel, the departure coefficients, $b_i = n_i^{\rm NLTE}/n_i^{\rm LTE}$ of the selected levels of Nd II and Nd III in the model atmosphere with $T_{\rm eff}/\log g/[{\rm M/H}] = 7700/4.2/0.1$ are shown as a function of continuum optical depth τ_{5000} refering to λ5000. Here, $n_i^{\rm NLTE}$ and $n_i^{\rm LTE}$ are the kinetic equilibrium and thermal (Saha-Boltzmann) number densities, respectively. Everywhere in atmosphere [Nd/Fe] = 3 is adopted.

Overionization of Nd II in the atmospheric layers above $\log\tau_{5000} = 0$ is caused by superthermal radiation of a non-local origin near thresholds of $4f^4$6p levels with $E_{\rm exc}$ from

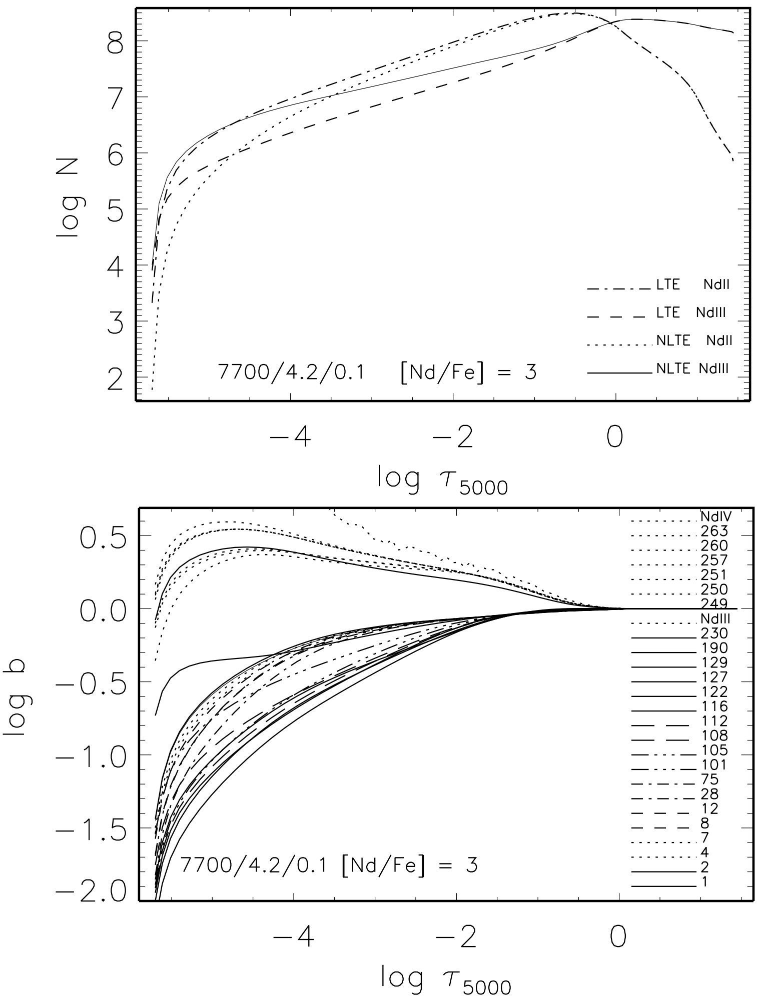

Figure 1. LTE and NLTE total number densities of Nd II and Nd III (top) and departure coefficients for selected levels of Nd II and Nd III (bottom) in the model atmosphere 7700/4.2/0.1. Everywhere in atmosphere [Nd/Fe] = 3.

3 eV to 4 eV ($\lambda_{thr} = 1600$ - 1850 Å). The Nd II lines are weakened compared with the LTE case at mild neodymium overabundances relative to the solar Nd abundance ([Nd/H] $<$ 2.5) but strengthened at greater [Nd/H] values. The Nd III lines are always stronger than with LTE. In Table 1 for the model atmosphere 7700/4.2/0.1 which represents the roAp star γ Equ, theoretical NLTE and LTE equivalent widths are given for several lines of interest together with NLTE abundance corrections $\Delta_{\rm NLTE} = \log \varepsilon_{\rm NLTE}$ - $\log \varepsilon_{\rm LTE}$. As expected, departures from LTE for the Nd II and Nd III lines grow with $T_{\rm eff}$ (Fig. 2).

2.3. *NLTE effects for a stratified* Nd *abundance distribution*

For the model atmosphere 7700/4.2/0.1 NLTE calculations were performed assuming [Nd/H] = 4 in the atmospheric layers above $\log \tau_{5000} \simeq -3.6$ and a steep change of Nd overabundance to [Nd/H]= 0 in the layers below $\log \tau_{5000} \simeq -2.7$. The calculated departure coefficients for the selected levels of Nd II and Nd III are shown in Fig. 3 and

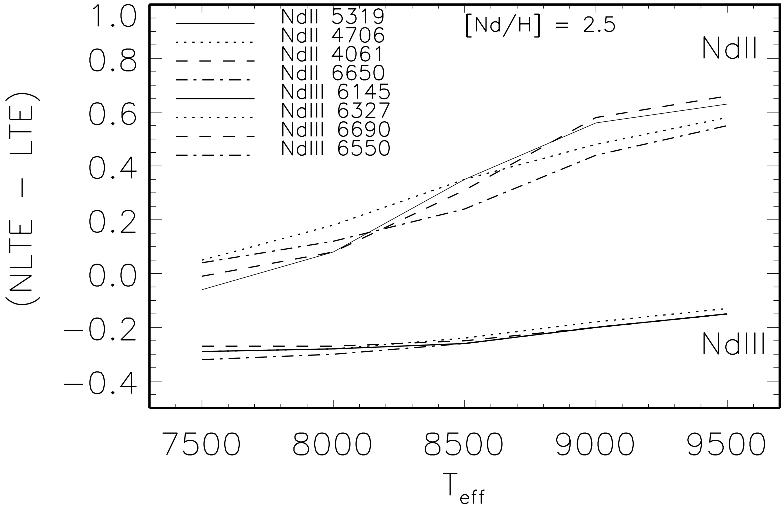

Figure 2. NLTE abundance corrections for the Nd II and Nd III spectral lines for different values of $T_{\rm eff}$. In all cases $\log g = 4$ and [Nd/H] = 2.5

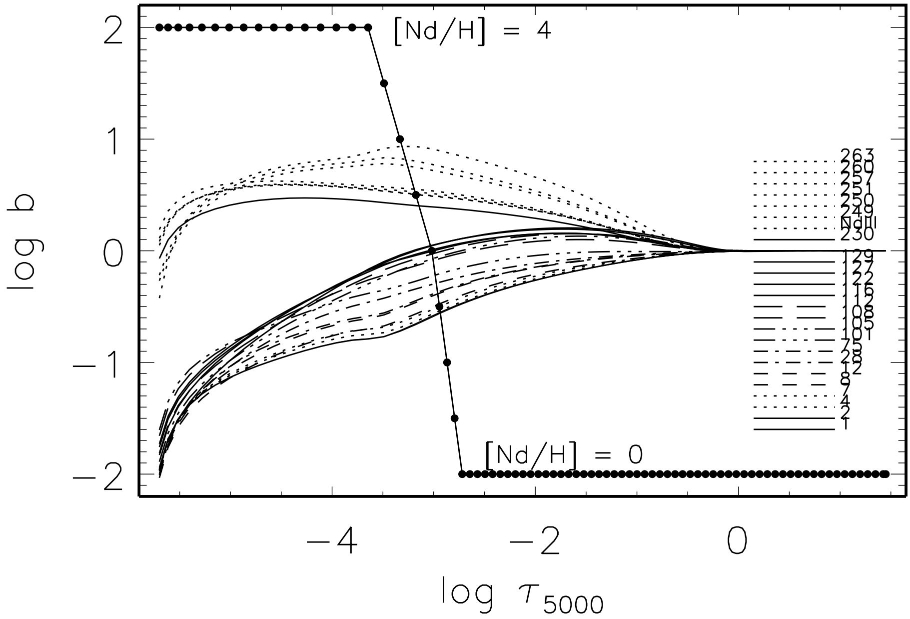

Figure 3. Departure coefficients for the selected levels of Nd II and Nd III in the model atmosphere 7700/4.2/0.1 with stratified Nd abundance distribution (the [Nd/H] ratio is shown by filled circles connected with the solid line).

theoretical NLTE and LTE equivalent widths as well as NLTE abundance corrections are given in Table 1 (columns "layer").

NLTE calculations show the overionization of Nd II and enhanced number densities of Nd III in line formation layers are similar to the homogeneous Nd abundance distribution. However, in contrast to Fig. 1, the Nd II low-excitation levels are strongly underpopulated above log τ_{5000} = -2 and their departure coefficients are smaller compared with the levels of intermediate energy. The Nd II lines are weakened compared with the LTE case and NLTE abundance corrections range from 1.07 dex to 1.42 dex for different lines. The Nd III lines are strengthened compared with the LTE case and have approximately the same values as for the homogeneous Nd abundance distribution.

2.4. *Influence of uncertainties of atomic parameters on the final results*

A first test concerns photoionization cross-sections for the Nd II levels since kinetic equilibrium of Nd II depends strongly on radiative b-f transitions. Test NLTE calculations have been made for the stratified Nd abundance distribution by multiplying photoionization cross-sections of the Nd II levels by scaling factors of 100 and 0.01. In the first case the overionization on Nd II is amplified and $\Delta_{\rm NLTE}$ increases by 0.09 dex - 0.14 dex for different Nd II lines. For the Nd III lines $\Delta_{\rm NLTE}$ increases by only 0.02 dex. Reducing photoionization cross-sections by 100 times has much larger effect: $\Delta_{\rm NLTE}$ decreases by 0.36 dex to 0.65 dex for different Nd II lines and by 0.10 dex to 0.14 dex in absolute value for the Nd III lines. However, we emphasize that even with such low photoionization cross-sections the ionization equilibrium Nd II/Nd III deviates significantly from thermodynamical value and a difference of neodymium abundances deduced from the Nd II and Nd III lines is reduced by about 1 dex if NLTE effects are taken into account.

For the homogeneous Nd abundance distribution NLTE calculations performed with increasing collision excitation cross-sections by a factor of 10 have show a small effect for the Nd II lines ($\Delta_{\rm NLTE}$ have reduced by 0.02 dex to 0.05 dex) and a slightly larger one for the Nd III lines, at the level of 0.1 dex of $\Delta_{\rm NLTE}$.

Table 1. Theoretical NLTE and LTE and observed equivalent widths (in mÅ) of the Nd II and Nd III lines for γ Equ. Computations were made for two cases: [Nd/Fe] = 3 everywhere in atmosphere (columns "[Nd/Fe] = 3") and enhanced Nd abundance with [Nd/Fe] = 4 in atmospheric layers outside log $\tau_{5000} = -3.6$ (columns "layer"). i and j are level numbers according to the model atom.

λ, Å	$E_{\rm low}$, eV	log gf	$i - j$	[Nd/Fe] = 3			layer			$W_{\rm obs}$
				$W_{\rm LTE}$	$W_{\rm NLTE}$	$\Delta_{\rm NLTE}$	$W_{\rm LTE}$	$W_{\rm NLTE}$	$\Delta_{\rm NLTE}$	
Nd II										
4706.54	0.00	-0.88	1 - 101	92	92	0.00	90	41	1.30	40
4811.34	0.06	-1.01	2 - 101	86	86	0.00	85	32	1.42	30
4061.08	0.47	0.55	7 - 122	127	128	-0.03	109	77	1.05	73
5319.82	0.55	-0.21	8 - 105	105	110	-0.12	103	53	1.31	47
5533.82	0.56	-1.23	8 - 104	67	67	0.00	63	12	1.39	9
5077.15	0.82	-1.04	12 - 114	62	62	-0.01	55	12	1.07	7
5399.09	0.93	-1.41	14 - 114	44	42	0.03	32	5	0.97	6
5033.51	1.14	-0.47	20 - 123	74	77	-0.07	69	22	1.05	24
6650.52	1.95	-0.17	75 - 129	66	71	-0.09	59	15	1.07	25
Nd III										
5294.10	0.00	-0.70	248 - 263	105	124	-0.42	106	127	-0.51	143
6550.23	0.00	-1.50	248 - 257	77	99	-0.40	86	112	-0.48	120
4796.49	0.14	-1.66	249 - 270	57	69	-0.27	53	70	-0.37	83
5633.55	0.14	-2.19	249 - 263	34	48	-0.26	31	55	-0.43	67
6327.26	0.14	-1.42	249 - 260	74	94	-0.37	81	104	-0.42	123
6145.07	0.30	-1.34	250 - 263	74	94	-0.36	78	99	-0.40	
5987.68	0.46	-1.27	251 - 266	67	87	-0.37	70	91	-0.38	108
6690.83	0.46	-2.36	251 - 263	20	32	-0.27	17	38	-0.46	53
5677.18	0.63	-1.43	252 - 271	54	68	-0.26	49	64	-0.27	90
5845.02	0.63	-1.18	252 - 270	63	82	-0.35	64	82	-0.33	110

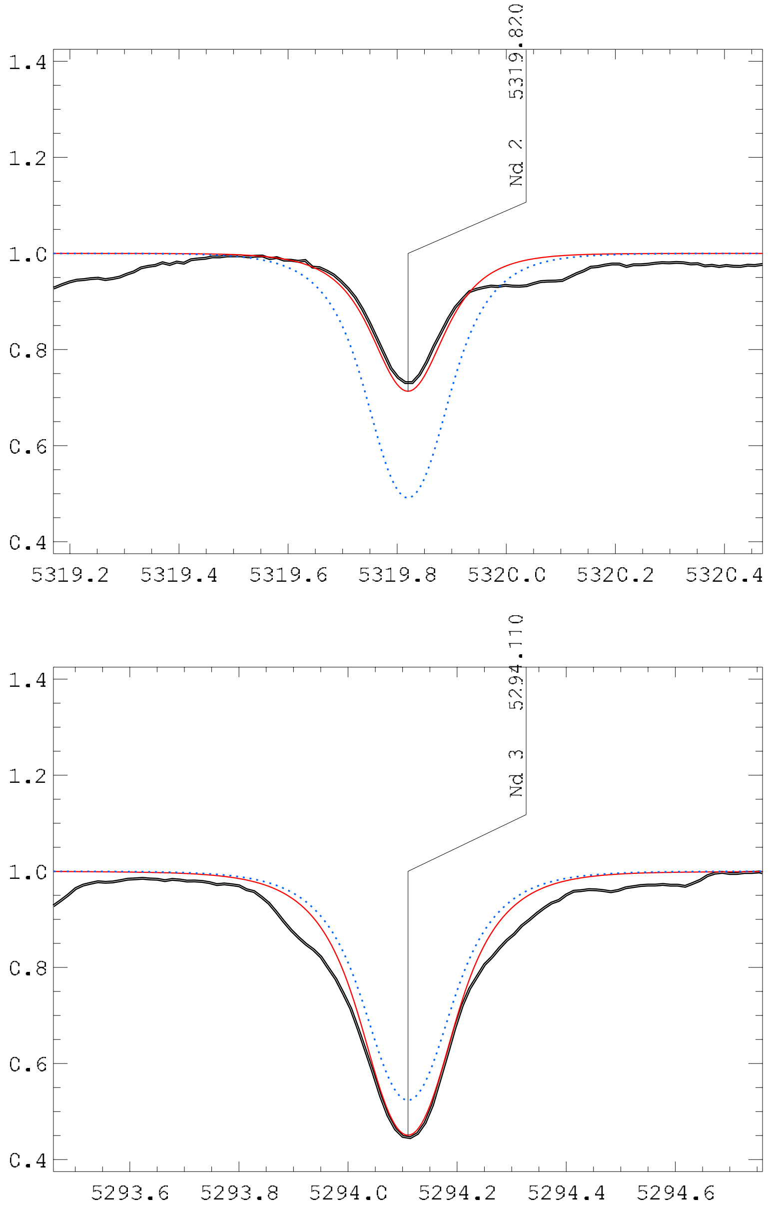

Figure 4. A comparison between the observed (double line) and theoretical NLTE (solid line) and LTE (dotted line) Nd II λ5319 (left panel) and Nd III λ5294 (right panel) line profiles calculated with the stratified Nd abundance distribution from Fig. 3.

3. Nd abundance distribution in the atmospheres of the roAp stars γ Equ and HD 24712

Ryabchikova *et al.* (2002) performed a stratification LTE analysis of Nd in the atmosphere of roAp star γ Equ and concluded that Nd should be concentrated above $\log \tau_{5000} = -8$ to fit the observed lines of Nd II–Nd III. This result was qualitatively consistent with the observed distribution of pulsational radial velocity (RV) amplitudes observed in spectral lines of different elements/ions. However, even with stratified Nd abundances the fit of line profiles was not good in many cases. New NLTE calculations were made of the Nd lines in γ Equ and in another roAp star HD 24712 (Sachkov *et al.* 2005). Equivalent widths in γ Equ were measured in the spectra described in Sachkov *et al.* (2004) and in Kochuknov *et al.* (2004) and are given in the last column of Table 1. Fig. 4 shows a comparison between the observed and synthetic NLTE and LTE line profiles for chosen Nd II and Nd III lines calculated with the Nd abundance distribution from Fig. 3.

The results of Table 1 and Fig. 4 demonstrate a fairly good agreement between observations and calculations and provide strong evidence for Nd concentrations above $\log\tau_{5000} = -3$. This new Nd abundance distribution is more realistic than Ryabchikova *et al.* (2001) with LTE. Curiously, we also get good agreement both in equivalent widths and in line profile fit for another roAp star, HD 24712, using the same Nd abundance distribution, although this star is cooler than γ Equ (Sachkov *et al.* 2005).

Line formation depths were calculated and applied to the pulsational analysis of γ Equ atmosphere (Kochukhov 2005).

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Discussion

G. Mathys: Have you taken the hyperfine structure into account in your determinations of abundance of Nd? It is definitely seen as a difference between the separation of the σ_{b^-} and π^- components, on the one hand, and of the σ_{r^-} and π^- components, on the other hand, in strongly magnetic Ap stars with magnetically resolved lines.

T. Ryabchikova: No, we have not. According to the laboratory analysis by Dolk *et al.* (2002, A&A 385, 111) the hyperfine structure of the two odd Nd isotopes, which represented 20% of the total terrestrial abundance, generally is not observable. Isotopic shifts are also small The heaviest ^{150}Nd isotope is only responsible for $\approx$ 6% of the terrestrial mixture. The observed asymmetry you have mentioned may be caused by line blending. The Nd III λ6145 line which you mean, I believe, is blended with weak Si I and Ca II lines. Both elements may be stratified, which increases the blending.

C. Cowley: Are there some cases (stars) where the Nd II and Nd III LTE abundances do agree? And if so, does this mean that if we do the calculations for them in NLTE that the Nd II and Nd III will no longer agree?

T. Ryabchikova: There are some cases where Nd II and Nd III seem to provide consistent results (mainly for effective temperatures above 8000 K), but the errors in the abundance determinations from Nd II lines are rather large, up to 0.5 dex, and may be of the order of NLTE effects.

N. Piskunov: Do you expect that the application of NLTE spectral synthesis to other rare-earth elements would bring down their formation depth as it did for Nd?

Ryabchikova: Yes, we expect it.