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Segregation of isotopes of heavy metals due to light-induced drift: results and problems

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Abstract. Atutov and Shalagin (1988) proposed light-induced drift (LID) as a physically well understandable mechanism to explain the formation of isotopic anomalies observed in CP stars. We have generalized the theory of LID and applied it to diffusion of heavy elements and their isotopes in quiescent atmospheres of CP stars. Diffusional segregation of isotopes of chemical elements is described by the equations of continuity and diffusion velocity. Computations of evolutionary sequences for the abundances of mercury isotopes in several model atmospheres have been made, using the Fortran 90 program SMART composed by the authors. Results confirm predominant role of LID in separation of isotopes.

Key words: processes: diffusion – stars: atmospheres – stars: chemically peculiar

1. Introduction

About two decades ago Atutov and Shalagin (1988), Nasyrov and Shalagin (1993) proposed light-induced drift (LID) as an effective physical mechanism for diffusional separation of isotopes of chemical elements in the atmospheres of CP stars. Thereafter in earlier papers (Sapar, Aret 1995; Aret, Sapar 2002; Sapar *et al.*, 2005) we investigated some general features of the LID phenomenon in the atmospheres of CP stars. We assumed that the initial abundance of the relevant chemical element and its isotopes is constant throughout the atmosphere, and that the isotope mixture corresponds to the solar (or terrestrial) one. Starting from corresponding initial and boundary conditions and using our computer code SMART (Sapar, Poolamäe, 2003; Sapar *et al.*, 2007), we have studied the evolutionary abundance changes of mercury and its isotopes due to gravity, radiative acceleration and LID.

LID appears due to asymmetry of radiative flux in spectral lines. It can be described as acceleration a_{LID} additional to usual radiative acceleration a_{rad}. The expression for a_{LID} is similar to the formula for a_{rad}, but instead of Voigt function there is its derivative relative to wavelength. The effectiveness of LID depends on the probability that electron stays on the upper level until the next collision (Sapar *et al.*, 2008).

2. Separation of isotopes of heavy metals due to LID

The asymmetry of flux in overlapping isotope lines generates different accelerations of isotopes, yielding their segregation. Isotopic spectral line splitting is similar in most spectral lines and thus the effect of LID is cumulative. LID causes rising of isotope with red-shifted lines and sinking of isotope with blue-shifted lines. For heavy elements the effect of field shift (due to nuclear volume) dominates over the mass shift in the opposite direction. Thus, spectral lines of their heavier isotopes are shifted to longer wavelengths. For heavy metals LID generally causes subsequent sinking of the lighter isotopes and rising of the heavier ones, leaving finally only the heaviest isotope in the atmosphere and its equilibrium abundance is then determined predominantly by the usual radiative acceleration. However, hyperfine splitting of spectral lines of isotopes with odd number of nucleons somewhat complicates the picture of diffusional segregation.

High–precision spectral data and high–resolution model computations are needed to model the LID. We have found that resolution $R = 5\,000\,000$, corresponding to Doppler shift 60 $\mathrm{m\,s^{-1}}$, can be considered as sufficient for the computations. Values of collision cross-sections for atomic particles determine effectiveness of LID and thus they are needed with the highest possible precision. However the data are yet of low accuracy.

The formulae used for LID computations are given in Sapar *et al.* (2008). The diffusion coefficient by Gonzalez *et al.* (1995) was used. The LID efficiency has been computed assuming long-range Coulomb interactions between ions, the hard core impact model for neutrals, and its extension outside the Debye sphere for impacts of ions with neutrals. We specified boundary conditions by using Lagrange 4th order interpolation polynomials for all model layers.

3. Computational software and results

The software used is the Fortran code SMART composed by us for modelling stellar atmospheres and studying different physical processes in them. The codename is acronym of Spectra and Model Atmospheres by Radiative Transfer.

Program SMART enables us to compute plain-parallel and static model stellar atmospheres, and the corresponding emergent spectra of O, B and A spectral classes in the temperature interval from 9000 to about 50 000 K. The lowest value of temperature is due to the circumstance that absorption only by H_2 and H^- molecules is taken into account. Restrictions in modelling are that the atmosphere is chemically homogeneous and LTE holds.

Capabilities of program SMART include: isotopes segregation; getting detailed radiative flux in all layers of stellar atmosphere; iterative correction of initial model; relaxational formation of NLTE in line spectra; accelerations of clumps in stellar wind; computation of detailed spectral limb darkening and hence the spectra of rotating stars and non-irradiated eclipsing binaries.

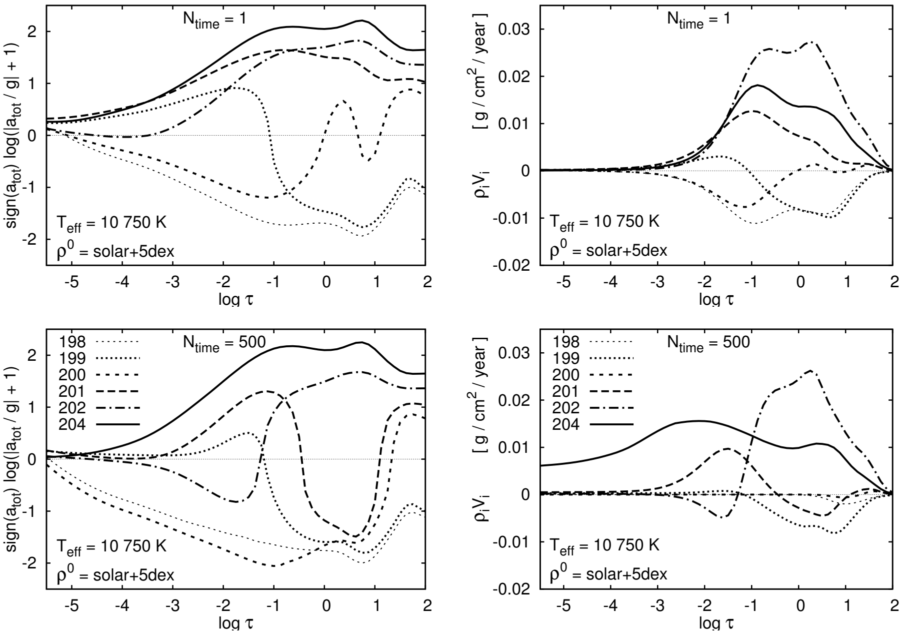

Figure 1. Change of acceleration $a_{\rm tot} = a_{\rm rad} + a_{\rm LID}$ (left column) and of flows of Hg isotopes (right column) from the first to the 500th time-step. The ratio $a_{\rm tot}/g$ is given in a modified logarithmic scale. Note the complicated change of the curves for intermediary isotopes and evolutionary damping of the flows.

SMART is a compact and simple software. Its former FORTRAN 77 code has been essentially improved and rewritten in Fortran 90. Using the code several evolutionary segregation scenarios for mercury isotopes in quiescent atmospheres of CP stars have been computed. Computation of one time step takes approximately 15 min on a PC with CPU 3.2 GHz, 2 GB RAM.

Model atmospheres have been computed with SMART, using sampling for moderate spectral resolution ($R = 30\,000$). Smooth transition from spectral line series to corresponding continua is a special feature of the code. It was achieved by introducing probability functions of continuum depression which are complementary to corresponding existence probabilities of high-excitation (Rydberg) electron states. Spectral line data from Kurucz file ``` ``gfhyperall.dat'' ``` have been used in computations. Spectral line data for Hg have been compiled using different sources and improved by adding isotopic splitting to all Hg lines. The line list used by us contains about 700 resonance and low excitation spectral lines for Hg I, Hg II and Hg III, i.e. for ion species, which are most important for LID.

Formation of evolutionary stratification of Hg isotopes has been computed for a set of three effective temperatures ($T_{\rm eff}$ = 9500 K, 10 750 K, 12 000 K) and three initial Hg abundances (ρ^0 = solar, solar + 3 dex, solar + 5 dex). We assumed homogeneous initial abundance of Hg throughout the atmosphere and solar (terrestrial) ratios of isotope abundances. The possible presence of stellar wind and microturbulence, both reducing or even cancelling the diffusional segregation of isotopes, has been ignored. The longest evolutionary sequence (500 time steps, à 1 year) has been computed for a model atmosphere with parameters $T_{\rm eff}$=10 750 K, $\log g = 4$ and initial Hg abundance solar + 5 dex. Due to much longer free paths in higher atmospheric layers the isotope segregation proceeds there much more rapidly than in the deeper and denser ones. Drastically different diffusion time scales in upper and lower atmospheric layers cause an essential computational problem: time-steps have to be chosen small enough to ensure stability of algorithms in upper layers, but a very large number of time-steps, which is necessary there, makes only small changes in deep layers.

Computed early evolutionary scenarios demonstrated rapid changes in the total acceleration due to LID and presence of relaxational damping of the isotopic flow. The results are illustrated in Fig. 1, where a modified logarithmic scale $\mathrm{sign}(a)\log\left(\left|\frac{a}{g}\right|+1\right)$ has been used for a sign-changing acceleration. The dependence of the evolution of Hg concentration on $T_{\rm eff}$ has been illustrated in the left column of Fig. 2, and the dependence on the initial Hg abundance is illustrated in the right column.

An evolutionary scenario has been computed also for a "pure mercury" case, where lines of all other elements were ignored. This evolutionary scenario has been computed for a model atmosphere with parameters $T_{\rm eff}$ = 10 750 K, $\log g =$ 4 and an initial Hg abundance solar + 3 dex, first ignoring the hyperfine splitting of spectral lines and thereafter taking it into account. The results are illustrated in Fig. 3.

4. Main conclusions and future outlooks

The computed evolutionary sequences of isotope segregation can help to explain the observed unusual or ever enigmatic ratios of isotopes of heavy elements in the atmospheres of CP stars, including their vertical abundance profiles. Radiative acceleration is dominant for a solar abundance of Hg. The role of LID increases with the increase of Hg abundance and it becomes dominant throughout the atmosphere at Hg abundance about solar + 5 dex. Separation of isotopes starts in the outer rarefied layers and then extends into the deeper layers. The process proceeds much slower at higher $T_{\rm eff}$ values and higher Hg abundances. Lighter isotopes with even number of nucleons sink rapidly. Hyperfine splitting of spectral lines of isotopes with an odd number of nucleons decelerates and weakens the segregation of isotopes. It also causes mixing of the order of isotope spectral lines and thus makes the picture of evolutionary isotope segregation

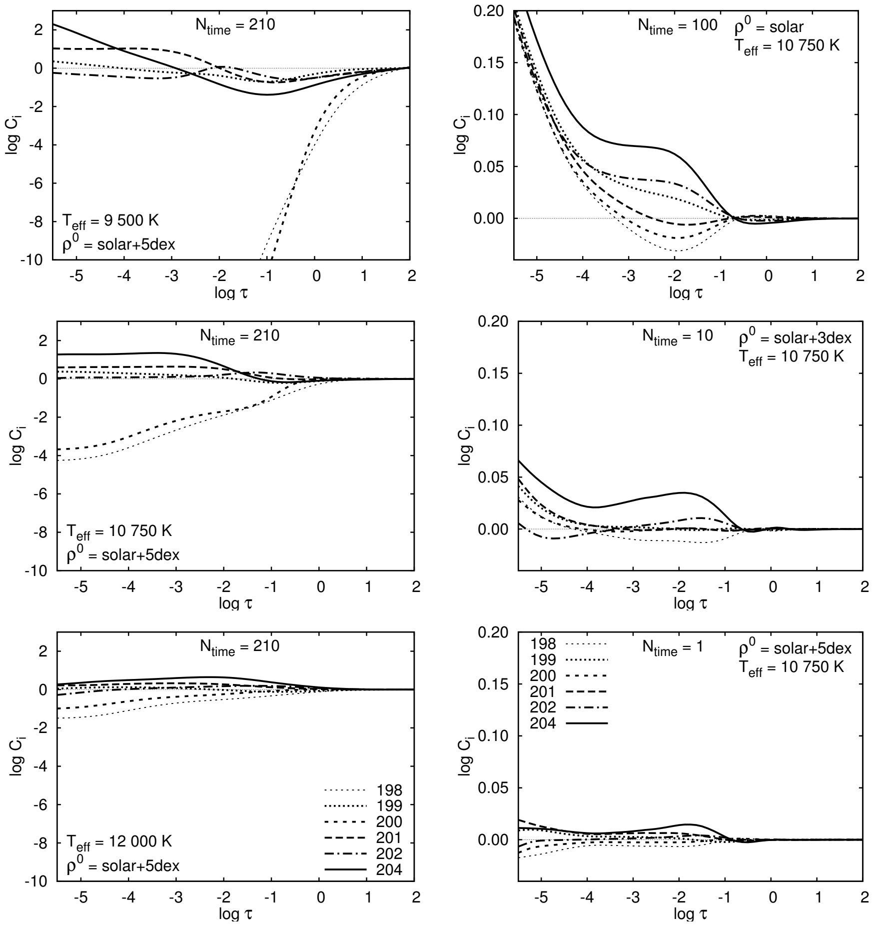

Figure 2. Evolutionary changes of Hg isotope concentrations relative to their initial values in a logarithmic scale. Left column: $T_{\rm eff}$ dependence (time=210 yr); right column: initial Hg abundance dependence (time=1 yr). Note the essential slowing of the segregation at higher $T_{\rm eff}$ and Hg abundance values.

more complicated. The overlapping isotopic spectral line profiles are sensitive to isotope abundance throughout the whole atmosphere.

Several improvements are required to obtain more realistic evolutionary scenarios. More complete and accurate data of spectral line strengths and their damping constants, more exact cross–sections for impact processes and the physically more adequate initial and boundary conditions are needed. Physically adequate inner boundary conditions can be specified only if deeper layers of stellar envelope are included in modelling. More realistic time scales can be obtained

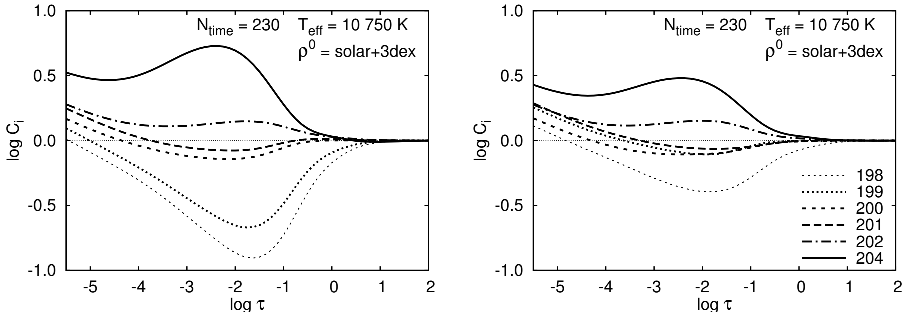

Figure 3. Evolutionary changes of "pure mercury" concentrations without hyperfine splitting give the uncrossed curves in the order of isotope masses (left panel), and with hyperfine splitting give slower diffusion and intersecting curves for intermediate isotopes (right panel).

by including the processes which hinder the diffusion (turbulence, stellar wind). Currently obtained diffusion time scales demonstrate only the maximal values for isotope segregation rates in absolutely quiet stellar atmospheres.

There are several possibilities to continue the studies of evolutionary segregation of isotopes of heavy elements. The simplest way is to compute longer evolutionary sequences for mercury. There are also no essential problems to include stellar wind into evolutionary computations (formulae are given in Sapar *et al.*, 2008). A complicated problem is to find the physically correct diffusion coefficient due to microturbulence. Serious problems are to elaborate new and more stable algorithms, enabling us to integrate over longer time steps and to find the final distribution of isotopes without evolutionary computations.

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