COMPARING MAIN SPECTROSCOPIC DATABASES

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Abstract: This article deals with comparing of data in the main world spectroscopic databases NIST and Kurucz. Our target was to calculate differences in the ratio of Stark broadening and function F which depends on electron density, temperature and pressure. Stark broadening is one of pressure broadenings of spectral lines which arise from the collisions of the emitters with neighboring particles. Stark broadening is due to charged perturbers. We developed the program NKrov for the comparison of databases with the help of regular expressions and the program awk. There were some differences found in input data for the silicon between NIST and Kurucz databases. Our results can be used in further research on silicon spectral lines.

Keywords: Stark broadening, NIST database, Kurucz database, unit system, regular expressions.

1 INTRODUCTION

Silicon is widely used material mainly in the semiconductor technology and this is the reason why there is an intensive research of silicon properties. A fundamental part of this research belongs to spectroscopic data which can be obtained for our research from main world databases. We can mention NIST [1] and Kurucz [2] databases which are the sources of our data. We calculated Stark broadening and shift of spectral lines of silicon in this article. We used above mentioned databases and examined the influence of differences in these databases to final Stark broadening of spectral lines. We developed the program NKrov. Our program examines data, transfers them to a comparable format and prepares the table of differences in the output file. The output of the program is a graph of Stark broadening of spectral lines dependent on temperature for both databases NIST and Kurucz.

2 OBSERVED QUANTITIES IN DATABASES

Comparison of quantities in databases could cause difficulties, which could arise from the unit system used in that databases. For example permeability of vacuum μ_0 has the value of $4\pi \times 10^{-7}$ and the dimension $\mathrm{H{\cdot}m^{-1}}$ in the system SI, for calculations according to Heaviside–Lorentz μ_0 is dimesionless and has the value of 1. Often used unit system (so called atomic) units includes fundamental constants chosen in the way to have the value of 1, [3]:

$$\hbar = m_e = e = 4\pi\varepsilon_0 = 1. \tag{1}$$

The central field approximation is used for multielectron atoms, we consider all electrons in the subshell as equivalent. These electrons have the same main quantum number. Every energy level according to the electron configuration is described not only by this electron configuration but also by the term which depends on the total angular momentum, including electron's spin. The spin–orbital interaction in the multielectron atom is described by the interaction between the spin vector $\vec{s}$ and the orbital angular momentum vector $\vec{l}$:

$$\vec{l_1} + \vec{l_2} + \vec{l_3} + \cdots = \vec{L}, \tag{2}$$

$$\vec{s_1} + \vec{s_2} + \vec{s_3} + \cdots = \vec{S}. \tag{3}$$

The interaction between $\vec{L}$ and $\vec{S}$ is known as Russell–Saunders interaction abbreviated as the spin–orbital L–S bond where the states of the atom are described as

$$^{2S+1}L_J, \tag{4}$$

where S is the total spin quantum number, $2S+1$ is the spin multiplicity, L is the orbital angular momentum number and J is the total angular momentum quantum number. The bond scheme of the L–S approximation is used until atomic number 30, after that spin–orbital bonds start to interact and the another bond scheme called j-j coupling must be used [4]. We observed and calculated these quantities in databases NIST and Kurucz for silicon:

Database			
NIST		Kurucz	
Quantity	Dimension	Quantity	Dimension
Ritz wavelength V_{ac}	nm	Wavelength λ	nm
Einstein coefficient A_{ki}	s^{-1}	calculated	s^{-1}
Oscillator strength f_{ik}	Dimensionless [5]	calculated	Dimensionless
Strength of line S	a.u.	calculated	a.u.
First energetic level E_i	cm^{-1}	First energetic level E_i	cm^{-1}
Second energetic level E_k	cm^{-1}	Second energetic level E_k	cm^{-1}
Statistical weight g_i	Dimensionless	calculated	Dimensionless
Statistical weight g_k	Dimensionless	calculated	Dimensionless
Total ang. momentum J_i	Dimensionless	Total ang. momentum J_i	Dimensionless
Total ang. momentum J_k	Dimensionless	Total ang. momentum J_k	Dimensionless

Table 1: Observed quantities in NIST and Kurucz databases.

3 USE OF DATABASES TO DETERMINE SOME PROPERTIES OF SPECTRAL LINES

There can be various types of displayed spectra, we recognize emission or absorption spectra. Stark broadening for element silicon is calculated from databases with our program NKrov. Energetic level splitting due to electric field is an important phenomenon which occurs in small scale semiconductor structures controlled by electric field. Utilization of these circuits in electrical engineering is one of the reasons of scientific research. Stark broadening and shift could be calculated from semiempirical formulas [6]:

$$\delta_S = F(T,p)\left[\sum_{J''}\frac{S\left(J'',J\right)}{2J+1}g_{se}\left(X_{J''J}\right)+\sum_{J''}\frac{S\left(J'',J'\right)}{2J'+1}g_{se}\left(X_{J''J'}\right)\right] \tag{5}$$

$$d_S = F(T,p)\left(\sum_{J''}\frac{\Delta E_{J''J}}{|\Delta E_{J''J}|}\frac{S\left(J'',J\right)}{2J+1}g_{sh}\left(X_{J''J}\right)-\sum_{J''}\frac{\Delta E_{J''J'}}{|\Delta E_{J''J'}|}\frac{S\left(J'',J'\right)}{2J'+1}g_{sh}\left(X_{J''J'}\right)\right), \tag{6}$$

where F is defined as:

$$F(T,p) = 16\left(\frac{\pi}{3}\right)^{2/3} cR_\infty a_0^3 N_e \left(\frac{hcR_\infty}{k_B T}\right)^{1/2}, \tag{7}$$

where the Rydberg constant $R_\infty = 109737.3\,cm^{-1}$, c is the speed of light, N_e is the electron density, a_0 is the Bohr radius, h is the Planck constant, k_B is the Boltzmann constant, g_{se} and g_{sh} are correction Kramers–Gaunt factors, $S\left(J'',J^*\right)$ is the line strength of transition between states with quantum

numbers J'', J^*: $J'' \rightarrow J^*$, J'' is the quantum number for energy level $E_{J''}$, J^* = J or J' are the quantum numbers for energy levels E_J or $E_{J'}$. The line strength S is available in NIST database, but for Kurucz it has to be calculated:

$$S_{J''J^*} = 3\left(2J'' + 1\right) f_{J''J^*} \lambda R_\infty \tag{8}$$

J'', J^* are quantum numbers of total momentum of atom, λ is the wavelength and $f_{J'''J^*}$ is the oscillator strength,

$$X_{J''J^*} = \frac{3k_B T}{2|\Delta E_{J''J^*}|}, \tag{9}$$

where $\Delta E_{J''J} = E_{J''} - E_J$. Stark broadening and shift depend on temperature. There could be calculated linear coefficients a,b resp. A,B for temperature dependence of width resp. shift of spectral line.

4 DESCRIPTION OF THE PROGRAM NKROV

We developed the program NKrov, which processes various data formats available in NIST and Kurucz databases. List of quantities used in the program is in table 1. Due to differences of data in databases it is necessary to calculate some quantities from other in the database. The problem with equivalence of dimensions was mentioned in the previous part of this article. The block diagram of the program NKrov, see fig. 1.

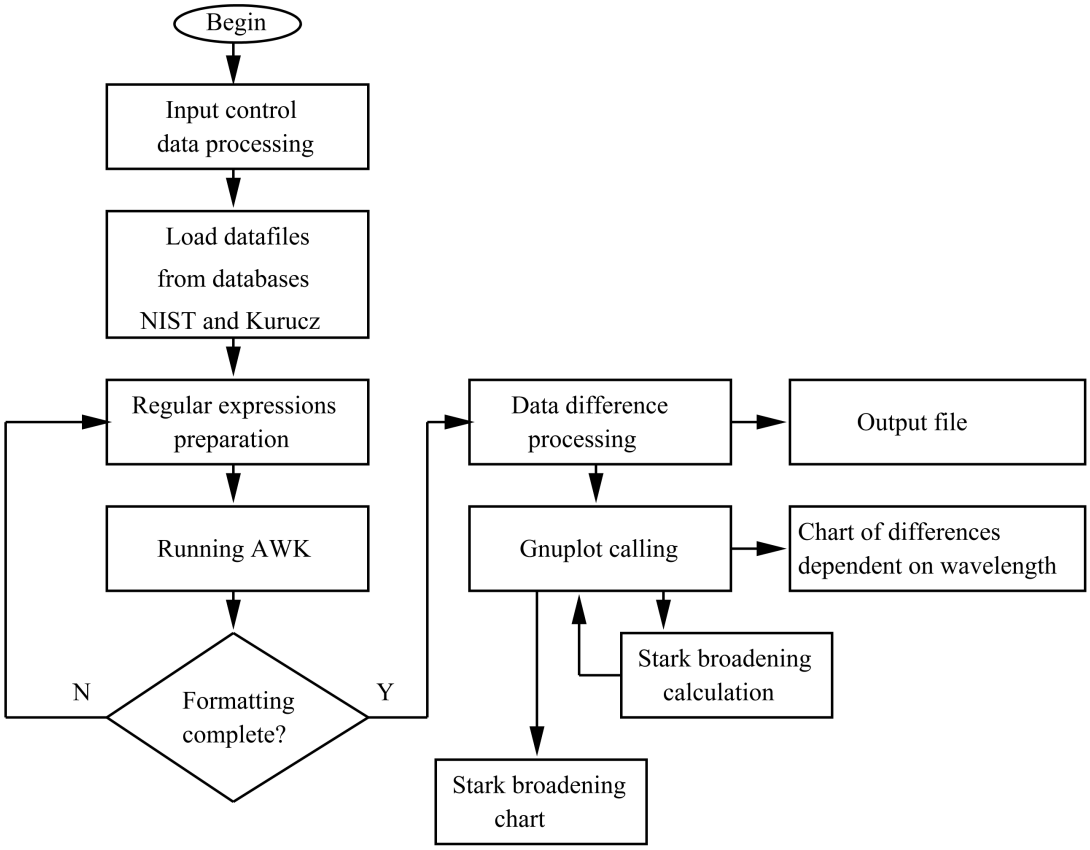

Figure 1: Program NKrov – block diagram.

After execution the program asks for input control data, path to files, wavelength range, degree of ionization and so on. The format of the datafile is transformed to unified format thanks to regular expres-

sions. This powerful programmer's tool for text files processing was introduced by american mathematician Stephen Cole Kleene [7]. We used the awk program for merging two quite different formats with rather big data collection, and it proved that it is an effective tool for quick processing of data. The whole task on the common dualcore 3 GHz processor takes almost 3 hours to complete.

After preparing necessary regular expressions the central program calls the standard Unix program awk, which can process large data collections, where common editors fail. Awk output is the data collection, awk is called in cycles until the expecting format is reached. The prepared datafile can now be used by the central program, which calculates mutual differences of input data from NIST and Kurucz databases, creates output textfile and automatically prints results in graphs with calling the Gnuplot program. The program Gnuplot is the free software and produces the graphical output. Gnuplot can be used and shared under GPL licence and is very often connected to LaTeXsystem for producing documents. The central program calls the graphical output Gnuplot with data for fig. 2, which compares data differences in databases for the input quantity – oscillator strength f_{ik} dependent on wavelength.

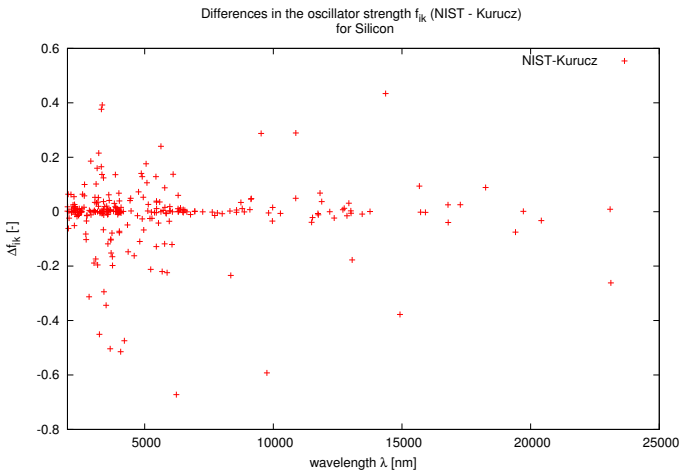

Figure 2: Differences in the oscillator strengths f_{ik} (NIST – Kurucz) for Silicon.

NKrov takes the input files and calculates Stark broadening of spectral lines for each of the databases NIST, Kurucz, and calls Gnuplot for producing the graphical output. The output of the NKrov program, which we developed, is then the graph of the ratio of Stark broadening and the $F(T,p)$ function dependent on temperature, fig. 3.

5 ACHIEVED RESULTS IN COMPARISON NIST AND KURUCZ DATABASES

In the above mentioned databases we chose silicon atom in 2000 to 25000 nm wavelength range. The ratio of Stark broadening and $F(T,p)$ function was calculated in 5000 to 50000 K temperature range. Fig. 2 compares input quantity oscillator strengths f_{ik} shows, that the best correspondence between NIST and Kurucz was till the wavelength of 10000 nm, although even here were significant differences. In fig. 2 in the wavelength range till 10000 nm the absolute value of maximum difference equals to 0.6. We obtain from the databases for this difference these parameters: the wavelength λ=6231.1 nm has for NIST oscillator strength f_{ik}=1.28 and for Kurucz f_{ik}=0.61. This means more than 50% difference. These differences influence, according to equations (5) and (8), the overall difference in Stark broadening of spectral lines, in fig. 3. Our results can be a good base for future research work, graphs describe some difficulties in accuracy of Stark broadening for silicon.

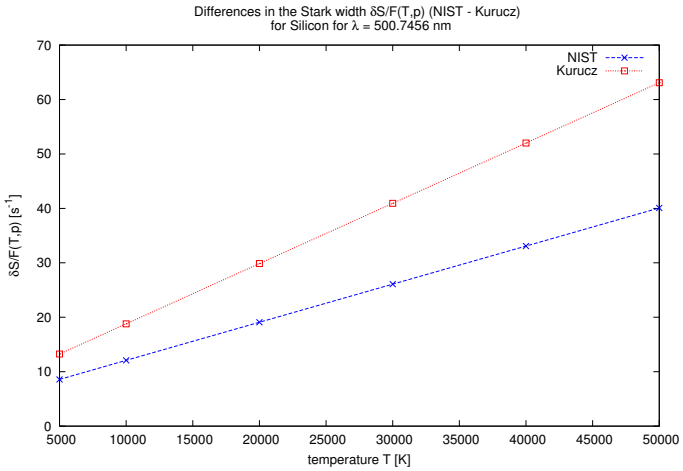

Figure 3: Differences in the Stark width $\delta S/F\,(T,p)$ (NIST – Kurucz) for Silicon.

6 CONCLUSION

The NKrov – program we introduced was designed to make the research work on silicon easier. The NKrov main feature lies in the capability to compare different formats in the main world databases (NIST and Kurucz). The program and it's utilities produce the graphical output of differences both on the input quantities and the output Stark broadening of spectral lines. It could be seen from the graphs, that some small part of spectroscopic data has non negligible differences, which should be the target of future scientific research.

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