

# SILICON IN SPECTROSCOPIC DATA OF WORLD DATABASES

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**Abstract.** This article deals with comparison of three world spectroscopic databases: NIST, Kurucz and Atomic Line List. Our target was to calculate the differences in input data and 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 to be able to compare data in databases. There were some differences in the database format and content. Our results could be used in science and technology.

**Keywords:** NIST database, Kurucz database, ALL database, Stark broadening.

## 1. Introduction

Some spectroscopic data could be found in several world databases. These data could be used in science and technology. The foundation of the semiconductor production is silicon, which atomic properties are under intensive research. We use the plasma and the lithography techniques such as EUV (Extreme Ultraviolet Lithography) in order to achieve the new horizons in the semiconductor design. The world leader IBM developed 5 nm semiconductor GaaFET structure as the first company in the world [1]. As the size of structures decreases then the importance of precise input physical quantities increases.

The introduced article compares selected spectroscopic quantities for silicon from three free-access world databases. We developed the program NKrov to compare various formats of the spectroscopic data. We produced the graphic output from the program to be able to observe how input data differences affect the results.

## 2. Database structure elements

Selected free-access spectroscopic databases comprise from various data structures and formats. This was the reason we chose for comparison these mutually similar databases: NIST [2], Kurucz [3], Atomic Line List (ALL) [4]. There is a problem that some of the databases do not offer whole data to be downloaded as e.g. txt file, but the data are fragmented to a number of webpages and must be downloaded individually. The ALL database has data fragmented this way.

You have to be careful about spectroscopic data units. For example vacuum permeability in various unit systems:

$$\mu_0 = \begin{cases} 4\pi \times 10^{-7} \text{N/A}^2, \text{ SI} \\ 4\pi, \text{ Gaussian} \\ 1, \text{ H - L.} \end{cases}$$

If the quantum properties of the objects are included in the database, then we can use Planck units. It is an advantage when there is clearly stated which methodology was used and what approximations were done [5].

When you choose mutually similar data from these databases you have to consider what is the surroundings, because the same electro-magnetic wave in the vacuum will have another wavelength in the air:

$$\lambda_{\text{vac}} = n \cdot \lambda_{\text{air}},$$

where  $\lambda_{\text{vac}}$  and  $\lambda_{\text{air}}$  are wavelengths in the vacuum and in the air,  $n$  is the refractive index, which empirical values are discussed by Edlen [6]:

$$(n - 1)_s \times 10^8 = 8342.13 + 2406030 (130 - \sigma^2)^{-1} + 15997 (38.9 - \sigma^2)^{-1},$$

where  $\sigma$  is the vacuum wave-number in  $\mu\text{m}^{-1}$ ,  $s$  means validity of the equation for "standard air" (i.e., 15°C, 101 325 Pa pressure, with 0.033% CO<sub>2</sub>).

For example for further mentioned wavelength  $\lambda_{\text{vac}} = 562.4 \text{ nm}$  in vacuum we get:

$$\sigma = 1/\lambda_{\text{vac}} = 1/0.5624 \mu\text{m}^{-1} = 1.778 \mu\text{m}^{-1}$$

$$(n - 1)_s \times 10^8 = 8342.13 + 2406030 (130 - 1.778^2)^{-1} + 15997 (38.9 - 1.778^2)^{-1},$$

$$n = 1.000278$$

$$\lambda_{\text{air}} = \lambda_{\text{vac}}/n = 0.5624/1.000278 \mu\text{m}$$

$$\lambda_{\text{air}} = 0.5622 \mu\text{m}$$

There is a problem that not all of the databases clearly states what conditions there were during wavelength measurement.

The multi-electron atoms are usually modelled with the central field approximation, which states that all electrons in the subshell are equivalent. Every energetic level depends on the electron configuration and term which describes also spins of electrons.

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  $\vec{l}$ :

$$\vec{l}_1 + \vec{l}_2 + \vec{l}_3 + \dots = \vec{L},$$

$$\vec{s}_1 + \vec{s}_2 + \vec{s}_3 + \dots = \vec{S}.$$

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 with terms in databases

$$^{2S+1}L_J,$$

or with main quantum number:

$$n^{2S+1}L_J,$$

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.

When distinguishing between states with the same  $L$  and  $S$  quantum numbers then the senior number  $\tau$  is used. For central field approximation is necessary to select coupling scheme, for silicon and other elements until atomic number 30 is used the Russell-Saunders bond scheme. Summary of notations used for describing structural entities in databases for L-S bond is in the tab. 1.

### 3. Database data for some spectral lines properties calculation

There are two main types of spectra: the absorption or the emission spectra. The spectral line structures could be divided according to energy ranges. The greatest energy ranges belong to the gross structures with energies between 1 to 10 eV. The fine structures with relativistic corrections belongs to  $10^{-4}$  to  $10^{-5}$  eV. The smallest structures are the hyperfine structures, where the spin of the atomic core plays it's role, these structures belong to  $10^{-7}$  to  $10^{-8}$  eV [8].

The influence of differences in data to the Stark broadening will be shown in our program NKrov. We can calculate the Stark broadening and shift with this semiempirical formulas [9]:

$$\delta_S = F(T, p)(P + Q), \quad (1)$$

where

$$P = \sum_{J''} \frac{\Re(J'', J)}{2J + 1} g_{se}(X_{J'' J}), \quad (2)$$

$$Q = \sum_{J''} \frac{\Re(J'', J')}{2J' + 1} g_{se}(X_{J'' J'}) \quad (3)$$

and function  $F$  is defined:

$$F(T, p) = 16 \left(\frac{\pi}{3}\right)^{2/3} c R_\infty a_0^3 N_e(p) \left(\frac{hcR_\infty}{k_B T}\right)^{1/2}, \quad (4)$$

where

$$X_{J'' J^*} = \frac{3k_B T}{2|\Delta E_{J'' J^*}|}, \quad (5)$$

where  $\Re(J'', J^*)$  is the line strength of transition between states with quantum numbers  $J'', J^*$ :  $J'' \rightarrow J^*$ ,  $J', J''$  are the quantum numbers of total angular momentum for energy levels  $E_{J'}$  and  $E_{J''}$ ,  $g_{se}$  and  $g_{sh}$  is Kramers-Gaunt factors,  $c$  is the speed of light, Rydberg constant  $R_\infty = 109737.3 \text{ cm}^{-1}$ ,  $a_0$  is the Bohr radius, variable  $N_e$  is the electron density,  $h$  is the Planck constant,  $k_B$  is the Boltzmann constant. Stark shift of spectral line:

$$d_S = F(T, p)(M - N), \quad (6)$$

where

$$M = \sum_{J''} \frac{\Delta E_{J'' J}}{|\Delta E_{J'' J}|} \frac{\Re(J'', J)}{2J + 1} g_{sh}(X_{J'' J}), \quad (7)$$

and

$$N = \sum_{J''} \frac{\Delta E_{J'' J'}}{|\Delta E_{J'' J'}|} \frac{\Re(J'', J')}{2J' + 1} g_{sh}(X_{J'' J'}), \quad (8)$$

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. Program NKrov description

We calculated important data from the infrared radiation, we focused from the SWIR (Short Wave Infra Red) up to the LWIR (Long Wave Infra Red) range, concretely from  $2 \mu\text{m}$  up to  $10 \mu\text{m}$ . We developed the program NKrov for the database comparison and the basic spectroscopic calculations. Program processes data from NIST, Kurucz and ALL databases and calculates differences of Stark broadening divided by function  $F(T, p)$ . The differences of the oscillator strength and the line strength are also calculated. We enter file paths to data and configuration files, wavelength range, degree of ionization to program control unit. Program (fig. 1) uses regular expressions, merges various data formats and creates output file of differences. The central program calls Gnuplot utility and produces graphical output of calculated data. There are these output quantities: the oscillator strength (fig. 2), the line strength (fig. 3) and the ratio of Stark broadening and function  $F(T, p)$  in temperature range from 5000 K to 50000 K (fig. 4).

Structural entity	Quantum numbers <sup>a</sup>	Group of all transitions
Configuration	$(n_i l_i)^{N_i}$	Transition array
Polyad	$(n_i l_i)^{N_i} \gamma S_1 L_1 n l$	Supermultiplet
Term	$(n_i l_i)^{N_i} \gamma S L$	Multiplet
Level	$(n_i l_i)^{N_i} \gamma S L J$	Line
State	$(n_i l_i)^{N_i} \gamma S L J M$	Line component

<sup>a</sup>The configuration may include several open subshells, as indicated by  $i$  subscripts. The letter  $\gamma$  represents any additional quantum numbers, such as ancestral terms, necessary to specify a particular term.

Table 1. Atomic structural hierarchy in  $L$ - $S$  coupling [7].

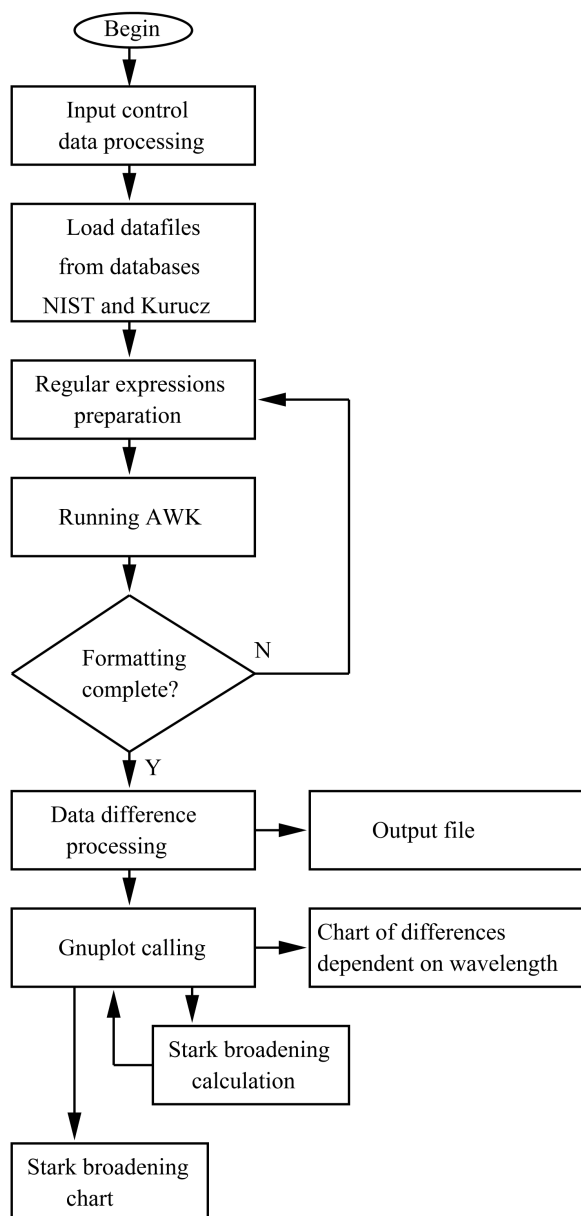


Figure 1. Program NKrov – block diagram.

## 5. Conclusions

The quantities in the basic world databases were inspected with our program NKrov. We targeted sili-

con data in the wavelength range 2000 to 10000 nm. NIST database states the wavelength with variable accuracy 1 to 4 digits after decimal point, Kurucz database uses 4 digits after decimal point accuracy and ALL database uses variable accuracy 1 to 4 digits after decimal point. Various accuracy in wavelength caused decrease in mutual intersection of data in databases and made the comparison more difficult. Even though there were such difficulties we compared data in the whole required range.

The difference in the oscillator strength at the wavelength of 3667.5 nm is largest for NIST–ALL with the value of 0.9. There can be seen in the fig. 2 that mutual differences in NIST–ALL databases are larger until 7000 nm than differences in NIST–Kurucz. In the range of 7000 nm up to 10000 nm the oscillator strengths  $f_{ik}$  are almost the same in all of the databases. In fig. 3 we can see that the largest differences in the line strengths are in the range 2000 to 6000 nm with the extreme 385 a.u. at 3729.021 nm for NIST–ALL. The NKrov output in fig. 4 shows differences in the ratio of Stark width and function  $F(T, p)$  for the silicon in the temperature range 5000 to 50000 K and wavelength of 562.4 nm. NIST data have the largest steepness in the figure. From this figure we can see how the data differences in the databases affect the theoretical calculations of spectral line width.

This article shows some differences in the observed free-access databases. The differences could be caused by the methods of measuring wavelengths, or maybe by corrections in theoretical calculations. Sometimes there is not clearly stated, if the data were measured or calculated. Data in the databases are constantly updated, e.g. in the database HITRAN [10] there were for H<sub>2</sub>O molecule 37432 transitions in 2008 and 142045 transitions in 2015, that means almost four times improved accuracy. This article shows that data unification for silicone is not finalized nowadays, so we have to care about the differences in data for our calculations.

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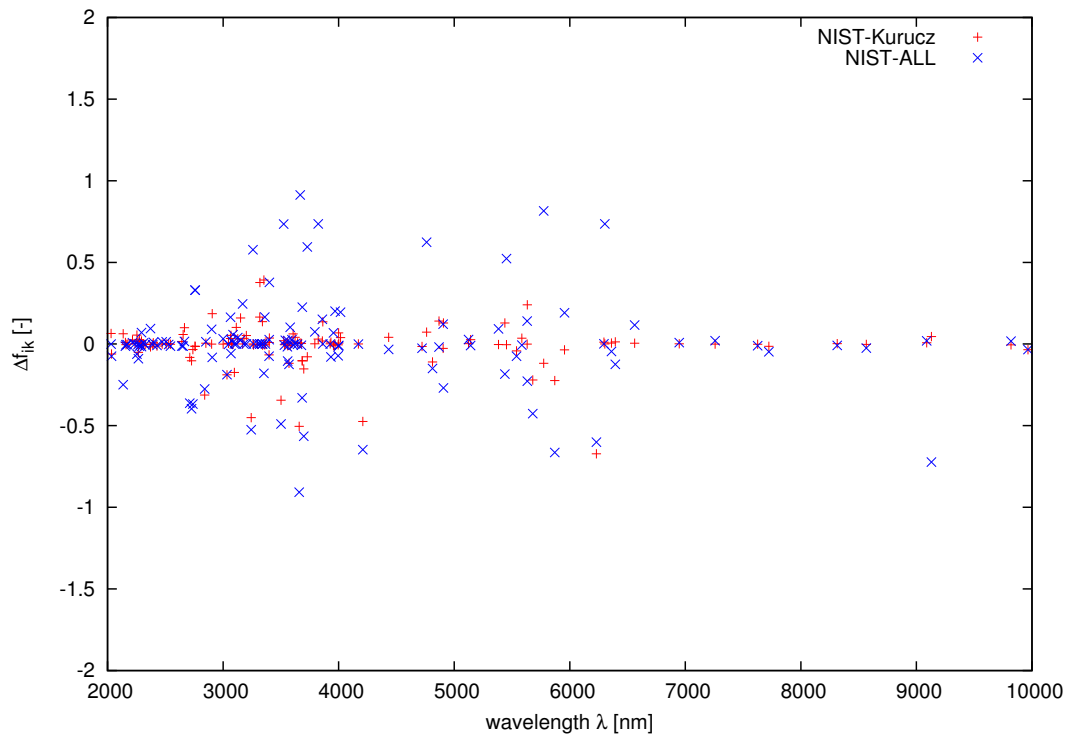


Figure 2. Differences in the oscillator strength  $f_{ik}$  for Silicon (NIST–Kurucz–ALL).

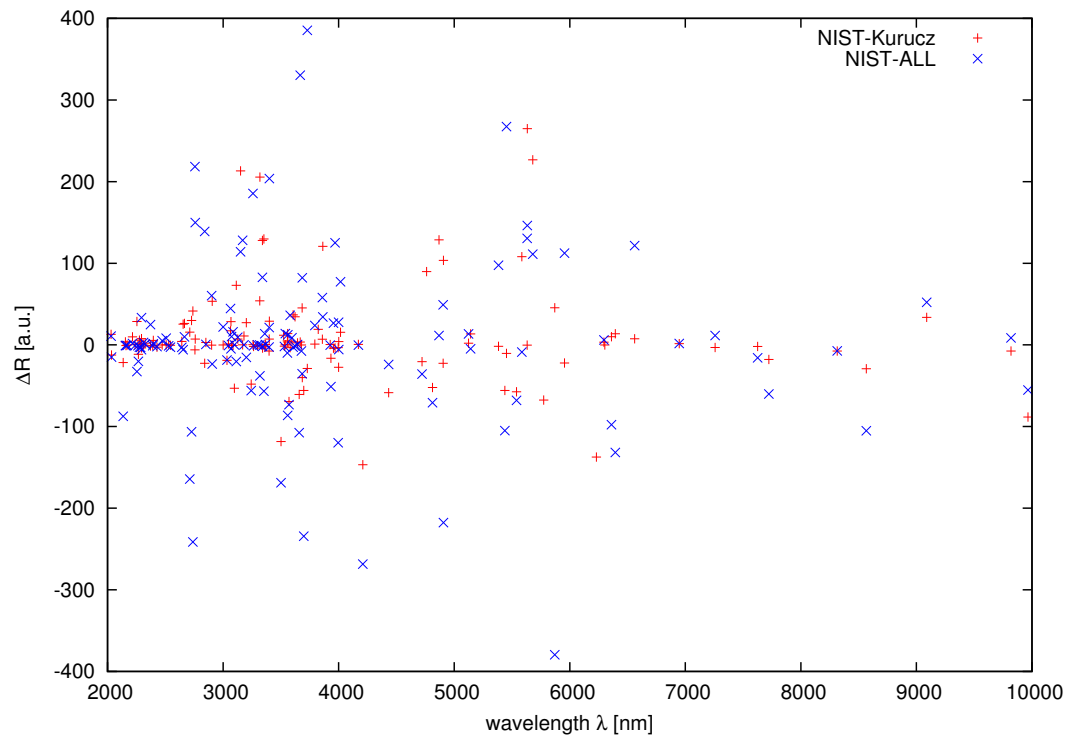


Figure 3. Differences in the line strength  $\mathfrak{R}$  (NIST–Kurucz–ALL) for Silicon.

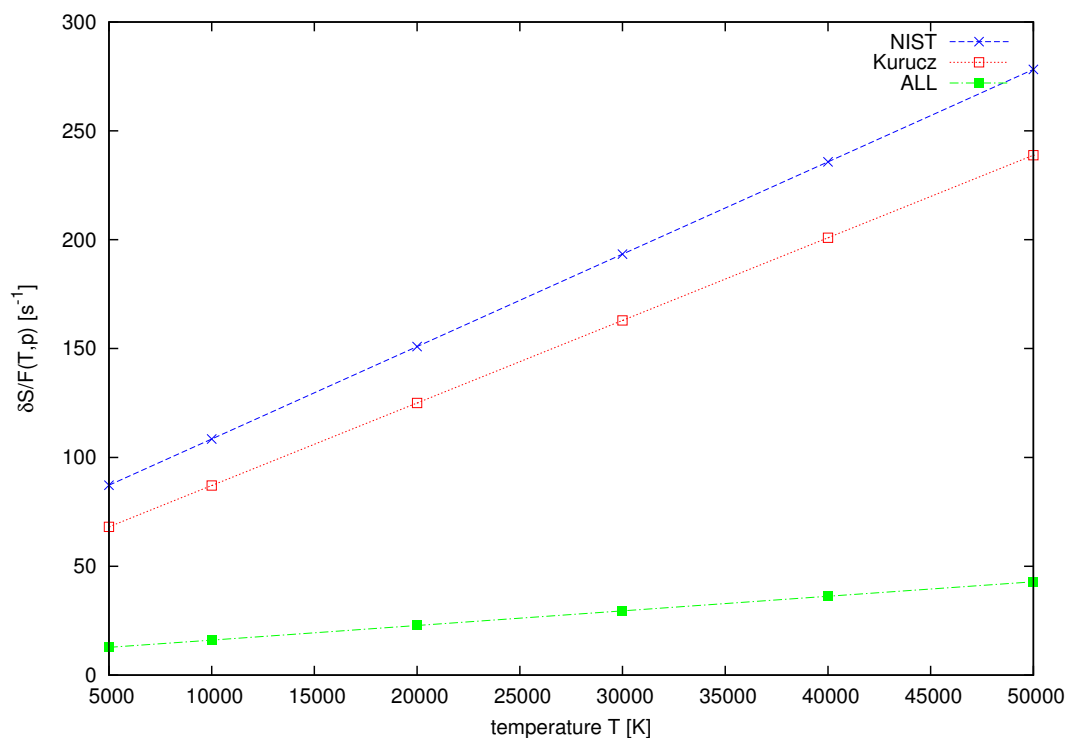


Figure 4. Differences in the Stark width  $\delta S/F(T,p)$  for Silicon (NIST–Kurucz–ALL),  $\lambda = 562.4$  nm.

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