

DETERMINATION OF ELEMENTS THROUGH GEOCHEMICAL LOGGING  
IN CRYSTALLINE ROCKS OF THE KTB-OBERPFALZ HB

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**Abstract**

Measurements of elemental concentrations contribute significantly to enhance interpretation of quantitative estimation of minerals which make up the complexity of crystalline rocks. Through recent developments, the most abundant and a few rare elements in the earth's crust can be determined in counting natural activity, delayed activation and prompt neutron-induced capture gamma rays. Whereas K and Al are obtained directly in weight percent through proper algorithms, a geochemical "closure model" is normally used to derive experimentally Si, Ca, Fe, Ti, S and Gd. This procedure is based on the fact that the rock elemental oxides, measured in weight %, sum up to 100%. Major unmeasured elements like O, C, Mg and Na are compensated in assuming that each element is present as one single oxide or carbonate and in using optimized oxide factors for those measured. The validity of this model, developed originally for sedimentary rocks, has been tested by comparison with data from an X-ray fluorescence analysis (XRF) on cuttings.

On the other hand, the densely spaced XRF data, sampled every 2m on average, made it possible to calculate the amount of oxides which can be measured with this tool string. Although lithology dependent, the sums of these oxides show little variation within each rock, so that their averaged values have been used in conjunction with the true oxide factors in the "KTB model". The agreement between the two models on one side and the XRF data on the other can be considered as very good.

**Introduction**

In the superdeep well of the German Continental Deep Drilling Project (KTB), the open hole section from 6018 to 3000m was recorded with the Geochemical Logging Tool (GLT) of Schlumberger in two sections. The first run took place on October 14, 1991, from 4450m to 3000m, the second on March 14, 1992, from 6007m to 4400m. Due to the large borehole diameter of 14 3/4" with increasing breakouts in the deeper part, the interest was focused on how to minimize and eventually correct these effects.

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The determination of elemental concentrations through logging provides continuous information on geochemistry and ultimately a better knowledge of quantitative mineralogy. It is achieved through an analysis that combines gamma ray intensities from natural activity, prompt thermal neutron capture reactions and delayed activation to obtain elemental concentrations for ten elements. Despite this fact, not all of the elements present in sufficient quantities can be measured when using NaI detectors. In this well, it is the case for such major elements like Na and Mg. Two models are therefore described to relate the concentrations of measured elements to the unmeasured ones.

### **Spectral processing of capture gamma rays**

It is assumed that the downhole capture spectrum can be represented as a linear combination of the spectrum of each individual element, the so called "standards". These standards represent the spectrum of each pure element. The way these coefficients or fractional elemental gamma ray "yields" are determined is through weighted least squares fitting and the results of the total spectral signal shown in Fig. 1.

This total signal is composed of a formation and a borehole signal. In general, information originating from the borehole is difficult to characterize and therefore not used in geochemical analysis. For this reason, yields from hydrogen and background are not used, although they represent roughly 40% of the total spectrum. The capability of eliminating yields which in the case of the KTB borehole do not contribute to the measured gamma ray spectrum and are below the tool's detection limits has been used to exclude chlorine and sulfur. This selective elimination improves the statistical precision of the elements remaining. The renormalized yields are displayed in Fig. 2.

### **Elemental processing**

To perform a comprehensive elemental analysis involves three separate modes of gamma ray spectroscopy. A set of spectrometers has been assembled to measure absolute elemental concentrations in the rocks. This includes a spectrometer for natural activity, one for delayed activation of Al and one for measuring prompt gamma rays following thermal neutron capture. With the present tool string this data is collected through a single run into the hole. At present, NaI-detectors are commonly used, as they can be operated up to 150°C.

### **Natural Spectroscopy: K, Th and U**

The concentrations of these elements are derived from the gamma ray spectrum recorded from naturally occurring radioactive elements and their daughter products. Among those elements only K is relevant for further elemental analysis, since its total is located within the percentage range. The count rates obtained are directly proportional to weight percent of that element in the formation.

### **Delayed Activation: Al**

In Al activation, the natural isotope Al-27 absorbs thermal neutrons and produces the isotope Al-28, which decays with a half-life of 2.24 min, emitting a 1779 keV gamma ray. Interference with other isotopes is reduced to a low level by using a Cf-252 source. During neutron irradiation, the Al radioactivity reaches saturation, at which point the rate of production and decay are in balance. The gamma rays are counted and the Al spectrum is determined by subtracting the natural gamma ray count rate from the detector situated above the source.

The aluminum count rates must be corrected for the complex effects of borehole environments on the neutron and gamma ray physics. Important factors influencing the gamma ray flux are the neutron slowing down length, the formation and borehole absorption cross section, formation density and the borehole size. The environmental correction algorithm taking care of the terms mentioned above, ignores however any varying stand-off between source/detector and borehole wall, which can be observed in break-out zones below 5000m.

Such a zone is depicted in Fig. 3, where the pronounced reduction in Al-measurement is due to stand-off.

### **Pulsed neutron-induced capture: Si, Ca, Fe, Ti, S and Gd**

The detectable gamma ray flux for each element is proportional to the product of its concentration and its thermal neutron capture cross section. Therefore an element which does not produce enough gamma rays or has a very low neutron capture cross section cannot be detected. For the two dominant rocks in this well, their respective sensitivity products (s.p.) of typical elemental concentrations (wt%) and thermal neutron capture cross sections [barns] divided by its atomic weight (A) are shown for certain elements in Table 1.

Table 1

Elem.	Capture Cross Section	A	Paragneiss		Metabasite	
			wt%	s.p.	wt%	s.p.
Si	0.16	28	30	0.17	24	0.14
Fe	2.56	56	4	0.18	7	0.31
Ca	0.43	40	1	*0.01	6	0.06
Ti	6.40	48	.5	0.06	1	0.13
S	0.52	32	.2	*0.003	.1	*0.001
Gd	49000	157	.0008	0.25	.0008	0.25
K	2.10	39	2	0.10	.7	0.04
Al	0.23	27	8	0.07	8	0.07
Na	0.53	23	2	0.05	3	0.06
Mg	0.06	24	2	*0.005	4	*0.01

Elements in this well which are below the present tool's threshold level of 0.025 for the sensitivity product are marked with an asterisk. Their determination will be difficult, as is the case for S and Mg in both dominant rocks and for Ca particularly in the paragneiss. Another point is the similarity between gamma ray spectra as is the case for Al and Fe. Their principal capture gamma ray energies fall within the resolution of the NaI-detector and can therefore not be separated. However, as discussed, Al is most efficiently detected through delayed activation. The same applies for Na, but its detection is not implemented.

The determination of absolute elemental weight fractions by gamma ray detection is very difficult in the borehole environment. However, relative concentration values can be obtained by dividing each elemental yield  $Y_i$ , by a relative spectral sensitivity factor  $S_i$ , which is a tool constant determined in the laboratory. These relative concentrations are then related to absolute ones, expressed as weight fractions  $W_i$ , by a depth dependent normalization factor  $F$ , such that  $W_i = FY_i/S_i$ . This normalization factor is a complex function of numerous parameters and cannot be calculated directly due to an unknown and variable neutron source output. Therefore

other approaches are needed to obtain F.

### Geochemical closure model

This method developed by Grau et al, 1989, is based on the fact that the sum of all elemental weight fraction is unity. It is intended for a broad applicability in all types of rocks, although originally conceived for clastic sediments. However assumptions must be made, as important elements like C, O, Mg and Na, which can contribute substantially to the total weight fraction, cannot be measured with this tool. The closure model takes care of the unmeasured C and O, in assuming that each of the measured element is present as one single oxide or carbonate, which is not true for Ca, Fe and S. The sum of these oxides/carbonates is then made equal to 100, in solving for the calibration factor F at each depth level. This method gives adequate results, except in cases, where Mg and Na is present.

Mathematically it can be expressed as:

$$F(\sum X_i Y_i / S_i) + X_K W_K + X_{Al} W_{Al} = 100$$

where:

F is the normalization factor  
Y<sub>i</sub> the yield attributable to element i  
S<sub>i</sub> the relative sensitivity for element i  
X<sub>i</sub> associated oxide/carbonate factor of element i  
W<sub>Al</sub> the aluminum weight fraction  
W<sub>K</sub> the potassium weight fraction

To account for other important unmeasured elements, such as Mg and Na, some oxide factors were optimized on core samples as listed in Table 2. By this method errors are minimized and dispersion from the ideal 100% fall within 5% on either side, comparable to the statistical precision of the downhole measurements. Fig. 4 depicts XRF data and log-derived weight fractions.

This condition satisfies all but one major mineral found in this well, with the exception being Ca feldspar. When using above stated equation, its closure sum amounts to 129%, therefore introducing an error of 6% from an estimated concentration of 20% Ca feldspar. The situation is worse for Pyrite with a closure sum of 156.7%, but since its concentration is small, the error it causes is negligible.

Table 2

Element	Oxide	Closure Model Oxide Factor	KTB Model Oxide Factor
Si	SiO <sub>2</sub>	2.139	2.139
Fe	Fe <sub>2</sub> O <sub>3</sub>	2.075	1.429
Ca	CaO	2.497	1.399
Ti	TiO <sub>2</sub>	1.668	1.668
K	K <sub>2</sub> O	0.615	1.204
Al	Al <sub>2</sub> O <sub>3</sub>	2.741	1.889

#### KTB model

A somewhat different approach has been adopted for this well. Its application is however limited to cases, where two preconditions are fulfilled, namely the availability of XRF data and a lithological profile containing only a few rock types. Being the case, the XRF oxides fractions were summed up for all measurable elements detectable through downhole spectroscopy. The histograms in Fig. 5 show that very little variation can be observed in the two main rocks. So for instance totals the mean in the paragneiss 90.7% with a standard deviation (sd) of 1.2 and in the metabasite 85.3% with a sd of 1.0. The sum of 100% in the above formula was therefore changed to these means and triggered according to the prevailing lithology. Using the true oxide factors eliminated also the uncertainty in the calculation with optimized factors for sediments in crystalline rocks.

One further improvement, although not limited to this model, is the possibility of applying a cut-off on unrealistic low values for Al concentrations in breakout zones. This allows a better fractional distribution for the other elements. The log-derived and XRF data are displayed in Fig. 6.

#### Discussion of results

The results of elemental processing from 3000 to 6010m are compared with XRF data analysed by the KTB field laboratory on cuttings. In general the agreement is good,

as can be seen in the annex in Plots 1a,b,c. Major discrepancies are observed for the elements Th and U. Especially for Th, the differences seem to worsen with increasing depth with XRF data probably too high in the metabasites. A comparison for the element Al reveals good agreement in the top section. Differences are limited to intervals where the borehole is severely ovalized, as below 5000m. Despite trials to orient the tool towards the short axis, which is more or less in gauge, occasional tool rotations into the long axis are responsible for this reduction in quality. For the other elements, the agreement is better for the first logging run than for the second.

### Conclusions

The availability of XRF data, although not compulsory, is useful to compare with the geochemical data from in-situ spectroscopy. Whenever differences occur, they might be attributed to cavings which contaminate the cuttings.

The differences between the two models are minor, and within the range of the differences of two consecutive runs using either model. This implies that the optimized oxidation factors of the geochemical closure model, developed for sediments, are also valid for the crystalline rocks encountered in the KTB well.

The results of elemental determination by both geochemical models are in good agreement with XRF data.

### Nomenclature

K	..potassium
Si	..silicon
Al	..aluminum
Ca	..calcium
Fe	..iron
Ti	..titanium
Gd	..gadolinium
Cf	..californium

### References

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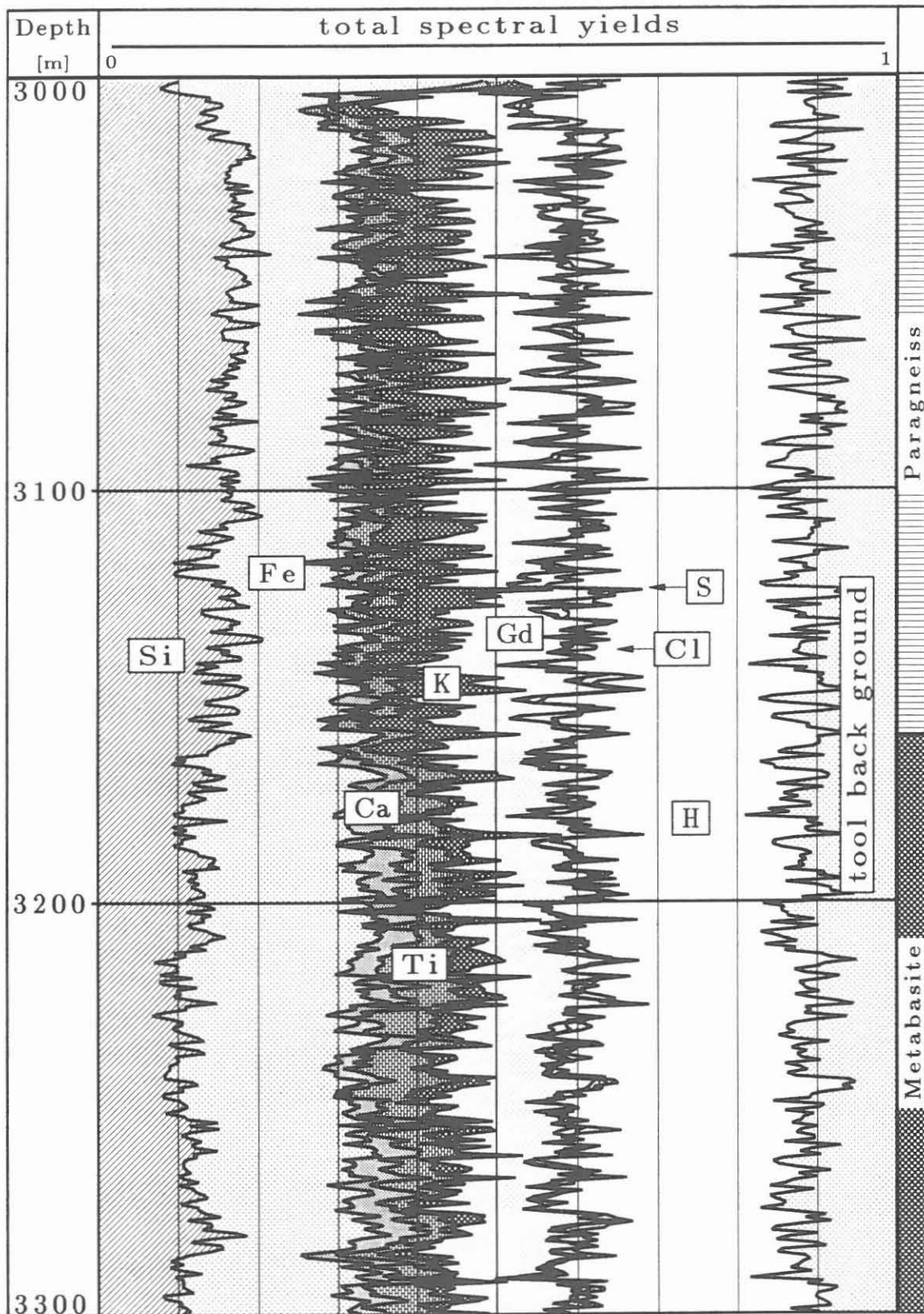


Fig.#1: Total spectral yields

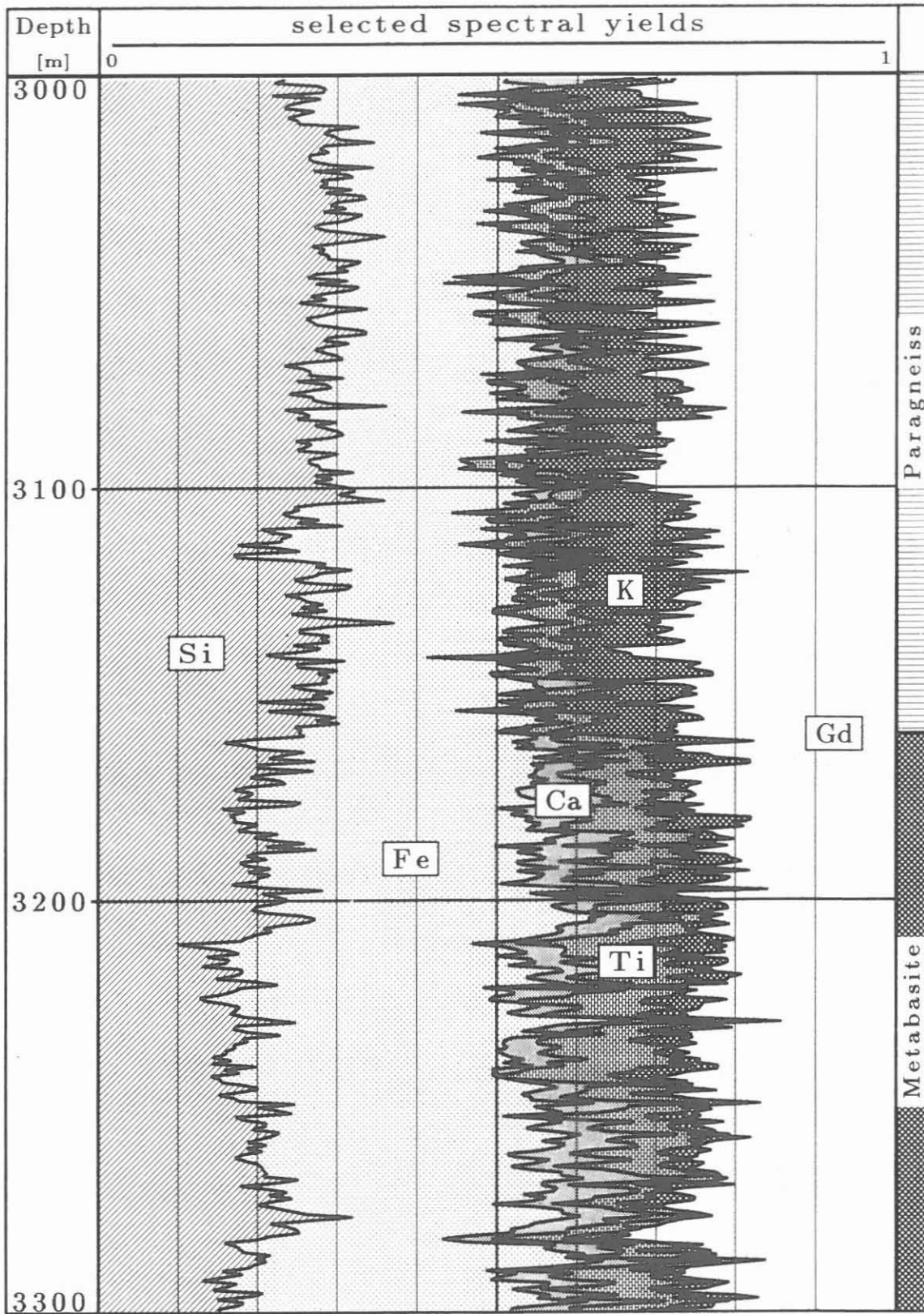


Fig.#2: Selected spectral yields (normalized)

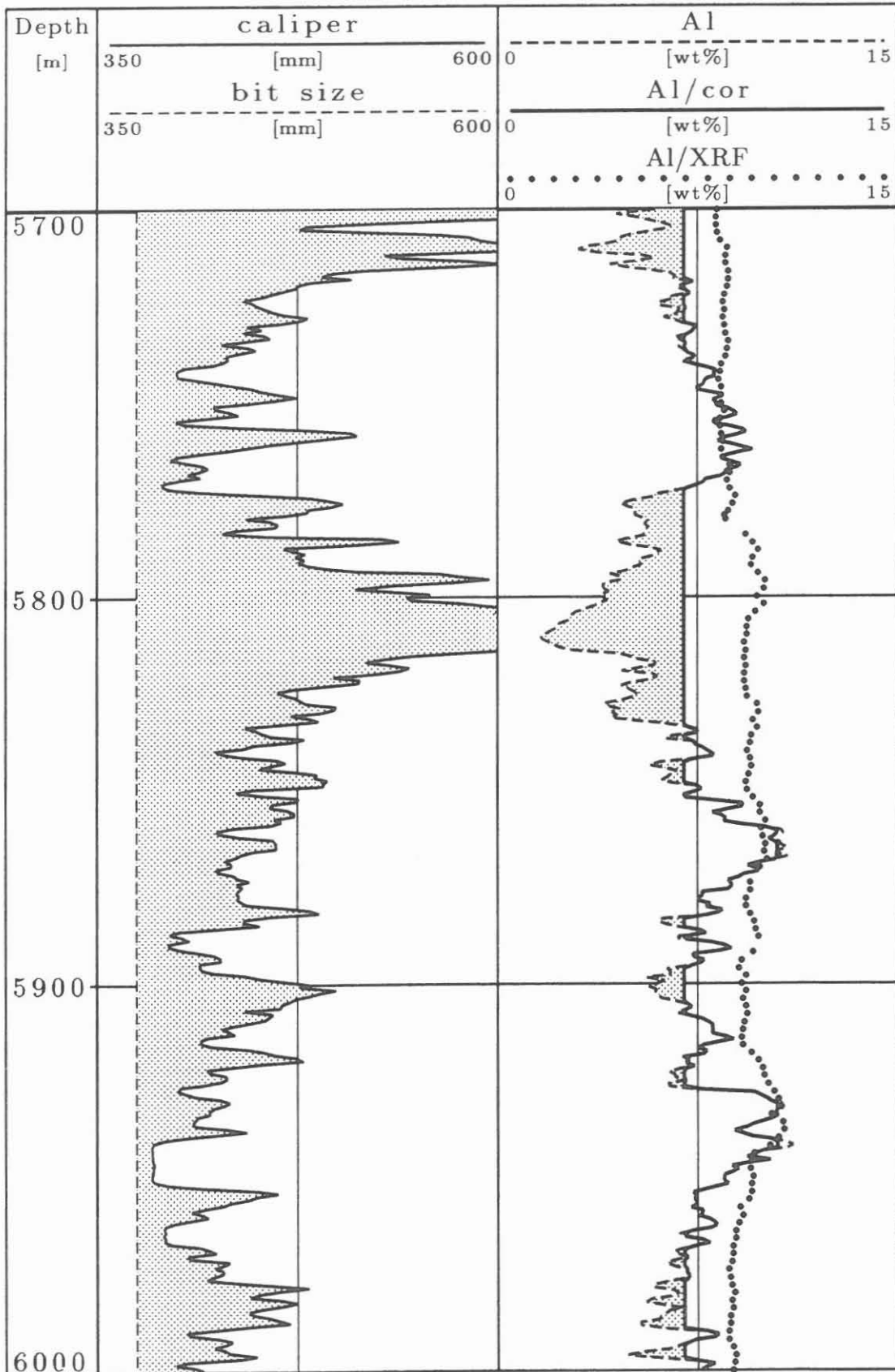


Fig.#3: Cut-off for unrealistic low Al values in break-outs

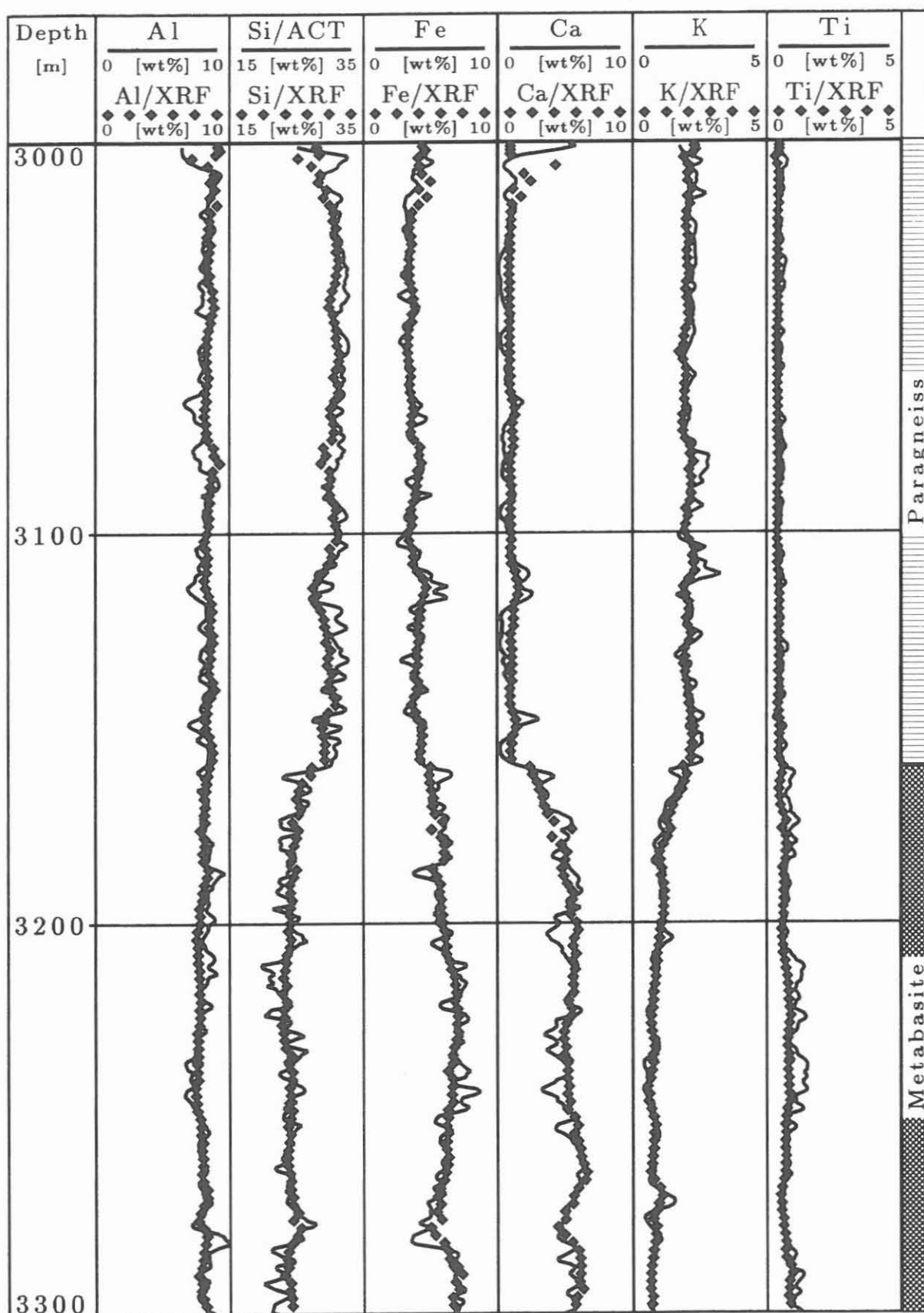


Fig.#4: Log-derived elements (closure model) and XRF

# Histogram

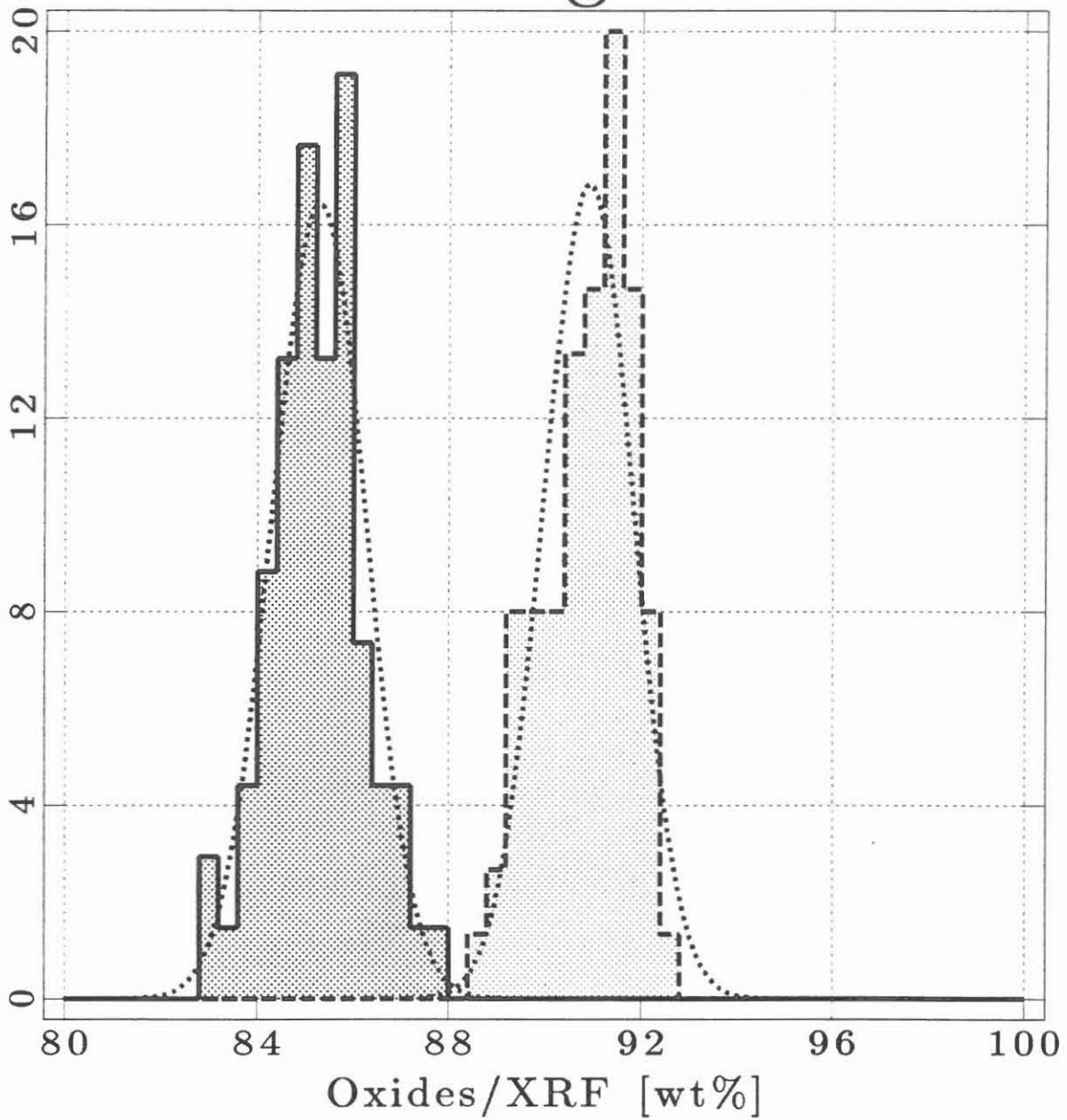


Fig.#5: Oxides/XRF sum of Al+Si+Fe+Ca+Ti+K  
in metabasite/ mean= 85.3, stand.dev.= 1.0  
in paragneiss/ mean= 90.7, stand.dev.= 1.2

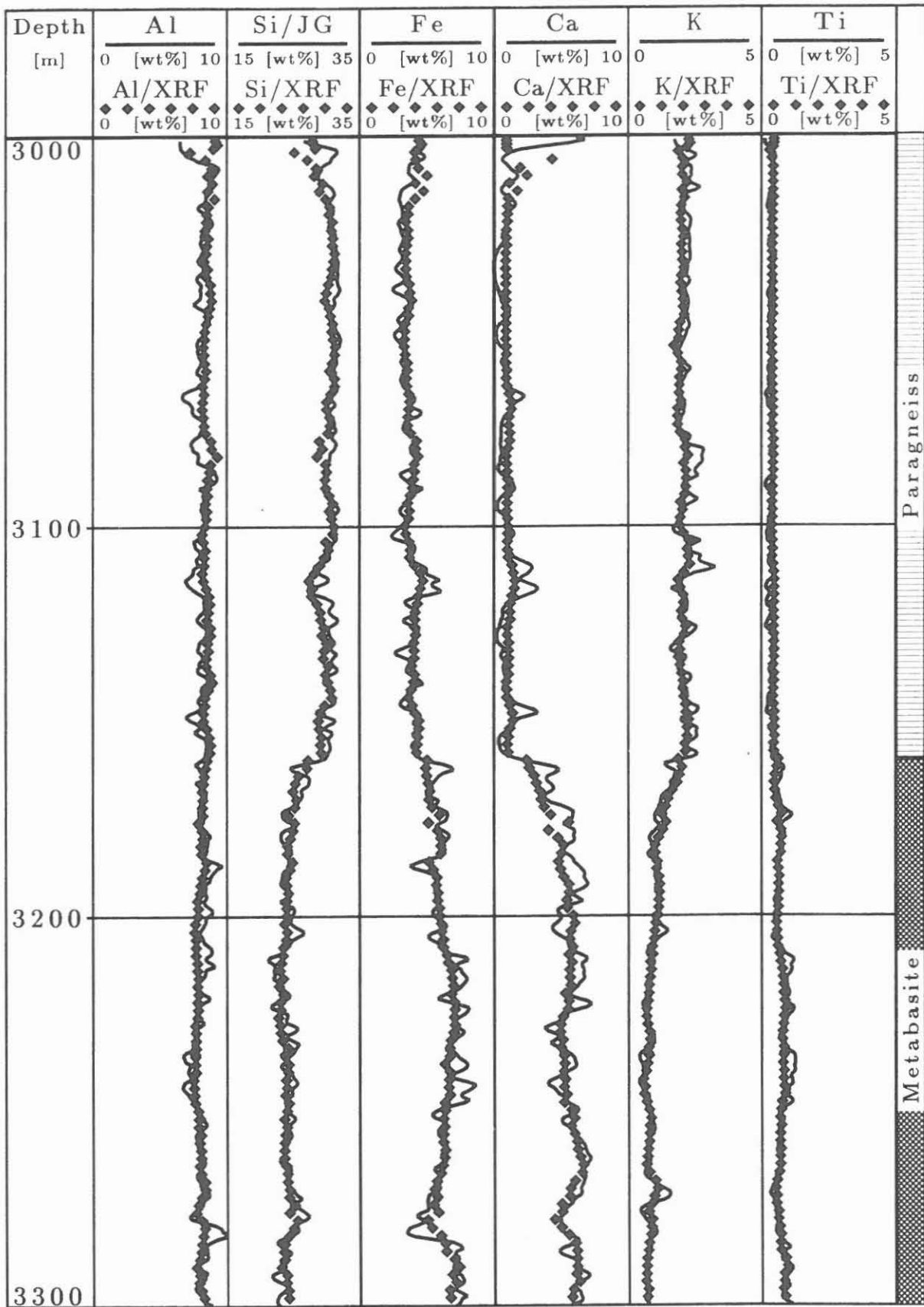


Fig.#6: Log-derived elements (KTB model) and XRF