



Graphitization degrees: information importance and scheme of their unification

Степени на графитизация: информационно значение и схема за унифицирането им

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Different deviations from ideal structure of hexagonal (2H) graphite have been used for determination of structural state (graphitization degree) of natural or synthetic carbon matters. The degree of graphitization (u and GD) increases with increasing temperature during regional or contact metamorphism. The general pressure, stress, chemical composition of fluids, origin of primary carbon matter, mineral and chemical composition of graphite-bearing rocks and duration of processes can also have an important effect on the graphitization degree. There are many diagrams for displaying the relationship between structural state of carbon matter, PT-conditions of metamorphism and facies of regional and contact metamorphic rocks. The most undoubted and informative structural geothermometer is d_{002} (Å) value of carbon substance. The structural disorder value (g) is closely connected with the interlayer distance d_{002} (Å) of natural carbon matter. The change of g from 0 to 1 corresponds to a variation of d_{002} from 3.354 Å (fully ordered graphite) to 3.440 Å (fully disordered graphite). The quantitative relationship between them was shown by Franklin (1951):

$$d_{002} (\text{Å}) = 3.440 - 0.086 (1 - g^2) \text{ and } u = 1 - g,$$

where u is the structural order degree.

The correlation between T °C of metamorphism and graphitization degree (GD) after Wada et al. (1994) is:

$$T \text{ °C} = 3.2 \times \text{GD} + 280$$

The following correlations are formulated by Vlahov (2015):

$$T \text{ °C} = 300 + (3.371 - d_{002}, \text{Å}) \times 24\,000$$

$$\text{DG} = (3.371 - d_{002}, \text{Å}) \times 8000$$

$$T \text{ °C} = 3 \times \text{GD} + 300.$$

The last three equations permit a conversion and unification of correlation between T °C, d_{002} (Å), u and GD after different authors (Table 1). The synthesis of graphite needs temperature as high as about 2700–2800 °C. All types of organic precursors transform partly to graphite at temperature of 500 °C as the complete graphitization of carbon matter occurs at 700 °C in conditions of regional metamorphism (Beysac et al., 2002). Different factors of the metamorphism as general pressure, stress, composition of fluids, origin and structure of primary organic matter can also have a certain influence on the temperatures obtained by XRD-graphite geothermometry and values of graphitization degree. This defect can be controlled by comparison of the results with values from other geothermometers and geobarometers, in combination with mineralogical and petrological data. The model proposed here (Table 1) is not absolute, but the last equations are tested during study of graphite from the Central and East Rhodopes. The temperatures of the regional metamorphism obtained by using d_{002} (Å), u and GD values are comparable to temperatures from other geothermometers after different authors (Vlahov, 2017).

References

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Table 1. Direct correlation between T °C of the metamorphism, d_{002} (Å) values and graphitization degrees of carbon matter after different authors and scheme of their unification

T °C after Vlahov (2015)	d_{002} (Å) of carbon matter after Vlahov (2015)	Graphitization degree (u) after Franklin (1951)	Graphitization stage after Landis (1971)	Graphitization stage after Grew (1974)	Graphitization degree (GD) after Wada et al. (1994)	Graphitization degree (GD) after Vlahov (2015)
<300 °C	>3.371	0.00 ($d_{002} > 3.439$ Å); 0.01–0.54 $d_{002} = 3.439$ – 3.372 Å	graphite d_3	not graphitized carbon matter	0 ($T \leq 280$ °C); 3 ($T = 290$ °C)	0
300 °C	3.371	0.55–0.56	graphite d_2, d_1	Ist graphitization stage	6	0
400 °C	3.367	0.61	graphite d_2, d_1	Ist graphitization stage	37–38	33
500 °C	3.363	0.67–0.68	graphite d_2, d_1 and fully ordered graphite	Ist graphitization stage	69	67
600 °C	3.359	0.75–0.76	fully ordered graphite	IInd graphitization stage	100	100
700 °C	3.355	0.87–0.91	fully ordered graphite	fully ordered graphite	131	133
800 °C	3.350	1.00	fully ordered graphite	fully ordered graphite	162–163	167

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