Abstract: The peak value as well as the full width at half maximum of the reflectivity of single crystal neutron monochromators may be expressed, besides thickness and mosaic spread, in terms of two material parameters: reflection number and penetration depth in the abscence of Bragg scattering. The values of these parameters, as functions of neutron wave length and reflection order, corresponding to reflection as well as to transmission geometry, are calculated for the most representative planes of Be, pyrolitic graphite, Al, Si, Cu, Zn, Ge, Pb and Bi single crystals.

The monochromator (as well as the analyser, if such be the case) plays the leading part in a thermal neutron crystal spectrometer. That is why several attempts have been done till now to draw up tables or diagrams describing the reflecting properties of various single crystals used for neutron monochromation (Hautecler & Pollak, 1958; Carvalho, Ehret & Gläser, 1957; Popovici, Gheorghiu & Gelberg, 1969; Stedman, Almqvist, Raunio & Nillson, 1963; Riste, 1970).

All the treatments, as well as that presented below, are based on the reflectivity formulae given, in the frame of the mosaic crystal model, for semi-infinite plane slabs, by Bacon & Lowde (1948) and by Dietrich & Als-Nielsen (1965) for the reflection (R) and, respectivelly, transmission (T) geometries. Using the notation rendered in Table 1 these formulae may be written, for the symmetric case, as follows:

$$R_R(\varphi) = \frac{a}{1+a+\sqrt{1+2a}.\mathrm{cth}(A_R\sqrt{1+2a})} \quad , \qquad (1)$$

in R-case, and:

$$R_T(\varphi) = \exp(-A_T f_T(1+a)).\mathrm{sh}(A_T f_T a) \qquad (2)$$

in T-case.

$R(\varphi)$ is expressing the reflecting probability of neutrons whose incident and final divergence angles are γ_i and γ_f, while $\varphi=(\gamma_i+\gamma_f)/2$

However, for calculation of resolution functions of neutron crystal spectrometers there is commonly used the Gaussian approximation of the reflectivity. Checking up for the validity of this procedure it has been shown that, in both R and T cases, the approximation of the reflectivity with a Gaussian, having the same peak value and the same full width at half maximum, is quite satisfactory provided the collimators defining the incoming and diffracted beams have the collimation angles smaller or of the same order of magnitude as the effective mosaic spread of the single crystal (Grabcev, 1979). Under these circumstances we can write:

$$R(\varphi) = P.\exp(-\varphi^2/2L^2) \qquad (3)$$

where:

$$P = R(o) \qquad (4)$$

is the peak reflectivity, while

$$L = \eta y_1 (\ln 2)^{-1/2} \qquad (5)$$

is the effective mosaic spread; $y=\varphi/(\sqrt{2}\eta)$ and y_1 is the solution of the following equation:

$$R(y_1) = R(o)/2 \qquad (6)$$

According to Eqs. (1)-(6) the quantities P and L/η, fully describing the crystal reflectivity in the limits of the Gaussian approximation, may be expressed in terms of only two parameters: β and A_R or A_T.

The dependence of peak reflectivity and effective mosaic spread upon β, for several values of A_R or A_T is illustrated

in Figs.(1)-(4). In Fig.(5) there is plotted the function $f_T(\beta)$.

From definition, β depends on the structural parameter η and on the reflecting number B; A_R and A_T, on the other hand, depend on the thickness of the crystal plate and on the penetration depths t_R and t_T. Consequently, the reflectivity is affected, besides thickness and mosaic spread, by the intrinsic crystal parameters B, t_R and t_T.

The calculation of B, t_R and t_T, as functions of neutron wave length, for a few reflecting planes of some single crystals largely used as neutron monochromators, is the aim of the present paper.

The lack in the literature of data concerning the attenuation cross sections of single crystals has determined previous measurements of μ for Al, Si, Cu, Zn, Ge, Pb and Bi (Grabcev, Todireanu & Cioca, 1978). For pyrolitic graphyte (PG) and Be there have been used the calculated values of μ reported by Bergsma & Van Dijk (1967) and, respectivelly, the experimental values of Durgal & Thaper (1962).

For computation it has been convenient to express μ in the following way:

$$\mu = C_{-2}/\lambda^2 + C_{-1}/\lambda + C_0 + C_1\lambda + C_2\lambda^2 , \qquad (7)$$

with C_i coefficients determined by a least squares fitting.

All the necessary physical data have been taken from the publications of the International Union of Crystallography (International Tables for X-ray Crystallography, 1962; Neutron Diffraction Comission, 1969 .

The C_i coefficients are listed in Table 2.

The values of B, t_R and t_T corresponding to the most representative reflecting planes of Be, PG, Al, Si, Cu, Zn, Ge, Pb and Bi single crystals as functions of neutron wave length and reflecting orders are given in Figs. (6)-(14), as follows:

Fig. 6 Be(1-1o), -(oo2), -(o11).

Fig. 7 PG(oo2).

Fig. 8 Al(111), -(2oo), -(22o).

Fig. 9 Si(111), -(311), -(22o).

Fig. 1o Cu(111), -(2oo), -(22o).

Fig. 11 Zn(oo2), -(1-1o), -(o11).

Fig. 12 Ge(111), -(22o), -(311).

Fig. 13 Pb(111), -(2oo), -(22o).

Fig. 14 Bi(11o), -(211), -(-1 1o).

These data enables us to find the values of β, A_R and A_T, and subsequently of P and L, for any mosaic spread and thickness of the crystal.

Table 1. Notation

φ = mosaic angle.

$w(\varphi) = \frac{1}{\sqrt{2\pi}\cdot\eta} \exp(-\varphi^2/2\eta^2)$ = normal distribution function of mosaic angles.

η = mosaic spread = standard deviation of $w(\varphi)$.

λ = neutron wave length.

μ = total macroscopic attenuation cross section = cross section corresponding to all neutron-crystal interactions except Bragg scattering.

= structure factor squared times Debye-Waller factor.

θ_B = Bragg angle.

V_c = unit cell volume.

$$Q = \frac{\lambda^3 F^2}{V_c^2 . \sin 2\theta_B}$$

$B = Q/\mu$ = reflecting number.

t = thickness of crystal.

$t_R = \sin\theta_B/\mu$ = penetration depth in the abscence of Bragg scattering in R-case.

$t_T = \cos\theta_B/\mu$ = penetration depth in the abscence of Bragg scattering in T-case.

$a = B.w(\varphi)$

$\beta = B.w(o)$

$f_T = \ln(1+2\beta)/2\beta$

$t_o = t_T . f_T$ = optimum thickness in T-case = thickness for which $R_T(o)$ is maximum.

$A_R = t/t_R$

$A_T = t/t_o$

Table 2. Values of C_{-2}, C_{-1}, C_0, C_1 and C_2.

Crystal	C_{-2}	C_{-1}	C_0	C_1	C_2
Be	-0.26695×10^{-1}	0.25370	-0.74148	0.86168	-0.10332
PG	0.84337×10^{-3}	-0.29607×10^{-3}	-0.10387×10^{-1}	0.16555×10^{-1}	0.31028
Al	-0.14883×10^{-2}	0.26042×10^{-1}	-0.72715×10^{-1}	0.13153	-0.32367×10^{-1}
Si	-0.14760×10^{-2}	0.20702×10^{-1}	-0.52731×10^{-1}	0.75099×10^{-1}	-0.97547×10^{-2}
Cu	0.24365×10^{-1}	0.23978×10^{-1}	0.22027	0.28712	-0.54864×10^{-1}
Zn	0.22146×10^{-1}	-0.10706	0.21233	0.14542	-0.53704×10^{-1}
Ge	-0.37201×10^{-2}	0.10563	-0.23246	0.46472	-0.11723
Pb	0.43527×10^{-2}	-0.40924×10^{-1}	0.92224×10^{-1}	0.26667	-0.67378×10^{-1}
Bi	0.37754×10^{-2}	-0.30734×10^{-1}	0.50447×10^{-1}	0.18372	-0.48521×10^{-1}

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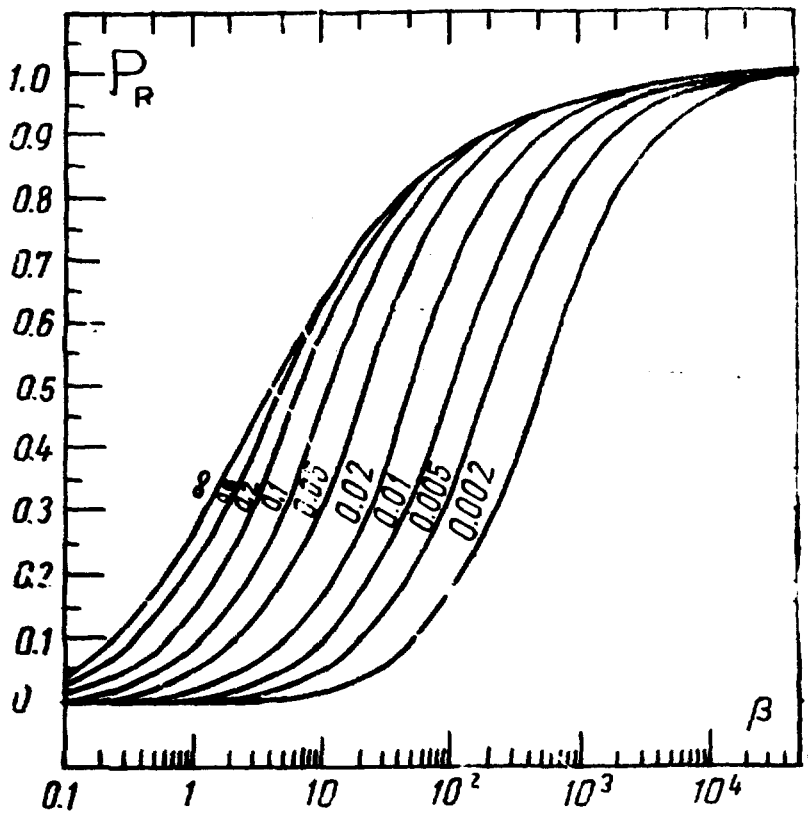


Fig.1 Peak reflectivity in R-case.

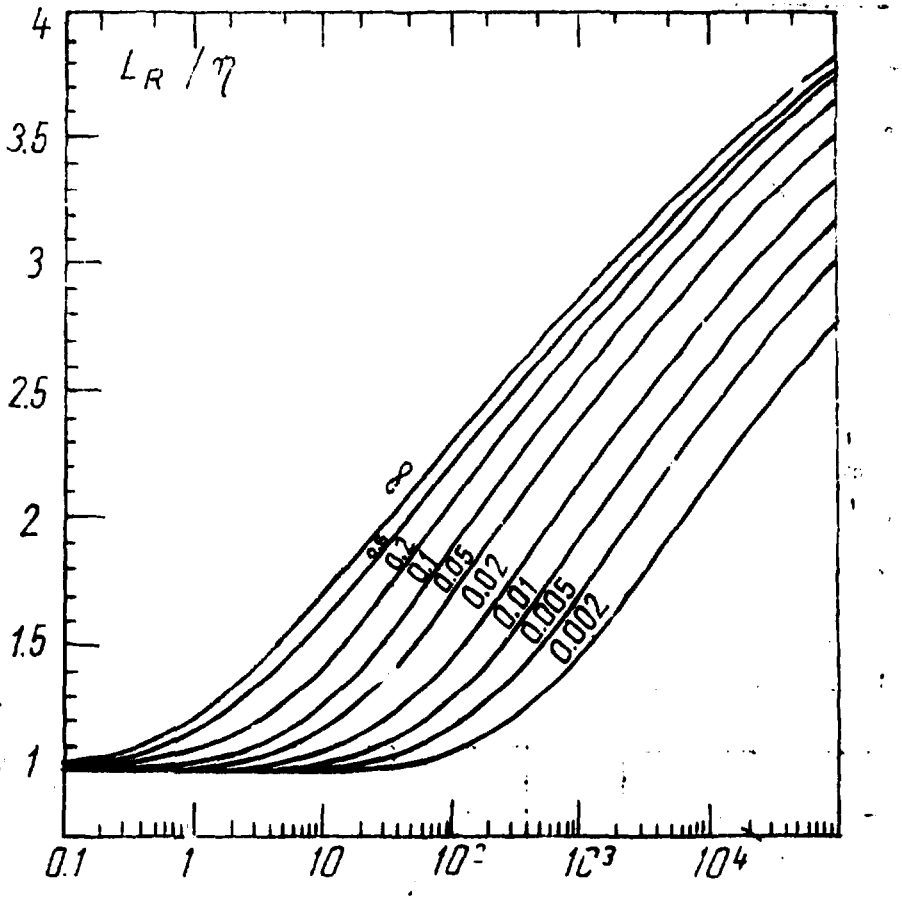


Fig.2 Mosaic ratio in R-case.

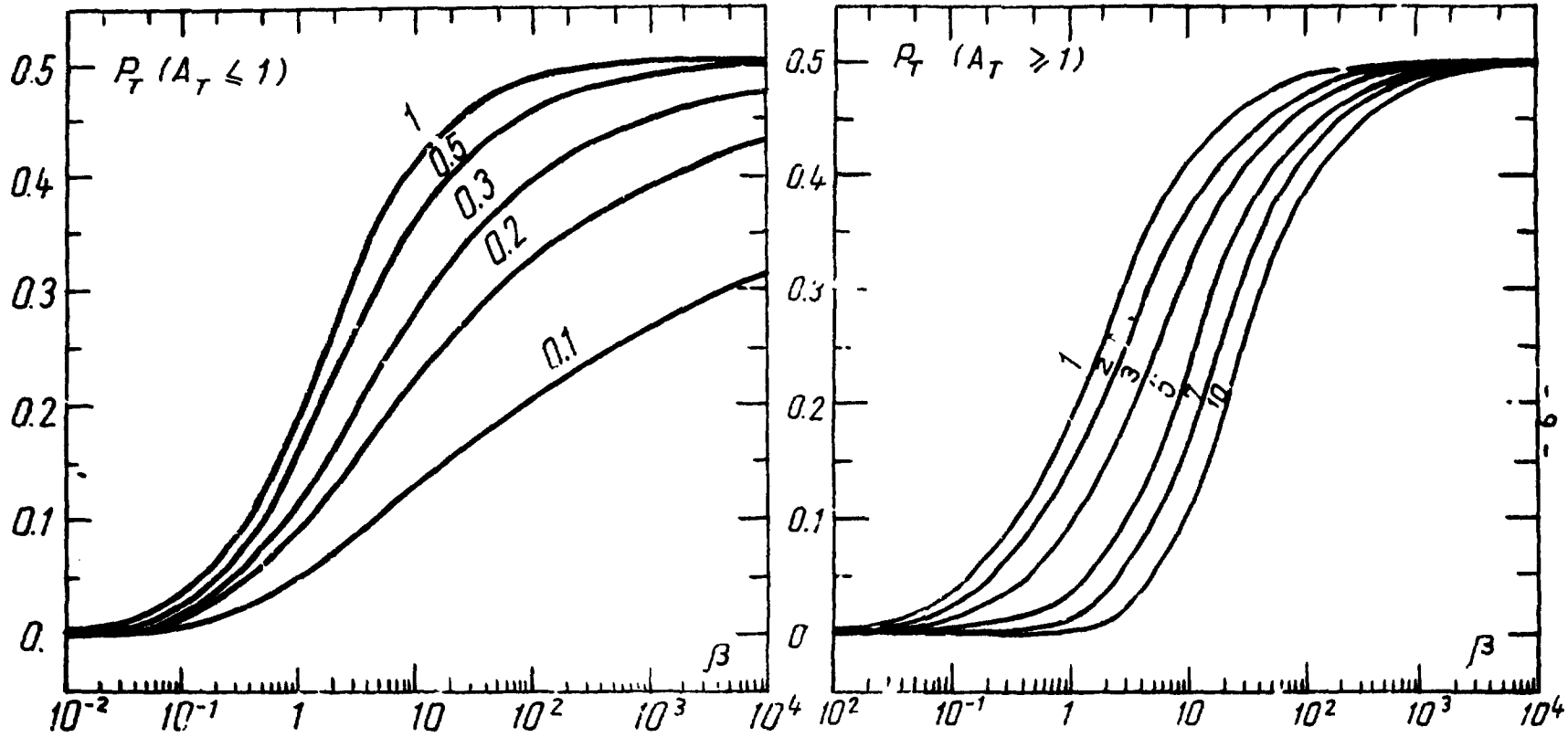


Fig.3 Peak reflectivity in T-case.

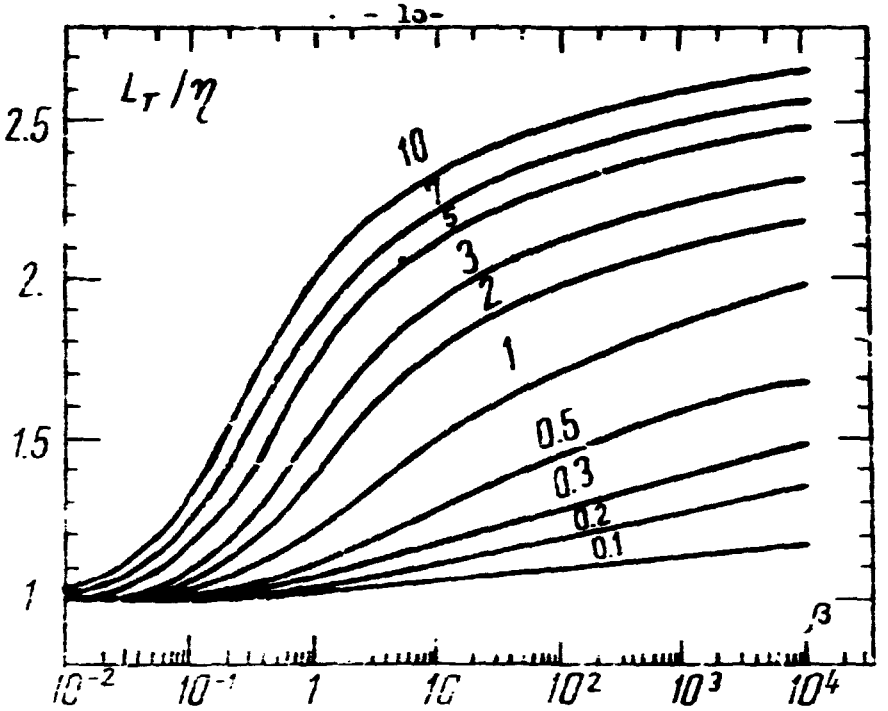


Fig. 4

Mosaic ratio in T-case.

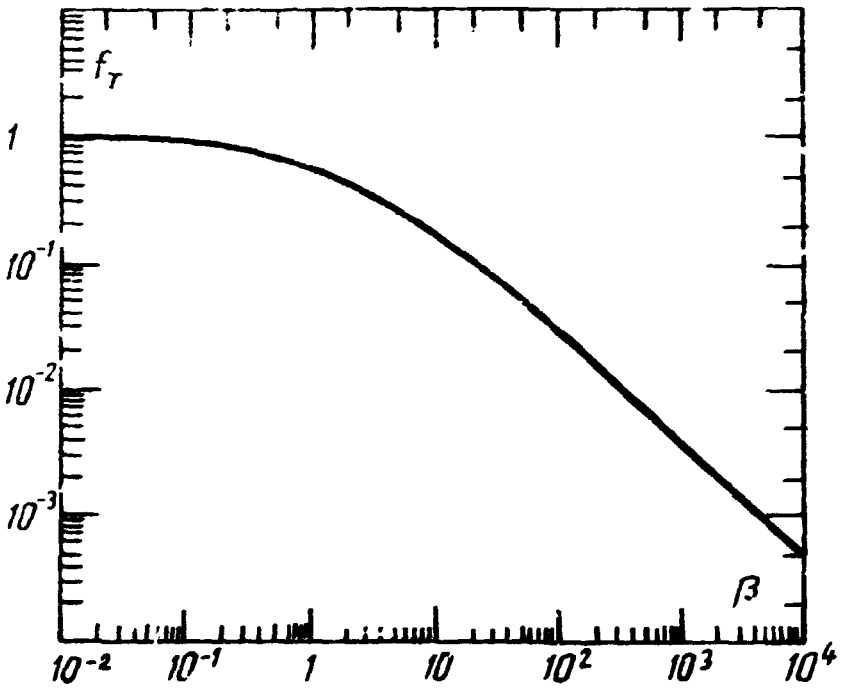


Fig. 5 Function f_T

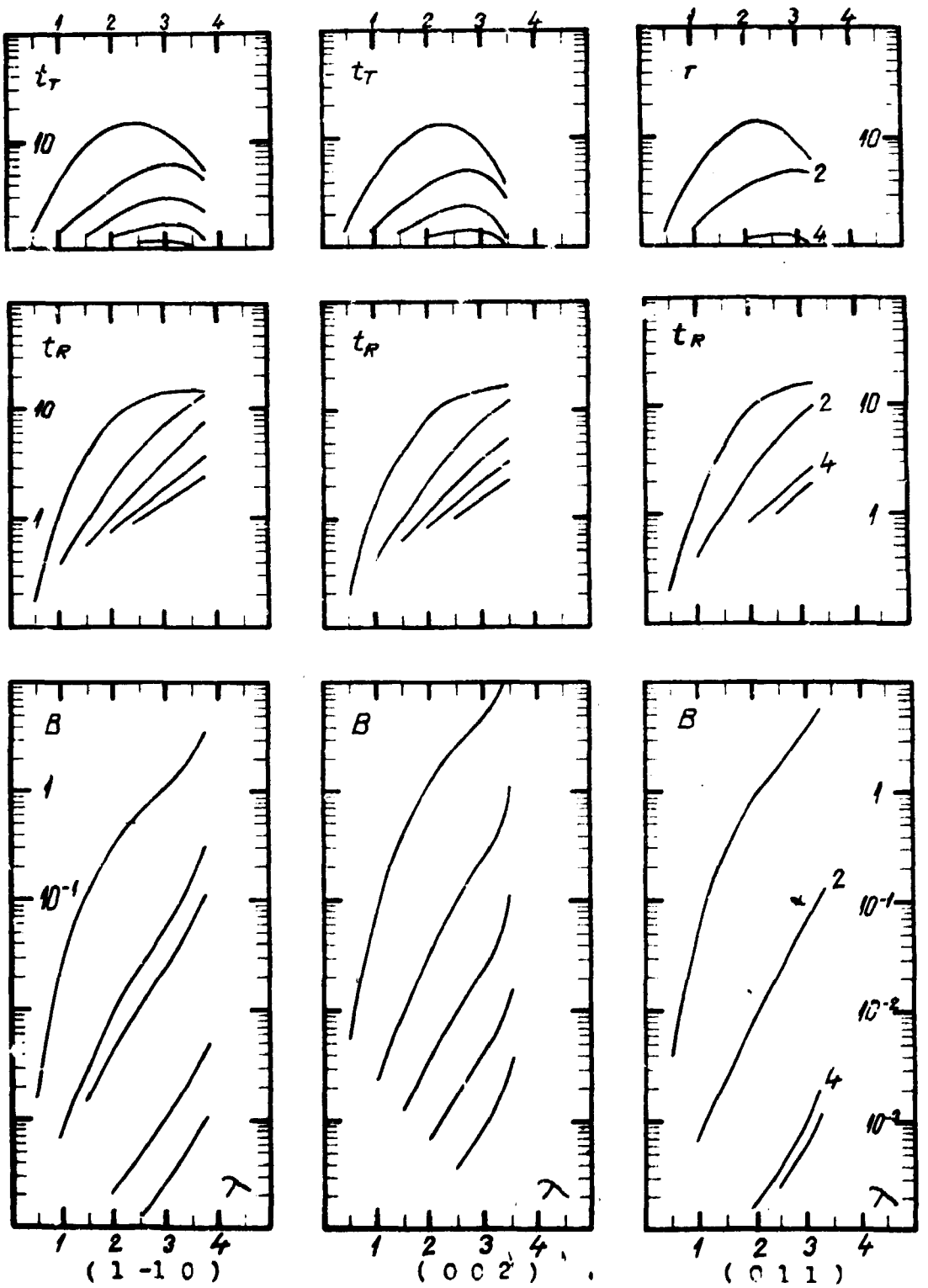
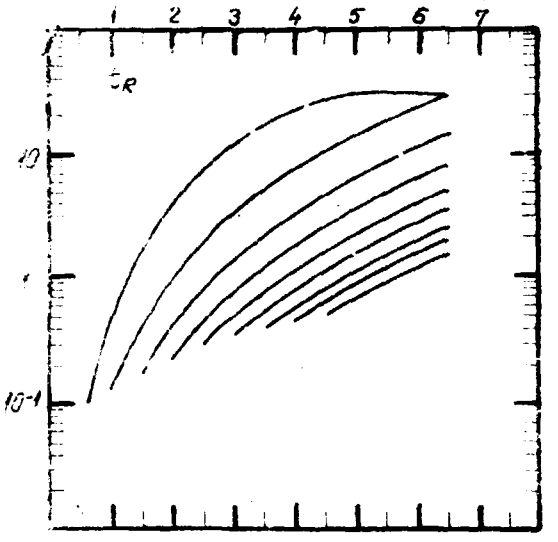
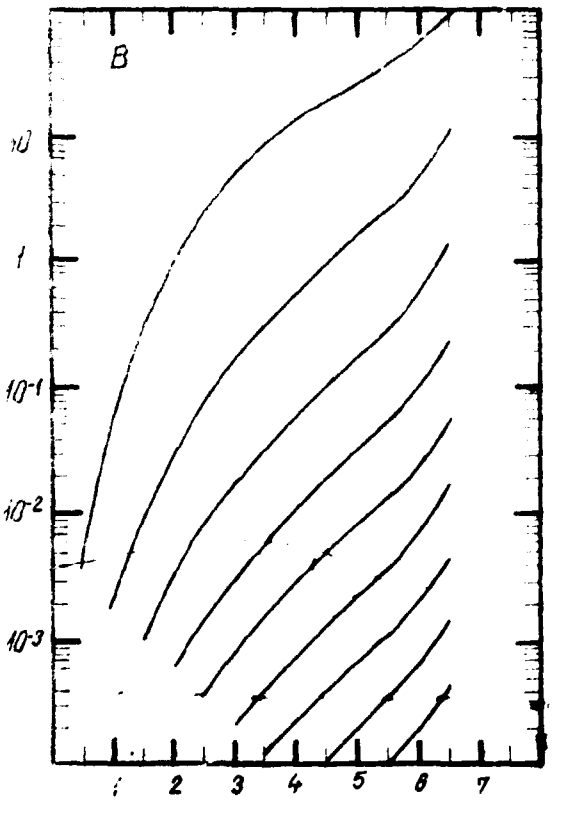


Fig.6 Values of B, t_R and t_T for Be.





(0 0 2)

Fig.7 Values of B and t_R for pyrolitic C.

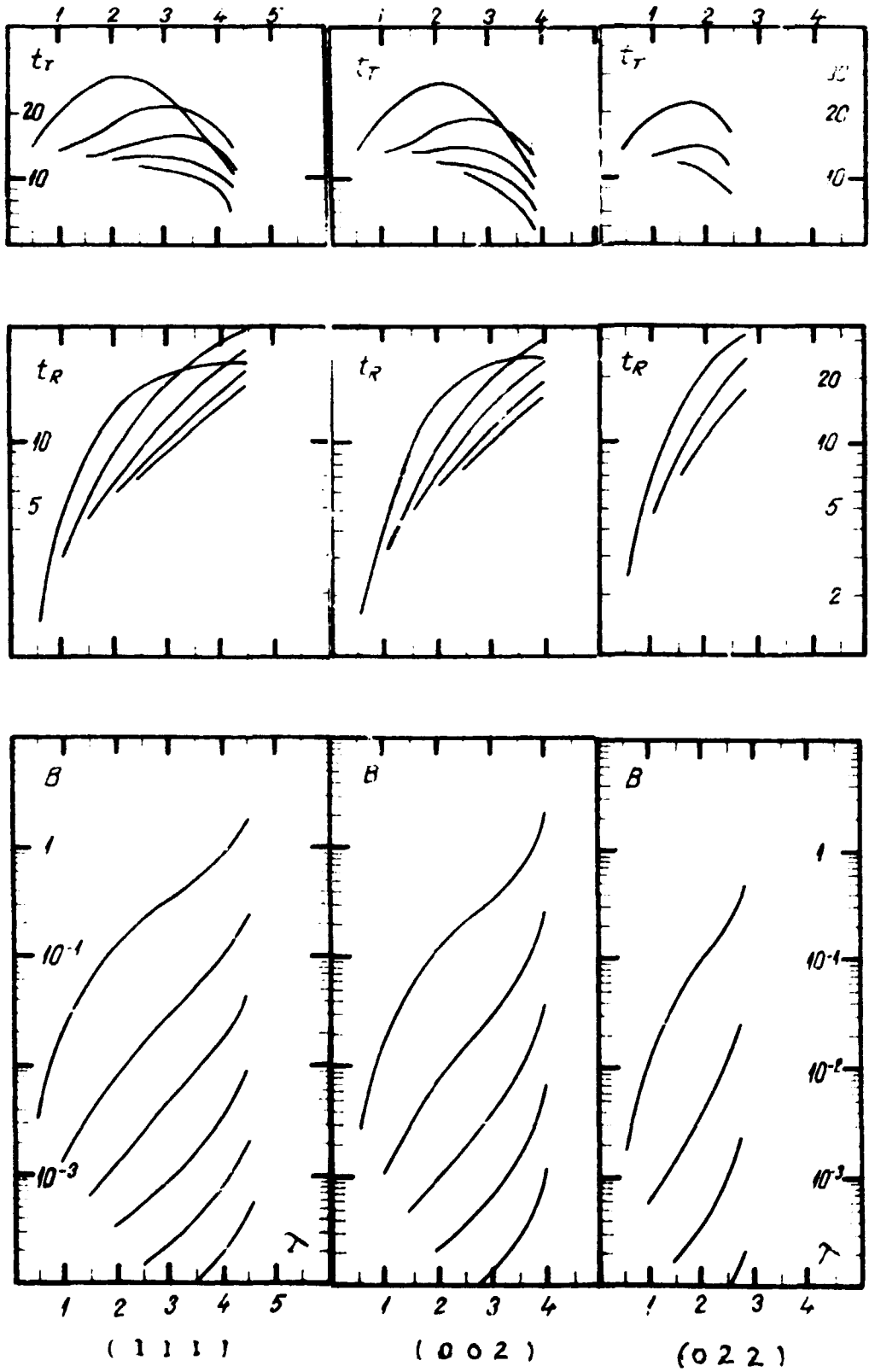


Fig.8 Values of B, t_R and t_T for Al

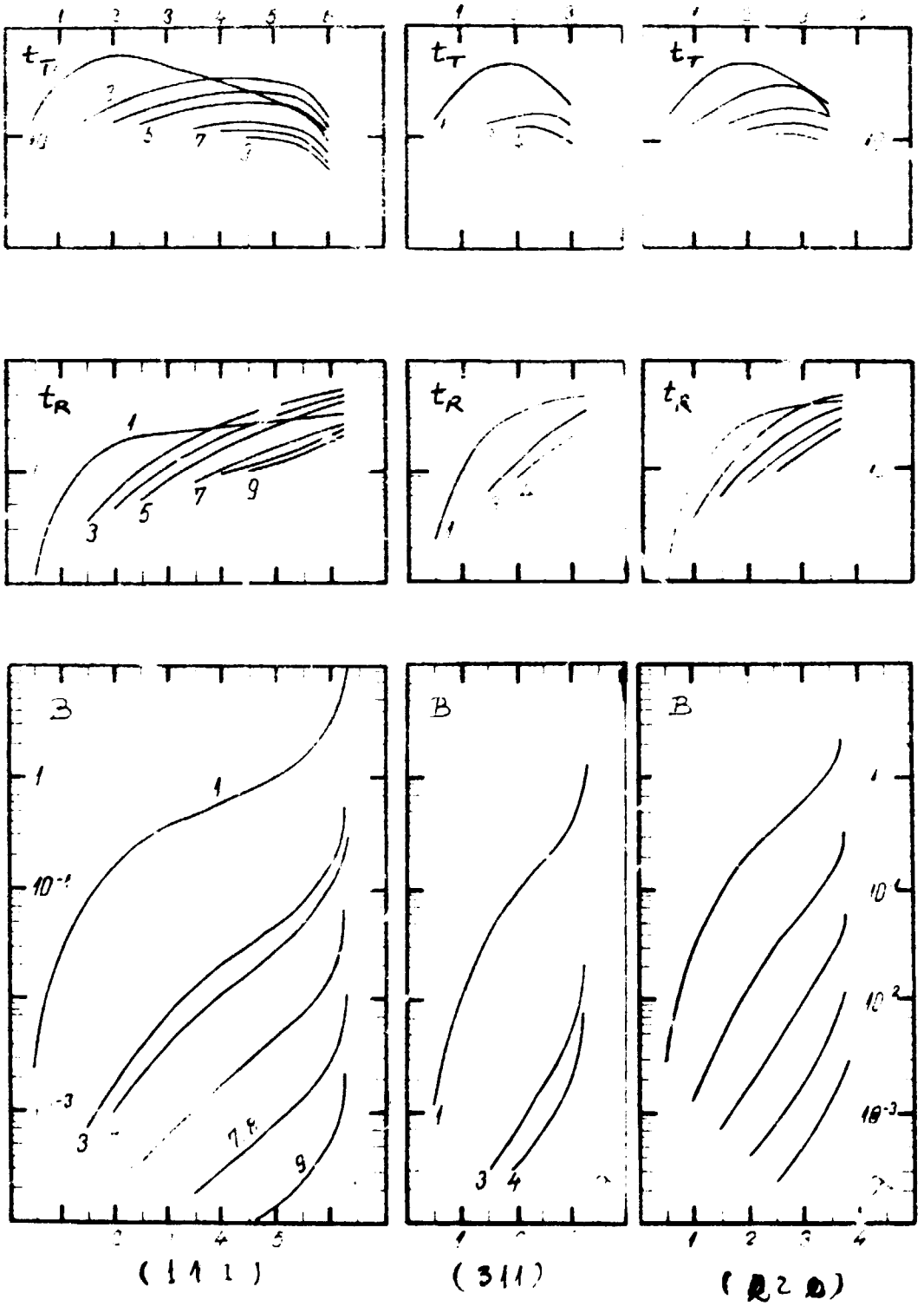
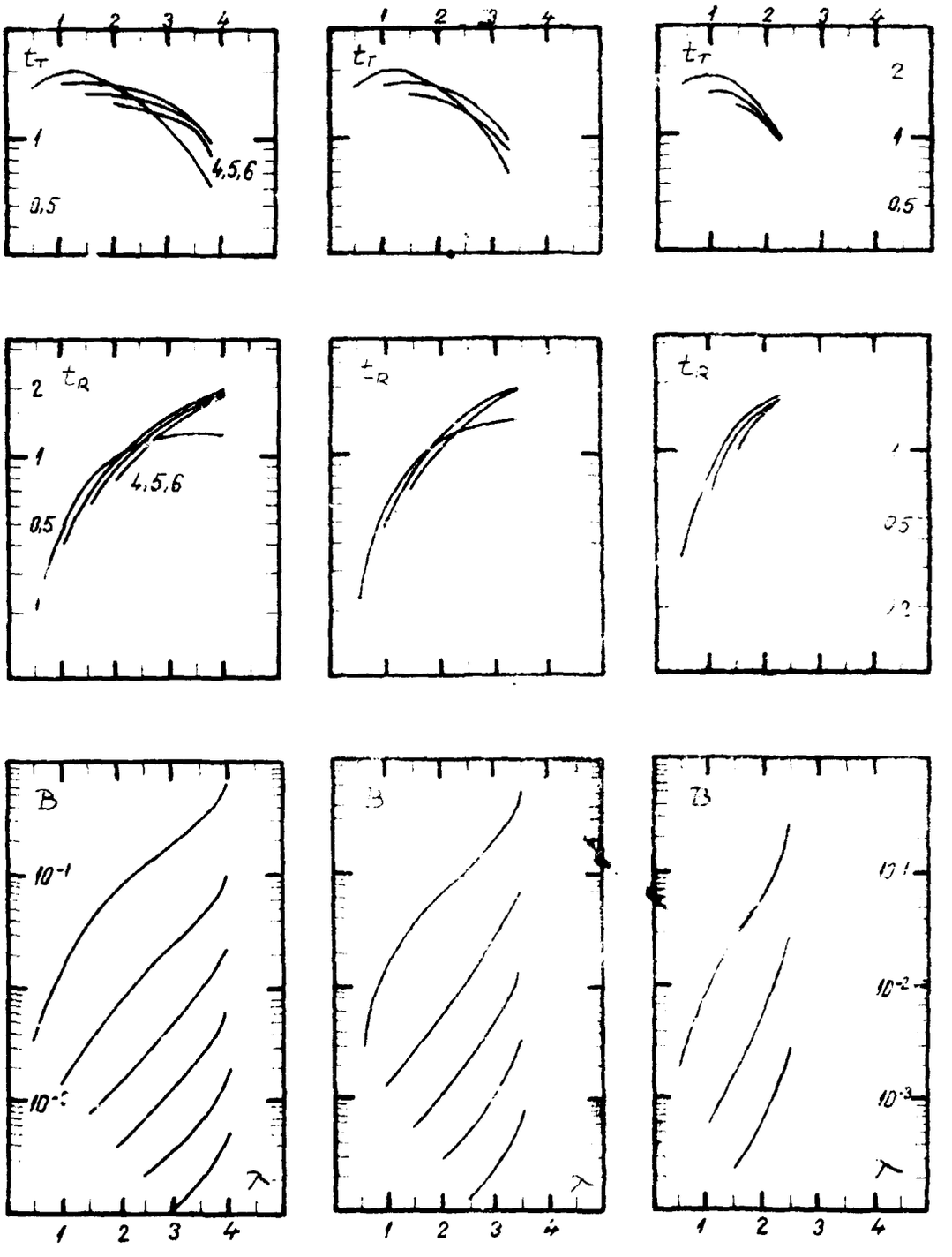


Fig 9. Values of B, t_R and t_T for Si



(1 1 1) (2 0 0) (2 2 0)

Fig. 10 Values of B, t_R and t_T for Cu.

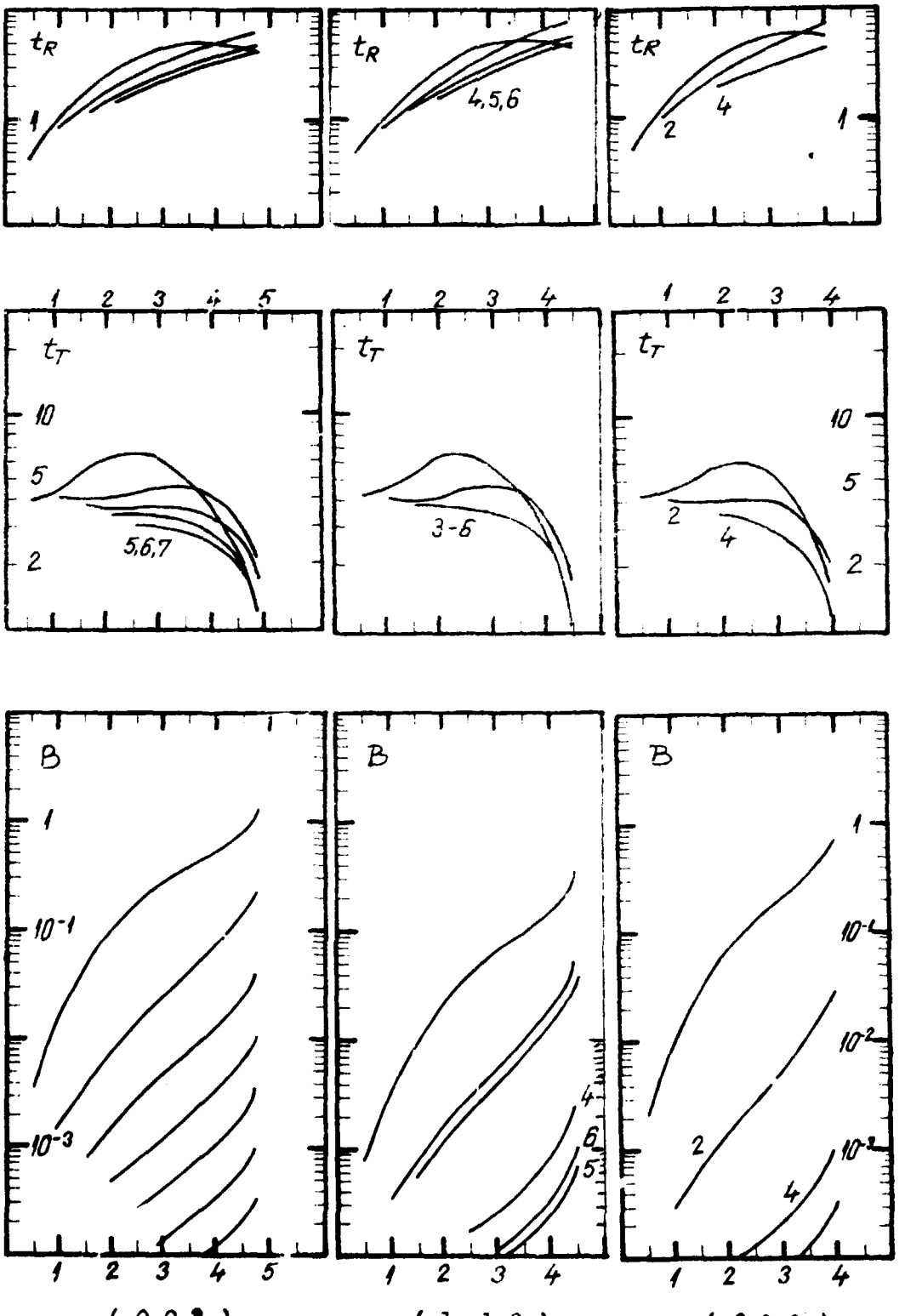


Fig.11 Values of B, t_R and t_T for Zn.

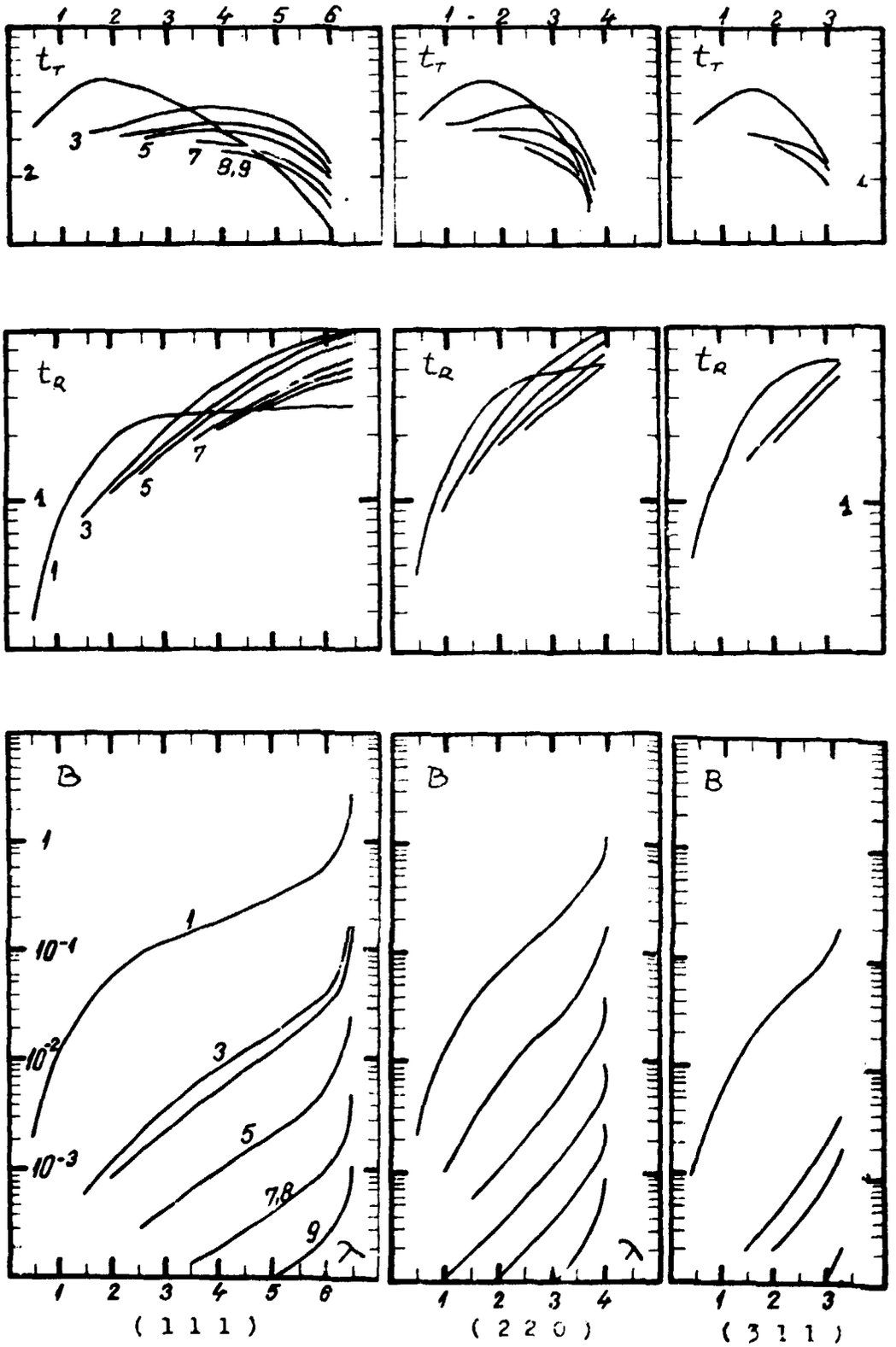


Fig.12 Values of B, t_R and t_T for Ge.

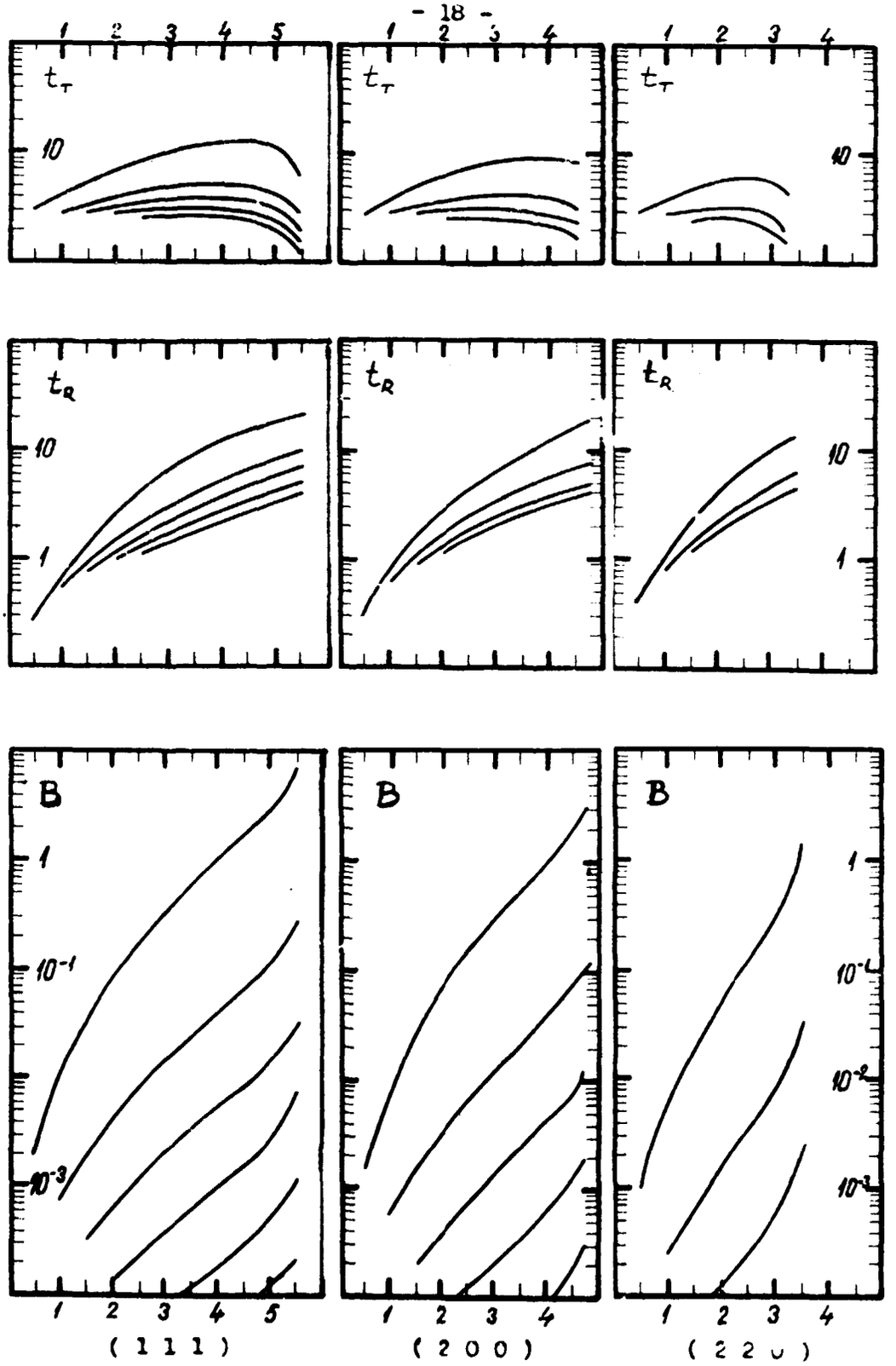


Fig.13 Values of B, t_R and t_T for Pb.

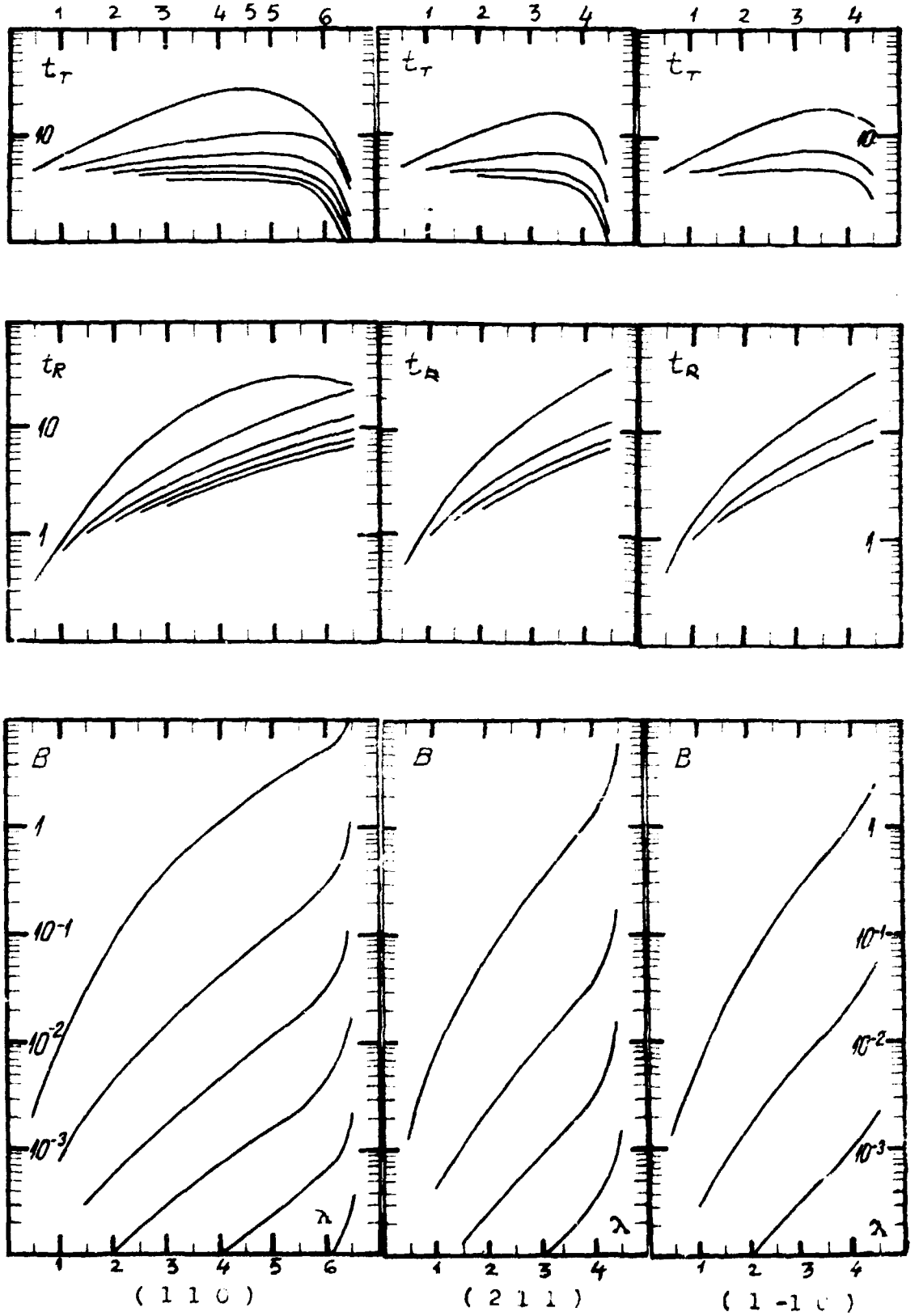


Fig.14 Values of B, t_R and t_T for Bi.

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