REVISED RUBY PRESSURE SCALE

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The ruby pressure scale where pressure is measured using the ruby R_1 luminescence line shift, is one of the most commonly used standards in diamond anvil cell experimental studies of *PV* relations of minerals on the room-temperature isotherm. Up to now the ruby pressure scale of Mao et al. [1], who have measured the ruby R_1 luminescence line shift in argon medium up to pressure 80 GPa, was the most widely used calibration. The pressure was determined from Cu and Ag room isotherms calculated by Carter et al. [2] from shock-wave data. As a result, the pressure scale in the following form gained acceptance in the literature

$$P = \frac{A}{B}[(1+\frac{\lambda}{\lambda_0})^B - 1], \quad (1)$$

where A=1904 GPa, B=7.665 (Fig. 1).

Almost at the same time Alexandrov et al. [3] have published a significantly different high pressure scale based on an *a priori* diamond equation of state. Alexandrov et al. [3] have performed simultaneous measurements of the ruby R_1 luminescence line shift in diamond anvil cell in helium pressure medium and a first-order Raman light scattering spectra in diamond up to compression $x=V/V_0$ =0.93. The scale with parameters A=1918 GPa, B=11.7 begins to differ from the scale of Mao et al. [1] at pressures above 20 GPa and results in significant differences in the pressure range above 50 GPa (Fig. 1).

Although Zha et al. [4] confirmed the scale of Mao et al. [1], recently on the basis of detailed analysis of the present X-ray, ultrasonic, theoretical and shock-wave data for diamond Holzapfel [5] has proposed a new ruby scale in the form:

$$P = \frac{A}{B+C}[\exp((\frac{B}{C}+1)(1-\frac{\lambda}{\lambda_0})^{-C}) - 1], \quad (2)$$

where A=1820 GPa, B=14, C=7.3 (Fig. 1).

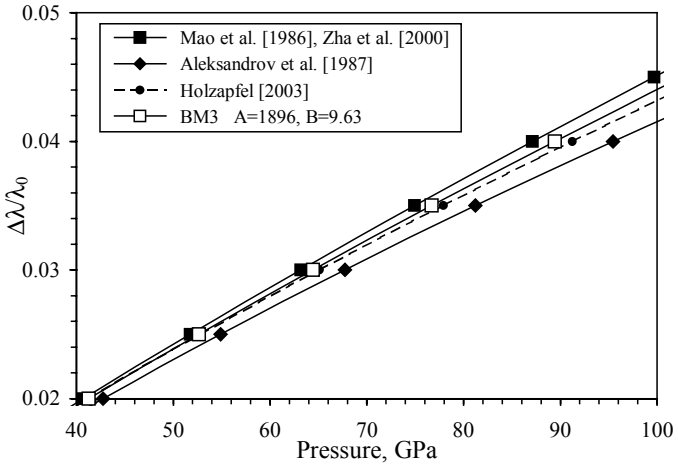

Fig. 1. Ruby pressure scales

In order to find the reasons for such discrepancy between scales [1], [3] and [5], it is necessary to check the Cu and Ag room isotherms from Carter et al. [2], which have been calculated only from shock-wave data. By now the range of shock-wave data on Cu and Ag has expanded, which together with ultrasonic, X-ray and thermochemical data allows one to obtain reliable equation of state for these metals. Therefore the purpose of our study is to develop an equation of state for Cu and Ag on the basis of contemporary data and comparison of calculated room isotherms with Carter et al. [2] isotherms. Then from Mao et al. [1] data we calculate the Cu and Ag volume that permits us to revise the pressure of the ruby pressure scale.

Thermal equations of state for Cu and Ag have been developed on the basis of recent thermochemical, X-ray, ultrasonic, theoretical and shock-wave data using formalism from [6]. Parameters of equation of state for Cu and Ag with cold isotherm according to a third-

Table 1. Parameters of the equation of state of Cu and Ag.

Parameters	Cu	Ag
V_0, cm^3	7.113	10.272
K_0, GPa	133.9	100.0
K'	5.24	5.99
Θ_{B1o}, K	47.24	120.72
d_1	1.990	39.325
m_{B1}	0.001	1.121
Θ_{B2o}, K	146.57	112.63
d_2	6.450	4.266
m_{B2}	0.471	0.436
Θ_{E1o}, K	286.65	191.86
m_{E1}	1.549	1.443
Θ_{E2o}, K	181.32	–
m_{E2}	0.980	–
γ_0	1.975	2.439
γ_∞	1.100	1.655
β	2.722	5.089
a_0, K^{-1}		-15.95E-6
g		6.495
e_0, K^{-1}	10.66E-6	23.27E-6

order Birch-Murnaghan equation are given in Tab. 1. Deviations of calculated functions from experimental measurements are 0.5-1.5% over the whole *PVT* range. Therefore hereinafter we will compare the calculated room isotherm of Cu and Ag with Carter et al. [2] data.

Fig. 2 shows the difference between newly calculated pressures on room isotherm and the pressures recommended by Carter et al. [2]. This figure suggests that equations of state for Ag from our data and [2] are close but at the same time differences between equations of state for Cu are significant and reach 2 GPa at pressure equal to 70 kbar. Thus, data from Fig. 2 suggest that the ruby pressure scale of Mao et al. [1] underestimates the pressure at each given ruby R_1 line shift by up to 2 GPa.

Pressures obtained at given ruby R_1 line shift may be approximated by a third-order Birch-Murnaghan equation with A=1896 and B=9.63 parameters. Here A-parameter was fixed according to initial slope of quasi-hydrostatic conditions [7]. Dependence obtained for the ruby R_1 line shift with pressure gives pressures intermediate between the Mao et al. [1] scale and the Holzapfel [5] independent scale.

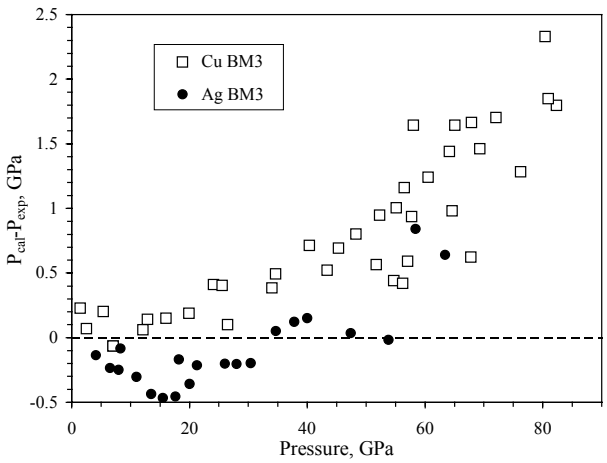

Fig. 2. Deviations of pressure on room-temperature isotherms of Cu and Ag from data Carter et al. [2].

Thus, equations of state for Cu and Ag have been developed, which in the range of experimental error are consistent with shock-wave, ultrasonic, X-ray and thermochemical data in the temperature range from 10-20 K to melting temperature and compression x=0.6. From comparison of calculated room isotherms with those recommended by Carter et al. [2], it follows that the latter deviates from our isotherm by up to 2 GPa at 70 Gpa-pressure, which implies a systematic error in the ruby pressure scale of Mao et al. [1]. We recommend a new ruby pressure scale, which is intermediate between the Mao et al. [1] scale and the Holzapfel [5] scale.

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