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The *P-V-T* equation of state of Au and Pt: An alternative pressure scale in high *P-T* experiments

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Abstract. The pressure-volume-temperature equations and state (EOS) of Au and Pt have been investigated to the relative volume change of 0.5–0.6 and temperature up to 3000 K based on experimental shock Hugoniot data and a simple thermal pressure model within the Mie-Grüneisen-type analysis framework. The calculated results have excellent agreement with the available volume compression data over a wide range of pressure and temperatrure. The comparison of the calculated results with the previous theoretical investigations also has been performed. The crosscheck on independent data and the excellent agreements with experimental data confirm that the present isothermal EOS for these pressure standard materials can be used as high-pressure scales for static DAC experiments.

1 Introduction

The pressure-volume-temperature equations of state (*P-V-T* EOSs) of relevant materials are important for various scientific fields [1]. In order to determine an accurate and reliable *P-V-T* EOS, the pressure and volume of the studied material should be known with high precision and accuracy. Nowadays, static diamond anvil cell (DAC) [2] and dynamic shock wave [3] experiments are two major methods to study the properties of materials at extreme experimental conditions. However, the particular difficulty with DAC experiments is to determine the exact pressure achieved in the experiment especially at various temperatures. Generally, the pressure, especially under high pressure and high temperature conditions, can be obtained from the diffraction line shifts of a standard material which is mixed with the sample and whose *P-V-T* EOS is well known. Therefore, the knowledge of the *P-V-T* EOS of relevant standard materials is one of the most basic information needed for pressure calibration [4,5].

However, tremendous differences in pressure can be achieved based on different pressure scales in the same DAC experiment. For example, Ono et al. [6] used both Jamieson's [7] and Anderson's [8] EOS of Au to determine the sample pressure in DAC experiment. These two equations give significantly different pressure for a given specific volume at high pressures. Recently, the measurements of Hirose et al. [9] show that the Au pressure scale [8] underestimate pressure with more than 10 GPa in comparison with MgO pressure scale [10] at pressure higher than 100 GPa and temperature up to 2330 K. From this point of view, crosscheck on relevant pressure scales is the key problem of the establishment of consistent pressure scales.

A method [11], for reducing shock-wave data to 0 K-isothemal EOS for metals, was proposed. Recently, this method is extended to calculate the *P-V-T* EOS of MgO through combining with a simple thermal pressure model [12]. We found that the calculated results is fully consistent with the available volume compression data. It gives us an impetus to calculate the *P-V-T* EOSs of Au and Pt because they are widely used as internal pressure scales in DAC experiments. The main purpose of the study is to establish a set of internally consistent pressure scales.

Table 1. Model parameters used in the present calculations for Au and Pt.

Material	$\rho_0/(\mathrm{g/cm^3})$	$C_l(\mathrm{km/s})$	S	γ_0	θ_D/K	$C_V/(\mathrm{J/kgK})$
Au	19.240	3.071 [29,30]	1.535 [29,30]	2.97 [29]	165 [31]	123 [8]
Pt	21.415	3.604 [27]	1.543 [27]	2.69 [28]	234 [28]	129 [32]

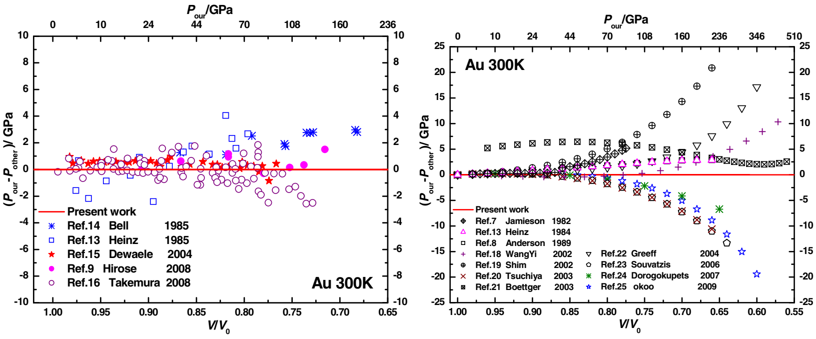

Fig. 1. Pressure difference between our calculation (P_{our}) and (a) the volume compression measurements and (b) other theoretical investigations (P_{other}).

2 Calculation results and discussions

Several different Au pressure scales have been proposed and the discrepancy between them often resulted in many arguments particularly in the earth science. Numerous investigations on the 300 K volume compression of Au have been performed in DAC experiments with the ruby scales or MgO scale. The large numbers of available experimental data are consistent with each other, and they can be used to verify the validity of different theoretical models. In the present calculation by using parameters listed in Table 1 and the method describled in Ref. [12], we calculated isothermal EOS of Au up to 500 GPa and 3000 K as shown in Fig. 1 and Fig. 2. For a comparison, the previous volume compression experimental [9,13–17] and other theoretical [7,8,13,18–25] data have been shown together.

As Fig. 1(a) shows, the 300 K isotherm obtained here has excellent agreement with the measured data by Dewaele et al. [15] up to 94 GPa, by Takemura et al. [16] up to 123 GPa based on the revised ruby scale [15], and by Hirose et al. [9] up to 140 GPa using MgO scale [10]. The maximum difference in the 300 K isotherm between the present and the measuremenets are less than 0.9 GPa, 2.5 GPa, and 1.5 GPa in the pressure range of 94 GPa, 123 GPa, and 140 GPa, respectively.

As Fig. 1(b) shows, all of the theoretical results have good agreement within the pressure range of 40 GPa except for the first-principles calculation by Boettger et al. [21]. However, the difference between these calculations increases gradually when pressure beyond 40 GPa, and the maximum difference reaches 30 GPa at about 230 GPa. The EOS models obtained from the first-principles calculations of Souvatzis et al. [23] and Tsuchiya et al. [20], and from the semi-empirical approach of Dorogokupets et al. [24] and Yokoo et al. [25] are in good agreement with each other. Unfortunately, the pressures determined by these four EOS models are much higher than experimental data [9,13–16]. In contrast, the proposed EOS model by Shim et al. [19], based on the inversion of quasi-hydrostatic compression and shock wave data, is significantly lower than all the other calculations. The first-principle calculations of Greeff et al. [22], shock-reduction results of Wang et al. [18] based on the first-principles mean-field potential approach, and semi-empirical calculations of Anderson et al. [8] and Heinz et al. [13] are in good agreement with our EOS model and experimental data in the pressure of 140 GPa.

In overall, the present calculated 300 K isotherm has excellent agreement with the available volume compression data and the theoretical investigations [8,13,18,22] over a wide range of pressure. Especially, the present 300 K isotherm and that of Wang are consistent, and the maximum deviation is less than 2.5%. The differences between our calculations and experimental data [15] are not beyond

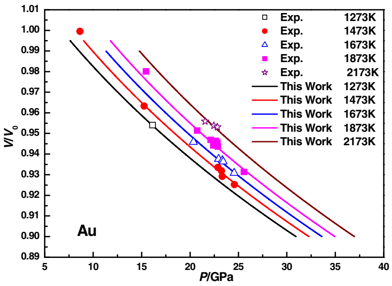

Fig. 2. The *P*-*V*-*T* EOS for Au. Comparison with experimental data at 1273 K~2173 K [28].

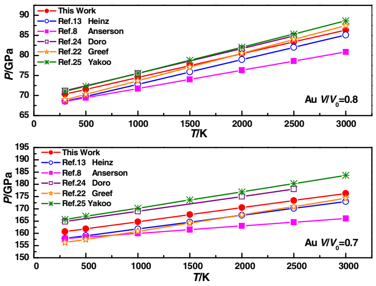

Fig. 3. Isochores for Au at $V/V_0 = 0.8$ and 0.7 upto 3000 K.

0.9 GPa up to 94 GPa which is used to recalibrate the ruby pressure scale. Thus, this study gives the supports to the revised ruby scale [15] at high pressure and room temperature.

It should be mentioned that the Pt scale of Holmes [26] predict higher pressure than other pressure scales. Matsui et al. [27] pointed out that it is duo to the Hugoniot parameters obtained by Holmes using the Hugoniot data over the pressure range of 32 GPa~660 GPa including the liquid region. Like that, the 300 K Au pressure scale proposed by Yokoo et al. [25], based on the shock Hugoniot data over the pressure range of 25 GPa ~ 580 GPa, are found to overestimate pressure at most 2% ($P < 100$ GPa) and 6% ($P < 350$ GPa). These overestimations are also mainly due to the differences in shock Hugoniot data used for modeling EOS.

Fei et al. [28] have measured the volume compression of Au at 1273 K, 1473 K, 1673 K, 1873 K, and 2173 K, and the pressure up to 25 GPa using the MgO scale [10]. We compared our calculations and these volume compression data at high temperature shown in Fig. 2. Our calculations are all in good agreement with these experimental data [28] over the wide pressure and temperature ranges up to 25 GPa and 2173 K. This is partly because the volume compression data measured by Fei et al. [28] is based on the Speziale MgO scale [10], which is in excellent agreement with our calculated *P*-*V*-*T* EOS of MgO [12] in the pressure and temperature range of 240 GPa and 3000 K.

We further compare our calculations with the other Au pressure scales at various temperatures. To do this two isochores are plotted at $V/V_0 = 0.8$ and 0.7 as a function of temperature from 300 K to 3000 K in Fig. 3. At $V/V_0 = 0.8$, our calculations have good agreement with the other four theoretical investigations up to 3000 K except for that of Anderson et al. [8], the difference is less than 2.5 GPa. However, in the more compressed region, the isochores begin to diverge widely. Although Anderson et al. pressure scale is consistent with our calculations at room temperature, it gives the lowest pressure at the temperatures above 1000 K at $V/V_0 = 0.8$ and 0.7. The comparison shows that the Anderson et al. EOS model is likely to underestimate the thermal pressure because of the larger value of q used in his study. The Yokoo et al. [25] and Dorogokupets et al. [24] pressure scales give the anomalously large pressure compared to the other pressure scales because of the reason mentioned above. The pressure scale of Heinz et al. [13] are in best agreement with our calculations in the entire volume compression and temperature ranges, as the results of the 300 K isotherm.

We also calculated isothermal EOS of Pt up to 500 GPa and 3000 K within the same theoretical framework. Cross-comparison among the present calculated *P*-*V*-*T* EOSs of Au and Pt, based on independent volume compression measurements at various temperatures, was conducted. The results show that the present calculated *P*-*V*-*T* EOSs of Au and Pt are mutually consistent. Their relative difference was found to be less than 1.0 GPa.

3 Summary

We calculated the *P*-*V*-*T* EOS of Au and Pt at pressures up to 500 GPa and temperatures up to 3000 K based on the shock Hugoniot data and a simple thermal pressure model within the Mie-Grüneisen-type analysis framework. All of the six parameters used in the present calculations can be measured with high accuracies. We found that the calculated *P-V-T* EOSs is fully consistent with the available volume compression data not only over a wide pressure range at 300 K, but also over a wide range of pressure and temperature. Of course, the present *P-V-T* EOSs of Au and Pt needs to be further verified by more EOS measurements at higher pressure and temperature region. The present calculated *P-V-T* EOSs of Au and Pt are mutually consistent, their relative difference was found to be less than 1.0 GPa. The crosscheck on the previous theoretical investigations and the excellent agreements with the experimental data confirm that the *P-V-T* EOS of Au and Pt can be used as a reliable pressure scale for high pressures and high temperatures DAC experiments.

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