Cascading crystallographic transitions $\alpha \rightarrow \omega \rightarrow \beta \rightarrow \beta' \rightarrow \beta''$ and melting curve of elemental zirconium

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Abstract

Applying Vinet equation of state (EOS) to analyze the experimental ambient isotherm data recently published by Stavrou et al. [1] for Zr metal, is reported. Precise fitting of the experimental data analyzed separately for each identified crystallographic phase ($\alpha$, $\omega$, $\beta$, $\beta'$ and $\beta''$) yield different bulk moduli $B_o$ and $B_o'$ and different zero pressure volumes ($V_o$) than those reported in the literature. Special attention is given to the bcc phases indicating cascading transitions $\beta \rightarrow \beta' \rightarrow \beta''$ associate with volume collapse. It is shown that the first order volume collapse at $\sim$58GPa ($\beta \rightarrow \beta'$) is followed by a moderate transition to the bcc-$\beta''$ phase. The $\beta'$ phase is stable up to 110GPa. Above 110GPa the bcc-$\beta''$ is dominant and stable up to $\sim$220GPa. By assuming isochoric conditions in the DAC the volume at the melt of the $\beta''$ phase is derived. The derived bcc-$\beta''$ bulk moduli are confirmed by the Lindemann-Gilvarry criterion as $B_o$ and $B_o'$ simultaneously fit both the P-V EOS and the P-T melting data points (combined approach). The calculated melting curve of elemental Zr which takes into account the thermal pressure shift $P_{oth}$ and the elevated melting $T_{mo'}$ at $P_{oth}$ yield very good fit of the experimental melting data which permits safe extrapolation to high pressures and temperatures. In addition, the combined approach lead to the direct determination of the Grüneisen parameter $\gamma_o$, needed for applying the approximated Lindemann-Gilvarry melting formula. In conclusion, the Zirconium $\beta''$ phase is analyzed within the combined approach, allowing the parametrization of reasonable bulk moduli, thus enabling the extrapolation the melting curve to high pressures and temperatures.

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Introduction - The physical-mechanical and melting properties of zirconium metal are of particular interest for the nuclear industry because of Zr’s low neutron absorption cross section and relatively high melting temperature (2128K). In addition, the bcc-to-bcc (β → β’) isostructural phase transition associated with volume collapse has attracted the scientific community during the last two decades. Pressure induced first-order isostructural transitions associated with volume collapse had been observed only in Ce, where an isostructural fcc→fcc phase transition with a substantial volume decrease up to a critical point is a well known effect [2,3]. The exact origin of the isostructural transition in Ce is still under debate, the general consensus, however, is that this transition is driven by a change in the degree of the localization and correlation of the one 4f electron. As early as in 1991 an isostructural bcc→bcc phase transition at ∼58 GPa in elemental Zr was suggested by Akahama et al. [4], speculating that this transition is triggered by s-d electronic transition.

Recently, Stavrou et al. [1] have performed at ambient temperature a precise XRD structural study of Zr up to 210GPa reconfirming the existence of an isostructural bcc-to-bcc phase transition claiming of first-order type. In addition, the bulk moduli of the β and β’ phases were derived utilizing the Birch-Murnaghan (BM) equation of state (EOS) [5]. Unfortunately, the fitting curves are not displayed in Fig.1 of Ref.1 and their results are only summarized there in Table I. In the present contribution I have performed accurate fittings of Stavrou et al. reported data using Vinet [6] and BM EOS. The fitting results revealed the existence of cascading β → β’→ β” bcc phases with different elastic constants reported in Ref.1.

The melting temperatures up to ∼80 GPa of Zr metal confined in a laser heated diamond anvil cell (DAC) were recently reported by Parisiades et al. [7]. Poor fittings of the experimental data by introducing the Lindemann-Gilvarry (LG) criterion and Simon-Glatzel procedure are depicted in the proposed phase diagram (there in Fig.5), the reason of which will be explained below.

In two recent publications [8,9] I have claimed that by assuming isochoric conditions in the DAC the LG criterion [10] is applicable for predicting the melting curves of metals. By introducing a constraint demanding that the fitting of the experimental EOS (P-V space) data will simultaneously fit the experimental melting results, consistent bulk moduli are obtained.

The LG criterion is not a theoretical model based on first principles but a phenomenological approach to the behavior of solids. Adopting the Lindemann criterion improved by Gilvarry, predictions of the melting curves
at high pressures and temperatures for metals were proposed [8]. The LG criterion needs the Grüneisen parameter $\gamma$. The procedure using the LG criterion together with the Grüneisen parameter $\gamma$, according to the Slater model [11] often does not fit the experimental melting results [12]. The LG formulation uses the bulk modulus $B$ and its pressure derivative $B'$ as fit parameters deduced directly from the EOS. However, the results are not unique reliant on the chosen EOS. The EOS [5,6] need two free parameters; the bulk moduli $B$ and $B'$ which are deduced from the P-V room temperature isotherm and are assigned $B_0$ and $B_0'$. Therefore, the reported values of $B_0$ and $B_0'$ for aluminum [13,14,15], copper [15,16], and uranium [18, 19,19,21,22] range up to $\sim 50\%$. In $\beta$-Zr the bulk moduli spread from 79 to 255GPa according to analysis reported by Greef [17], Stavrou [1] and Akahma [4]. Thus, the question remains, which of these bulk moduli should be addressed?

In the present paper the experimental data of Zirconium phases are analyzed according to the cascading $\alpha \rightarrow \omega \rightarrow \beta \rightarrow \beta' \rightarrow \beta''$ phases (P-V space). The $\beta''$ phase is analyzed using the combined approach [8], allowing the deduction of reasonable bulk moduli and enabling the extrapolation the melting curve to high pressures and temperatures.

**Lindemann-Gilvarry approximation** According to Lindenmann’s criterion
The melting temperature $T_m$ is related to the Debye temperature $\Theta_D$ as follows:

$$T_m = C \frac{V^{2/3}}{\Theta_D^2}$$  \hspace{1cm} (1)
Where \( V \) is the volume and \( C \) is a constant to be derived for each specific metal. In the Debye model the Grüneisen parameter \( \gamma \) is defined by 
\[
\gamma = \frac{\partial \ln \Theta_D}{\partial \ln V}.
\]
As shown by Anderson and Isaak [4] combining (1) and (2), inserting \( V_o/V = \rho/\rho_o \), and integrating one gets the form of the LG criterion for the melting temperature \( T_m \):

\[
T_m(\rho) = T_{mo} \exp \left\{ \int_{\rho_o}^{\rho} [2 \gamma - 2/3] d\rho/\rho \right\} \tag{2}
\]

Where \( \rho_o \) is a reference density, \( \rho \) is the density at the melt and \( T_{mo} \) is the melting temperature at the reference density. Integrating (2) assuming that \( \gamma = \gamma_o (\rho_o/\rho)^q \) and \( q = 1 \) one gets:

\[
T_m(\rho_o, T_{mo}) = T_{mo} (\rho_o/\rho)^{2/3} \exp[2 \gamma_o (1 - \rho_o/\rho)] \tag{3}
\]

where \( \gamma_o \) is defined as the Grüneisen parameter at ambient conditions [10].

Equation (3) states that if \( \rho(P) \), \( T_{mo} \) and \( \gamma_o \) are known the melting curve \( T_m(P) \) can simply be determined assuming that the relation between \( P \) and \( \rho \) is known.

It is well accepted that the pressure in the P-V-T space is given by:

\[
P(V,T) = P_C + \gamma_{lattice} C_v \rho \left[ T-T_o + E_o/C_{v \text{ lattice}} \right] + \frac{1}{4} \rho_o \gamma_e \beta_o (\rho/\rho_o)^{1/2} T^2 \tag{4}
\]

Here \( P_C \) is the cold pressure, \( C_v \) is the lattice specific heat above \( T_o \), \( T_o \) is the ambient temperature. \( C_{v \text{ lattice}} \) is taken as constant (usually at room temperature, following the approximation of Altshuler et al. [13] ) , \( E_o \) is the lattice thermal energy at \( T_o \) and \( \gamma_{lattice} \) is the lattice Grüneisen parameter. \( \gamma_e \) is electronic Grüneisen parameter and \( \beta_o \) is the electronic specific heat coefficient (Altshuler [13] and Kormer [24]). In most experiments, the material is compressed at room temperature and then heated to the melting point. The results obtained are known as the cold melting curve forming \( P_C \). In the second stage the actual pressure is obtained by adding the thermal pressure demanding that the shock wave data must serve as anchor to the fitting procedure. This two stage procedure have been confirmed for Al, Cu and U melting curves in reference [8].

The relation between \( P_C \) and the density \( \rho(P) \) for the room temperature isotherms are given by Vinet [5] and Birch-Murnaghan [6] equations of state. \( \rho \) is density and \( B = -V (\partial P/\partial V) \) is the definition of the bulk modulus and \( B' \) is the pressure derivative of the bulk modulus (\( B' = \partial B/\partial P \)). B and \( B' \) are fit parameters of the room temperature isotherm assigned as \( B_o \) and \( B_o' \). As stated
in the introduction, the best fit solutions are not unique and occasionally depends on the chosen EOS. This is the reason why diverse results are obtained by different authors.

Thus, it make sense to introduce a different procedure in order to improve the fittings of the data in the P-V and the P-T planes.

The following four step procedure to determine the correct melting curve (the combined approach) was proposed in [8]:

1. Utilize Lindemann-Gilvarry criterion (eq.3) with $\gamma_{\text{eff}}$ as a free parameter [8] and optimize $B_0$ and $B_0'$ by choosing the appropriate EOS which best fit simultaneously, the experimental P-V data (isotherm 300K) and the experimental melting P-T data. In this way obtaining $P_c$ and forming the cold melting curve. In LG eq.3 $T_m$ and $V_o$ are the melting temperature and volume at ambient pressure.

2. Adding the calculated thermal pressure $P_{\text{th}}$ to $P_c$ obtaining the LG melting curve accounting for the actual pressure (isochoric condition) sensed by the investigated sample. Demanding that the thermally corrected melting curve will include the shock wave melting data as anchor. The Grüneisen parameter $\gamma_o$ is derived accordingly.

   In the present Zr case the calculated thermal corrected melting curve should be applied [7].

3. Plotting of the volume compression $V/V_o$ vs. the thermally corrected melting temperatures obtained in 2.

4. Extrapolating the derived thermally corrected melting curve to high pressures and temperatures.

In DAC experiments, the material is compressed at room temperature and then heated to the melting point. In this case the claimed pressure is not the actual pressure and the $\gamma_o$ should be replaced by $\gamma_{\text{eff}}$ in eq.3 when fitting the
as measured experimental data thus forming the cold melting curve. By applying this procedure safe extrapolation of the melting curves to high pressures and temperatures done for Al, Cu, or U metals [8].

Assuming isochoric condition in the DAC upon heating the sample confined in a cell, thermal pressure develops associated with the increase of the melting temperature. The calculated thermal pressure ($P_{th}$) and the melting point $T_{m_{0}'}$ at ambient pressure are derived by calculating $P_{th}$ according to eq.4 and adjusting $\gamma_{o}$ to match the shock wave data forming the actual melting curve. To clarify, $P_{th}$ is the pressure shift from ambient pressure and $T_{m_{0}'}$ is the melting temperature at $P_{th}$. For Zr the calculated pressure shift is 8GPa and $T_{m_{0}'}=2300$K. The textbook melting point 2128K at zero pressure as derived in the open space simply does not exist in the heated DAC.

**Results** - The precise DAC measurements of the EOS elemental zirconium at ambient temperature (isotherm 300K) as reported by Stavrou et al. in PRB (2019) [1] is the first measurement performed with no transmission media (PTM). In other words, Zr metal fine powder is the PTM preventing uniaxial stress leading to a reliable EOS.

The analysis of this data using VIN or BM EOS are depicted in Fig.1 (solid lines). The experimental data of the hcp-$\alpha$ phase best fitted with the VIN EOS suggest bulk moduli $B_{o}=160$GPa and $B_{o}='=1$ and $V_{o}=23$ Å$^{3}$/at. (red solid line). The best fit of the hex-$\omega$ phase is obtained with the BM EOS suggest $B_{o}=190$GPa and $B_{o}='=3.3$ and $V_{o}=25$ Å$^{3}$/at. (green solid line). Increasing the pressure to above 34GPa the hexagonal crystallographic phase transforms to the bcc-$\beta$ phase. Further increasing the pressure reveal cascade of transitions to bcc phases, namely to $\beta'$ and $\beta''$. The $\beta$ phase is fitted with the bulk moduli parameters $B_{o}=203(20)$ GPa and $B_{o}='=3.3(2)$ in accord with Akahama [4]. Extrapolating to zero pressure yield $V_{o}=20(1)$ (Å$^{3}$/at.) (solid brown line). The second phase assigned $\beta'$ is fitted with $B_{o}=230(20)$ GPa and $B_{o}='=2.0(2)$, extrapolation to zero pressure lead to $V_{o}=18.3(2)$ (Å$^{3}$/at.) as the best fit. The third phase $\beta''$ is fitted simultaneously (combined approach steps 1and 2) with the bulk moduli parameters $B_{o}=265(10)$ GPa and $B_{o}='=3.3(1)$ where $V_{o}=16.8(2)$ (Å$^{3}$/at.), in agreement with $B_{o}$ claimed in [1], nevertheless, different $B_{o}'$ and $V_{o}$ are obtained. The cascade of transitions $\beta \rightarrow \beta' \rightarrow \beta''$ is clearly demonstrated in the inset of Fig.1 using the VIN EOS.
Fig.1: EOS of the elemental zirconium room temperature isotherm. The experimental data points are taken from Stavrou et al. [1] and are fitted with the VIN or BM EOS. The successive transformation from hcp to hexagonal to bcc structures are observed. The derived bulk moduli are assigned $B_o, B_o'$ and $V_o$ pointed with arrows. Above 30GPa the $\beta$ phase is dominant and a successive cascade to bcc-$\beta'$ and bcc-$\beta''$ are clearly demonstrated. The bcc-$\beta$ structure is stable up to ~58GPa, where a first order phase transition occurs with a volume collapse of ~5% which is stable up to ~105GPa (inset blue solid line). Above 105GPa and up to 220GPa a stable bcc-$\beta''$ exists (magenta solid line). The magenta solid line represents the simultaneous best fit of the experimental data in the P-V and P-T planes (see Fig.2) according to the combined approach (see text). The dashed blue line is the BM fitting of the $\beta''$ phase (see discussion).

Summary of the parametrized bulk moduli and the volumes at zero pressure are given in Table I:

| Zr Phase | $B_o$ (GPa) | $B_o'$ | $V_o$ (Å³/at.) | Fitting Procedure |
|----------|-------------|--------|----------------|------------------|
| $\alpha$-hcp | 160(5) | 1.0(0.3) | 23(2) | VIN |
| $\omega$-hex | 190(5) | 3.3(2) | 25(2) | BM |
| $\beta$ bcc | 203(7) | 3.3(2) | 20(2) | VIN |
| $\beta'$ bcc | 230(7) | 2.0(2) | 18.3(3) | VIN |
| $\beta''$ bcc | 265(5) | 3.3(1) | 16.8(4) | VIN simultaneously LG |
| $\beta''$ bcc | 255(10) | 3.3(2) | 21.3(3) | BM dashed blue line Fig.1 |

The thermally corrected (actual pressure) experimental melting data reported by Prisiades et al. [7] is in accordance with our calculations. However, the
thermal contribution upon raising the temperature experienced by the Zr sample confined in the DAC, $P_{th}$ and $T_{m,0}$, are not taken into account. Thus, poor fittings of LG or Simon-Glatzel are obtained (there in Fig.5). Applying the present combined approach, namely the LG criterion using $B_0$ and $B_0'$ determined above, deriving $P_{th}$ and $T_{m,0}$ and adjusting $\gamma_0$ accordingly, reveals the excellent fit of the thermally corrected experimental melting points. This allows the extrapolation of the melting curve to high pressures and temperatures shown (Fig.2):

![Melting curve of elemental Zr. The experimental melting data points (red O) are the thermally corrected pressure values reported by Prisiades et al.[7]. The square black are B. Radousky et al. [27]. The solid blue line stands for VIN and LG combined approach fitting procedure with the parameters $B_0$=265GPa and $B_0'$= 3.3 and $\gamma_0$=1.82 assigned VIN 265/3.3/1.82 arrow pointer inserted in the figure. V/Vo vs. melting temperature is depicted in the inset. V/Vo=16.8 (Å³/at.) is derived by the extrapolation to zero pressure shown in Fig.1 (magenta solid line β” phase). The calculated melting vs. the relative volume is depicted in the inset. Assuming isochoric condition in the DAC, the calculated thermal pressure shift $P_{th}$ and the melting temperature at $P_{th}$, $T_{m,0}$= 2300K, are the correction needed for the Zr sample confined in the DAC.

The choice of VIN EOS for the fittings the experimental melting points within combined approach, results from the fact that by no means the use of BM EOS can predict the melting curve of Zr metal. The parametrized bulk moduli $B_0, B_0'$ do not simultaneously fit the β” phase and the melting data.
Discussion – The EOS elemental zirconium at ambient temperature (isotherm 300K) reported by Stavrou et al [1] was performed in a DAC where the pressure transmitting medium (PTM) was fine powder of Zr, namely, no PTM was used. The influence of the PTM on the high pressure results was debated since the early studies using the DAC technique and is under discussion up to date [26]. The decision of Stavrou et al. to use fine powder of Zr as PTM remove uniaxial stress and possible misleading EOS. These excellent data warrant a precise analysis which utilize both VIN or BM EOS as shown in Fig.1. The bulk moduli $B_o$, $B_o'$ are derived separately for each of the crystallographic phases $\alpha, \omega, \beta, \beta'$ and $\beta''$. The $\beta''$ phase, fitted by both BM and VIN equations of state, shows that by no means $\beta'$phase can be denied. However, it can be argued that within the error bars, which are not depicted in Ref.1, the fittings of the EOS data using BM or VIN are both acceptable. Nevertheless, the BM formalism do not simultaneously fit the data of melting and the $\beta''$ phase according to the combined approach constraint. Therefore the use of VIN EOS shown in the inset of Fig.1 is the correct choice.

The analysis of any experimental point is referred to the center of mass of the error bars. What should be looked at is the trend of the experimental points relative to the fitting lines. In the present case all points in the region from 60 to 100GPa are above the VIN EOS fitting line. The fitting parameters, including the extrapolated $V_o$, are summarized in table I. Generally, best fit solutions are not unique and strongly depend on the chosen EOS and on the initial $B_o$ and $B_o'$ parameters inserted in to the fitting program. Thus, the derived bulk moduli given in Table I indicate an alternative best solutions for the P-V equations of state. This specially applies to the parameters proposed for $\alpha, \omega, \beta, \beta'$ phases. As shown in Fig.1 the transition $\omega \rightarrow \beta$ seems to be of first order type with volume collapse of ~10%. In the case of the $\beta''$ phase the derived bulk moduli $B_o,B_o'$ simultaneously best fit both, the EOS (Fig.1) and P-T phase diagram (Fig.2 ). Parisiades et al. [7] failed to fit their data with LG criterion because they used as an anchor the handbook ambient melting pressure (2128K) measured in the open space. Miss fitting has been reported recently by
B. Radouský [27] for the same reason. This melting point do not exist in the DAC. By introducing the thermally corrected $P_{th}$ and $T_{m_o}'$, and adjusting $\gamma_o$, a perfect fit is obtained according to the constraint of the combined approach. Thus allowing safe extrapolation of the melting curve of Zr metal to high pressures and temperatures shown in Fig.2.

The present analysis room temperature EOS data reveal a cascading bcc to bcc, pressure dependent volume transitions $\beta \rightarrow \beta' \rightarrow \beta''$ in the pressure region 34-200GPa. The first order volume collapse $\beta \rightarrow \beta'$ is followed by a smooth transformation to the $\beta''$ phase at $\sim$135GPa, in contradiction to the claim made in [1]. The $\beta''$ phase is the stable and dominant for Zr above 110GPa at 300K and is the phase approaching the melt, briefly described by Parisiades et al. [7].

Stavrou et al. applied first-principles combined density-functional theory (DFT) and finite temperature quantum molecular dynamics (QMD) calculating the EOS of Zr metal. Their results support the idea of a first-order pressure-induced isostructural phase transition which is triggered by un-harmonic motion. These simulations, as shown by the green line (there in Fig.1), do not pronounce the volume cascades $\alpha \rightarrow \omega \rightarrow \beta$ and the followed $\beta \rightarrow \beta' \rightarrow \beta''$ transitions. Crystal structures are typically relaxed in DFT electronic structure calculations as shown by the green solid line in Fig. 1 of Ref 1. In addition, the present analysis reveal that the $\beta'$ phase smoothly transform to $\beta''$, apparently by a second order type. It could be argued that the QMD calculations could predict higher temperatures isotherms rather than the 300K isotherm. It is expected that increasing the temperature will eliminate all the transitions like in the case of Ce [3].

**Conclusions** – Analysis of the experimental isotherm 300K data of Zr metal EOS, separately, for each identified crystallographic phase reveal different bulk moduli and zero pressure volumes $(V_o)$ to those reported previously in the literature. The cascade $\alpha \rightarrow \omega \rightarrow \beta$ phases are followed by additional $\beta \rightarrow \beta' \rightarrow \beta''$ bcc phases. Upon increasing the pressure at $\sim$135GPa, $\beta'$ phase smoothly transform to $\beta''$ phase indicating a moderate second order phase transition. The derived bulk moduli of the bcc-$\beta''$phase, are confirmed simultaneously by the approximated Lindemann-Gilvarry formula according to the procedure suggested in steps1 and 2 (combined approach). Inserting the actual pressure $P_{th}$ and the actual melting temperature $T_{m_o}'$ and
adjusting $\gamma_0$, yield a perfect fit of the reported melting data [2] allowing the extrapolation to high pressures and temperatures. The existence of the two crystallographic structures bcc-\(\beta'\) and $\beta''$ below the first order collapse at 58GPa, is here reported for the first time.

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