Theory for Pressure-dependent Melting Temperature of Metals

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Key Points:

- A theory for pressure-dependent melting curve of metals is developed to describe the solidification of metal under different pressures.
- The proposed theoretical model reveals the inner relationship between melting temperature and pressure.
- The model provides insights into the fundamental understanding of quantitative effect of pressure on melting temperature.

Abstract

We present a theory of pressure-dependent melting temperature to describe the physical fact that both cooling and pressurization can cause the solidification of liquid metal. Based on the Force-Heat Equivalence Energy Density Principle, an equivalent relationship between the heat energy variations during cooling and the mechanical work during pressurization is established as the molten metal solidifies. Then, this equivalent relationship is applied to develop a pressure-dependent melting temperature model without any adjustable parameter for metals. The model reveals the inner relationship between melting temperature, pressure, the bulk modulus and its first pressure derivative at zero pressure. The predicted results by our model are in good agreement with the available experimental data. Moreover, this study provides insights into the fundamental understanding of quantitative effect of pressure on melting temperature, which is in contrast to the well-known Lindemann's and Simon's equations that are both empirical melting temperature equations. It is worth noting that the melting curve of metals to very high pressure can be well predicted by our model only needing two experimental data at low pressures.

1 Introduction

The melting behavior of metals to very high pressure is an important field in geophysics (Errandonea, 2013), which helps to understand the properties of planetary interiors (Vočadlo and Alfè, 2002). Melting processes in the deep mantle of Earth have important implications for the origin of the deep-derived plumes believed to feed hotspot volcanoes (Andrault et al., 2012). Extensive experimental and theoretical studies have been performed on the melting behavior of metals (Boehler, 1993; Yoo et al., 1993; Alfè et al., 2004; Zhang et al., 2016). At low pressure, the experimental results of melting temperature (T_m) are mainly measured using diamond-anvil cells (DAC) method, which presents relatively few problems (Boehler, 1993; Alfè et al., 2004). However, the DAC experiments become progressively more difficult when the pressure increases above about 100 GPa (Alfè et al., 2004). When the pressure is above 200 GPa, the shock wave (SW) experiments is the only available measurement method of getting melting temperatures (Alfè et al., 2004). Nevertheless, the temperature cannot be obtained directly through SW experiments because this kind of experimental method needs to use some assumptions of the Grüneisen parameter and the specific heat (Yoo et al., 1993; Alfè et al., 2004). Therefore, the significant error exists when estimating by the SW method (Alfè et al., 2004). To better understand the melting behavior of metals to very high pressure, theoretical calculation is an alternative and convenient approach to obtaining of metals to very high pressure (Laio et al., 2000). To date, many theoretical methods have been proposed to predict in different pressure ranges (Laio et al., 2000; Belonoshko et al., 2000; Zhang et al., 2016). First principles and molecular dynamic (MD) simulations (Laio et al., 2000) have been used to forecast the melting temperature of solids, but they show difficulties in complex computation using different potential energy functions (Belonoshko et al., 2000; Zhang et al., 2016). In addition, the simulation results do not always meet the experimental results (Belonoshko et al., 2000; Errandonea, 2010, 2013; Zhang et al., 2016). The estimations of the melting temperature still mostly depend on several well-known empirical melting equations, including Lindemann's equation (Wang et al., 2001) and Simon's equation (Errandonea, 2010). However, the empirical melting equations generally stem from the earlier melting measurements at the relative lower pressure ranges (Wang et al., 2001), and bring large uncertainties for the assessment of melting curves under extremely high pressure. Moreover, even though empirical equations can describe the experimental results, they do not have reliable predictive ability. The reliable prediction of melting temperature to very high

pressure is still a challenging problem (Errandonea, 2013, Zhang et al., 2016). Thus, this study aims to establish a unified model to quantitatively characterize the inner relationship between melting temperature and pressure for metals, and then achieves the reliable prediction of the melting temperature of metals to very high pressure.

2 Method and model

In the previous work, Li et al. (2010) has proposed the Force-Heat Equivalence Energy Density Principle, which established the equivalent relationship between mechanical work and heat energy in the contribution to material failure. For a certain material, both the mechanical work and heat energy can change the chemical bonds between atoms. And the principle has been successfully applied to quantitatively characterize the temperature dependence of mechanical properties of materials, such as fracture strength (Li et al., 2010), critical resolved shear stress (Ma et al., 2018) and yield strength (Li et al., 2019). For liquid metals, they can be solidified either by cooling or by pressurization. Here, the energy variations of metal caused by cooling and pressurization can be represented by heat energy and mechanical work of pressure, respectively. Based on the Force-Heat Equivalence Energy Density Principle, we can assume that: the heat energy variations during solidification with isobaric cooling have an equivalent relationship with the mechanical work during isothermal pressurization for metals. In the isobaric solidification process, the heat energy variations can be evaluated by potential energy between atoms and kinetic energy of atomic motion at different temperatures (Zhang et al., 2018). Thus, the equivalent relationship between heat energy variations and mechanical work is expressed as:

$$W(P)\big|_T^{\,n} = \alpha\, E_{ke}(\Delta T)\big|_P + \beta\, E_{pe}(\Delta T)\big|_P \tag{1}$$

where $W(P)$ is the mechanical work under the pressure P, ΔT is the temperature difference. $E_{ke}(\Delta T)$ and $E_{pe}(\Delta T)$ are the kinetic energy variations of atomic motion and potential energy variations of atoms in per unit mass, respectively. α and β are the equivalent coefficients, n is an equivalent index.

The average kinetic energy of atoms is equal to the average potential energy between atoms for the periodical change of vibrating atoms. The kinetic energy and potential energy density in per unit mass at different temperatures can be expressed as:

$$E_{pe}(T)\big|_P = E_{ke}(T)\big|_P = \frac{3}{2} k N_0 T / M\big|_P \tag{2}$$

where T is the temperature (in Kelvin), k is the Boltzmann constant (1.381×10^{-23} J K^{-1}), N_0 is the Avogadro's constant (6.023×10^{23} mol^{-1}), M is the molar mass.

In the isothermal compression process, the volume of the object will change under the influence of external pressure. The amount work of the external pressure acting on a unit mass object can be expressed as (Callen, 1985):

$$W(P)\big|_T = -\int_v P(v)\,\mathrm{d}v\big|_T \tag{3}$$

where v is volume per unit mass.

If the melting temperatures at P_1 and P_2 are obtained, substituting Equation (2) and Equation (3) into Equation (1), one can get that:

$$-\left(\int_{V_1}^{V_2} P(v)\,\mathrm{d}v\big|_T\right)^n = \frac{3}{2}(\alpha+\beta)\,kN_0(T_{\mathrm{m2}}-T_{\mathrm{m1}})/M\big|_P \tag{4}$$

where V_1 and T_{m1} are the volume per unit mass and melting temperature at pressure P_1, respectively. V_2 and T_{m2} are the volume per unit mass and melting temperature at pressure P_2, respectively.

The relative volume under applied pressure can be calculated by the Murnaghan equation (Akella and Kennedy, 1971) using the bulk modulus B_0 and its first pressure derivative B_0' at $P=0$, which can be given as:

$$P = \frac{B_0}{B_0'}\left[\left(\frac{v_0}{v}\right)^{B_0'} - 1\right] \tag{5}$$

where v_0 denotes the specific volume at zero pressure.

Substituting Equation (5) into Equation (4), one can conclude that:

$$\alpha+\beta = -2M\left(\frac{V_2(P_2+B_0)-V_1(P_1+B_0)}{1-B_0'}\right)^n \Big/ \left[3kN_0(T_{\mathrm{m2}}-T_{\mathrm{m1}})\right] \tag{6}$$

For the melting temperature at arbitrary pressure, the following relationship can be obtained:

$$-\left(\int_{V_1}^{V} P(v)\,\mathrm{d}v\big|_T\right)^n = \frac{3}{2}(\alpha+\beta)\,kN_0(T_{\mathrm{m}}-T_{\mathrm{m1}})/M\big|_P \tag{7}$$

where T_{m} is the melting temperature at pressure P. Substituting Equation (5) and Equation (6) into Equation (7), T_{m} can be expressed as:

$$T_{\mathrm{m}} = T_{\mathrm{m1}} + \left(\frac{(\frac{B_0'P+B_0}{B_0'P_1+B_0})^{-\frac{1}{B_0'}}(\frac{P+B_0}{P_1+B_0})-1}{(\frac{B_0'P_2+B_0}{B_0'P_1+B_0})^{-\frac{1}{B_0'}}(\frac{P_2+B_0}{P_1+B_0})-1}\right)^n (T_{\mathrm{m2}}-T_{\mathrm{m1}}) \tag{8}$$

Utilizing Equation (8), the melting temperature of ten kinds of metals are predicted and the predictions are compared with the recent experimental values measured by Errandonea (2010) as well as previous theoretical results. During the calculation, the bulk modulus B_0 and its first pressure derivative B_0' used in this study are given in Table 1. And the first and last experimental data of melting temperature which were also measured by Errandonea (2010) are taken as the reference values to predict those ten metals. As we can see in figure 1, the predicted

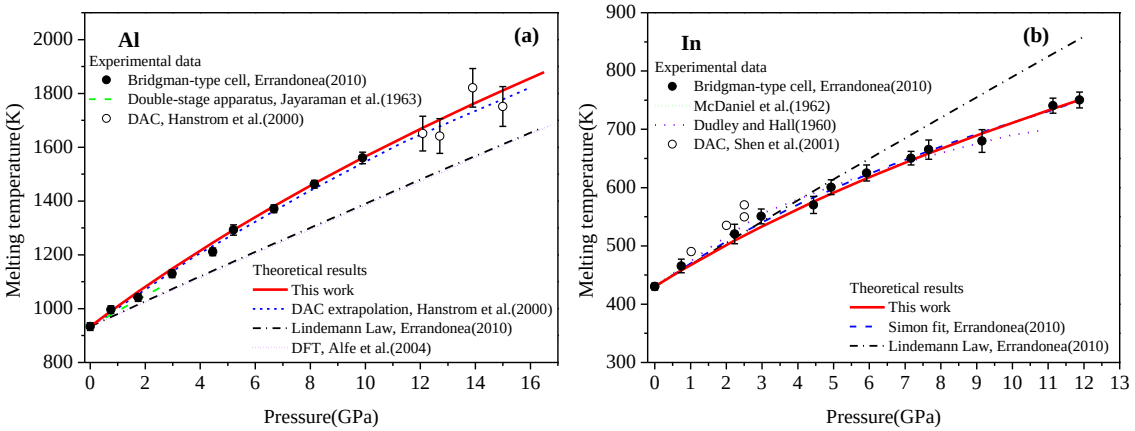
results of Mg, Mn, Cu, Ag, Au, Zn, Cd, Al, In, and Pb by our model agree well with these measurements (Errandonea, 2010) when the index n in Equation (8) is 1/2. Thus, the index n is determined as 1/2, and the final form of the proposed pressure-dependent melting temperature model is:

$$T_{\mathrm{m}} = T_{\mathrm{m1}} + \left(\frac{(\frac{B_0' P + B_0}{B_0' P_1 + B_0})^{-\frac{1}{B_0'}} (\frac{P + B_0}{P_1 + B_0}) - 1}{(\frac{B_0' P_2 + B_0}{B_0' P_1 + B_0})^{-\frac{1}{B_0'}} (\frac{P_2 + B_0}{P_1 + B_0}) - 1} \right)^{1/2} (T_{\mathrm{m2}} - T_{\mathrm{m1}}) \quad (9)$$

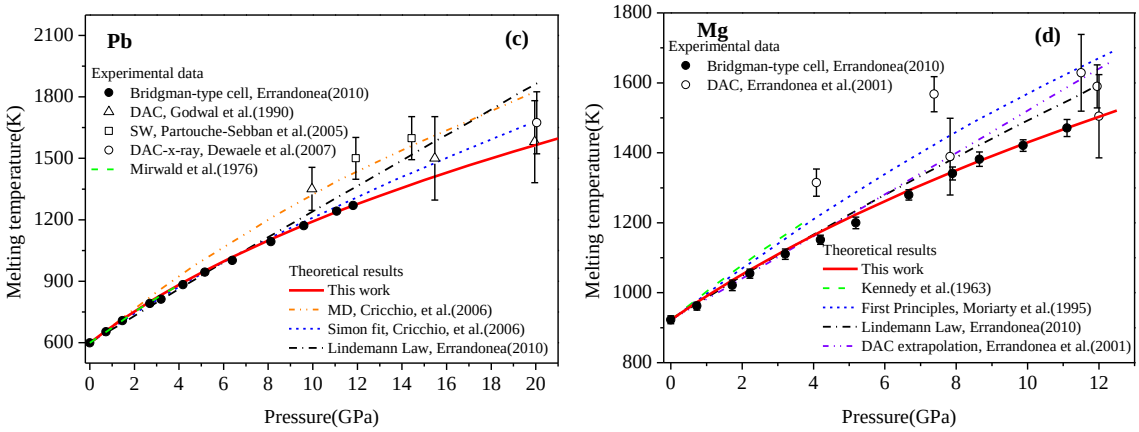
Table 1. Bulk modulus B_0 and pressure derivative B_0' of the metals

Metal	B_0 (GPa)	B_0'	Reference	Metal	B_0 (GPa)	B_0'	Reference
Au	167	6.00	Dewaele et al., (2004)	Ag	101	6.2	Holzapfel and Nicol (2007)
Pt	277	5.08	Dewaele et al., (2004)	Mg	36.8	4.3	Errandonea et al., (2003)
Ta	194	3.52	Dewaele et al., (2004)	Ni	183	6.2	Guinan and Steinberg (1974)
W	296	4.30	Dewaele et al., (2004)	Mo	263	4.4	Guinan and Steinberg (1974)
Cu	133	5.30	Dewaele et al., (2004)	γ-Fe	166	5.29	Guinan and Steinberg (1974)
Al	73	4.54	Dewaele et al., (2004)	Pd	193	5.35	Guinan and Steinberg (1974)
In	41.8	4.81	Takemura, (1991)	Tl	35.7	5.09	Guinan and Steinberg (1974)
Cd	42	6.5	Takemura, (1997)	Co	190	4.26	Guinan and Steinberg (1974)
Zn	65	4.6	Takemura, (1997)	Cr	162	4.89	Guinan and Steinberg (1974)
Mn	158	4.6	Fujihisa and Takemura, (1995)	α-Sn	52.13	4.18	Cui et al., (2008)
Ti	155.87	2.73	Srivastava et al., (2011)	Pb(fcc)	43.20	4.87	Vohra and Ruoff (1990)
V	132.06	2.49	Srivastava et al., (2011)				

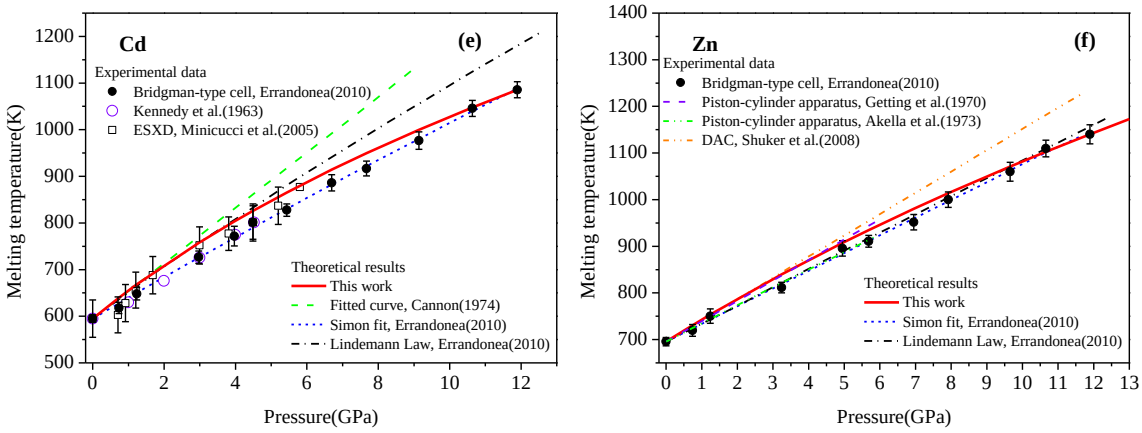
One can see that the model (Equation (9)) does not include any adjustable parameter, which uncovers the quantitative relationship between the melting temperature at different pressures, the bulk modulus and its first pressure derivative at zero pressure. And since the bulk modulus and its first pressure derivative at zero pressure of metals can be conveniently obtained from material handbooks or literatures, the melting curve of metals to very high pressure can be easily predicted by our model only using two easily obtained melting temperatures at low pressures.


Al
(a)
Experimental data
Bridgman-type cell, Errandonea(2010)
Double-stage apparatus, Jayaraman et al.(1963)
DAC, Hanstrom et al.(2000)
Theoretical results
This work
DAC extrapolation, Hanstrom et al.(2000)
Lindemann Law, Errandonea(2010)
DFT, Alfe et al.(2004)
Melting temperature(K)
Pressure(GPa)
In
(b)
Experimental data
Bridgman-type cell, Errandonea(2010)
McDaniel et al.(1962)
Dudley and Hall(1960)
DAC, Shen et al.(2001)
Theoretical results
This work
Simon fit, Errandonea(2010)
Lindemann Law, Errandonea(2010)
Melting temperature(K)
Pressure(GPa)

136


Pb
(c)
Experimental data
Bridgman-type cell, Errandonea(2010)
DAC, Godwal et al.(1990)
SW, Partouche-Sebban et al.(2005)
DAC-x-ray, Dewaele et al.(2007)
Mirwald et al.(1976)
Theoretical results
This work
MD, Cricchio, et al.(2006)
Simon fit, Cricchio, et al.(2006)
Lindemann Law, Errandonea(2010)
Melting temperature(K)
Pressure(GPa)
Mg
(d)
Experimental data
Bridgman-type cell, Errandonea(2010)
DAC, Errandonea et al.(2001)
Theoretical results
This work
Kennedy et al.(1963)
First Principles, Moriarty et al.(1995)
Lindemann Law, Errandonea(2010)
DAC extrapolation, Errandonea et al.(2001)
Melting temperature(K)
Pressure(GPa)

137


Cd
(e)
Experimental data
Bridgman-type cell, Errandonea(2010)
Kennedy et al.(1963)
ESXD, Minicucci et al.(2005)
Theoretical results
This work
Fitted curve, Cannon(1974)
Simon fit, Errandonea(2010)
Lindemann Law, Errandonea(2010)
Melting temperature(K)
Pressure(GPa)
Zn
(f)
Experimental data
Bridgman-type cell, Errandonea(2010)
Piston-cylinder apparatus, Getting et al.(1970)
Piston-cylinder apparatus, Akella et al.(1973)
DAC, Shuker et al.(2008)
Theoretical results
This work
Simon fit, Errandonea(2010)
Lindemann Law, Errandonea(2010)
Melting temperature(K)
Pressure(GPa)

138

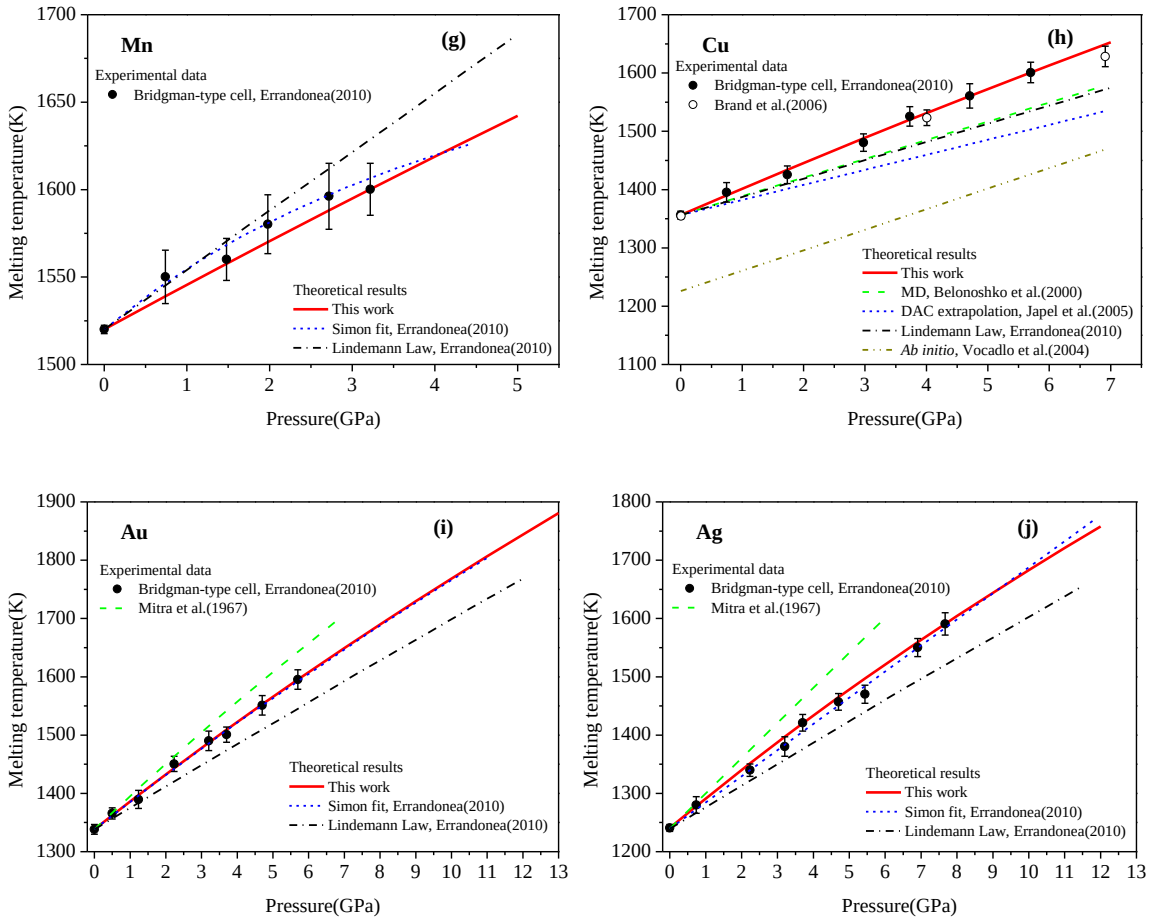


Figure 1. Comparison of predicted results and experimental data of pressure dependent melting temperature of Al, In, Pb, Mg, Cd, Zn, Mn, Cu, Au and Ag

3 Results and discussions

As we can see from figure 1, the predictions by our model are in better agreement with available experimental data than Lindemann Law, first principles and MD simulations results. To further verify the predictive ability and accuracy of our model, the extrapolation of prediction results of Cu and Al to higher pressures are also forecasted. As shown in figures 2 and 3, the predictions of Cu and Al by our model are more consistent with the experimental results than previous theoretical methods such as MD, generalized pseudopotential theory (GPT) and *Ab initio* calculations. In figure 3, the theoretical results of Al by using density functional theory (DFT) and Harrison local pseudopotential (HLP) models are also highly consistent with experimental data. However, the DFT and HLP methods rely on accurate calculation of interatomic interactions using quantum mechanics techniques (Alfè et al., 2004) which are difficult to apply.

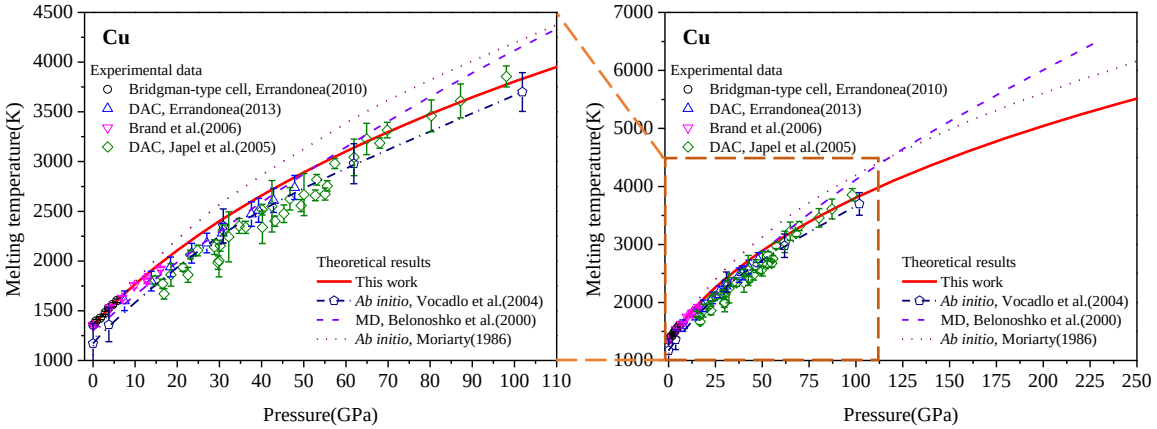


Figure 2. The predicted melting temperature of Cu to higher pressures by our model compared with the experimental data and previous theoretical results.

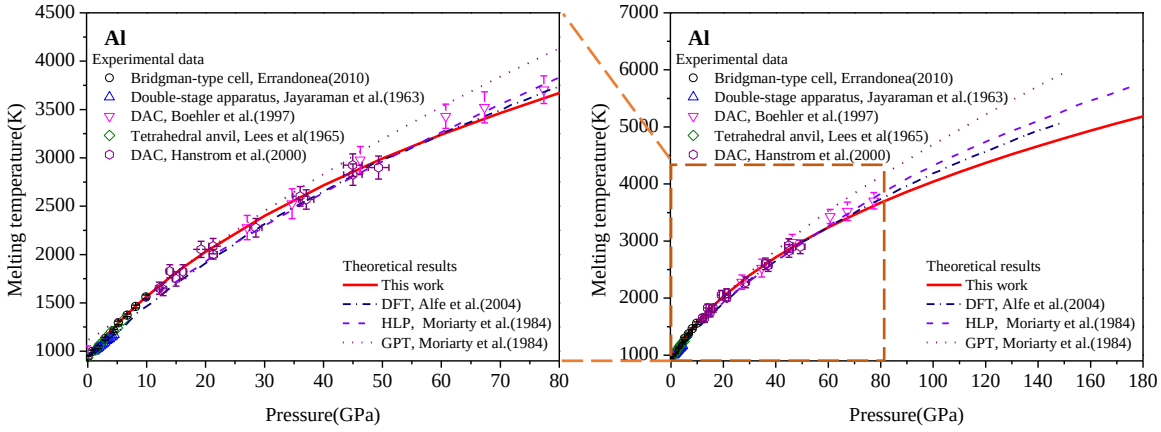


Figure 3. The predicted melting temperature of Al to higher pressures by our model compared with the experimental data and previous theoretical results.

Besides, the melting temperatures of Pd, Pt, Co and Ni at different pressures are also predicted and compared with the experimental data as well as previous theoretical results. In Equation (9), the selection of the reference point (T_{m1} and T_{m2}) is arbitrary. For convenience, we can choose one melting temperature at atmospheric pressure and the other melting temperature near atmospheric pressure as reference points. In figures 4, 5 and 6, the reference melting temperatures are marked with the dotted oval. The predicted results of Pd by our model are in better agreement with experimental results than MD and two-phase (TP) methods, as shown in figure 4. For Pt in figure 5, the *Ab initio* simulation results varying linearly with pressure also agree well with the experimental values up to 30 GPa. It can be also found that the predicted results by our model are not only in excellent agreement with experimental data but also reflect the nonlinear relationship between the melting temperature and pressure. The prediction results of Co and Ni to higher pressures are highly consistent with experimental data, as shown in figure 6 (a) and (b).

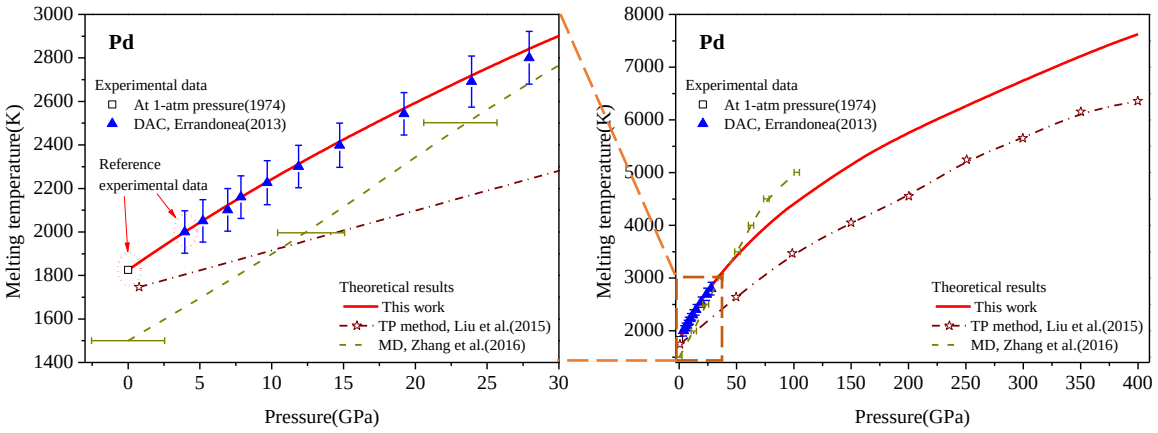


Figure 4. The predicted melting temperature of Pd to higher pressures by our model compared with the experimental data and previous theoretical results.

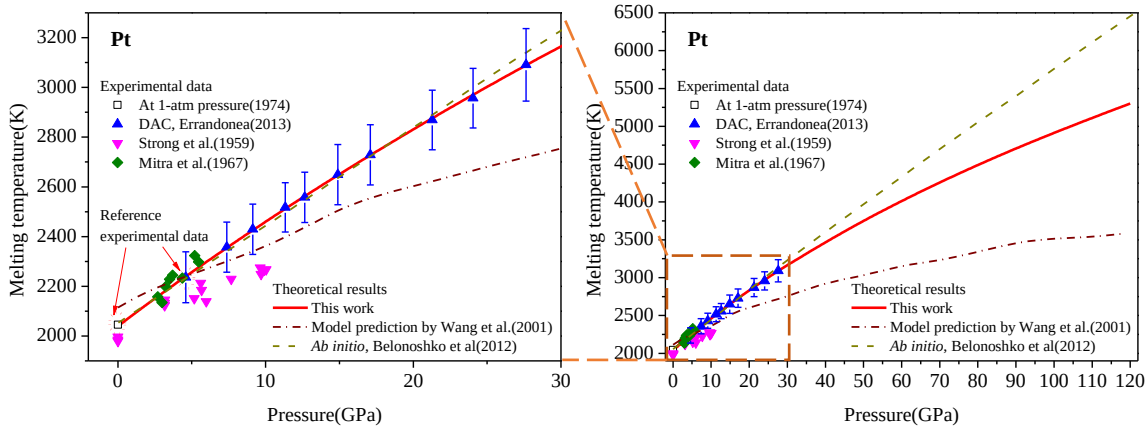


Figure 5. The predicted melting temperature of Pt to higher pressures by our model compared with the experimental data and previous theoretical results.

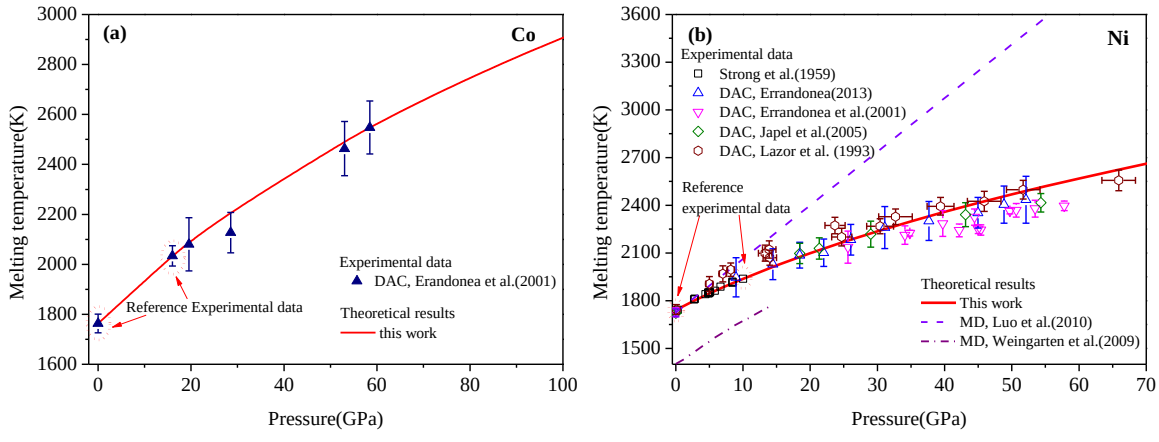


Figure 6. The predicted melting temperature of Co and Ni to higher pressures by our model compared with the experimental data.

Furthermore, the melting temperature of Tl, Sn and In at different pressures are predicted by our model, and the predictions are compared with the experimental data measured by McDaniel et al. (1962), as shown in figure 7(a). The predicted results of γ-Fe are shown in figure 7(b) and are compared with the experimental data measured by Boehler et al. (1990). Besides, the pressure dependence of melting temperature of W, Ta, Mo, V, Ti, and Cr up to 100GPa are also predicted, and compared with the experimental data measured by Errandonea et al. (2001), as shown in figure 8. The reference melting temperatures used in Equation (9) are also marked with the dotted oval in these figures. In all these cases, one reference melting temperature is at normal atmospheric pressure, and the other reference melting temperature is nearest to normal atmospheric pressure except W and Ta. The average data at around 17GPa for W and around 10GPa for Ta are set as reference melting temperature because of the dispersion of experimental data. The predicted results of above metals are all in good consistency with the experimental data, which further proved the predictive ability and accuracy of the pressure-dependent melting temperature model proposed in this study.

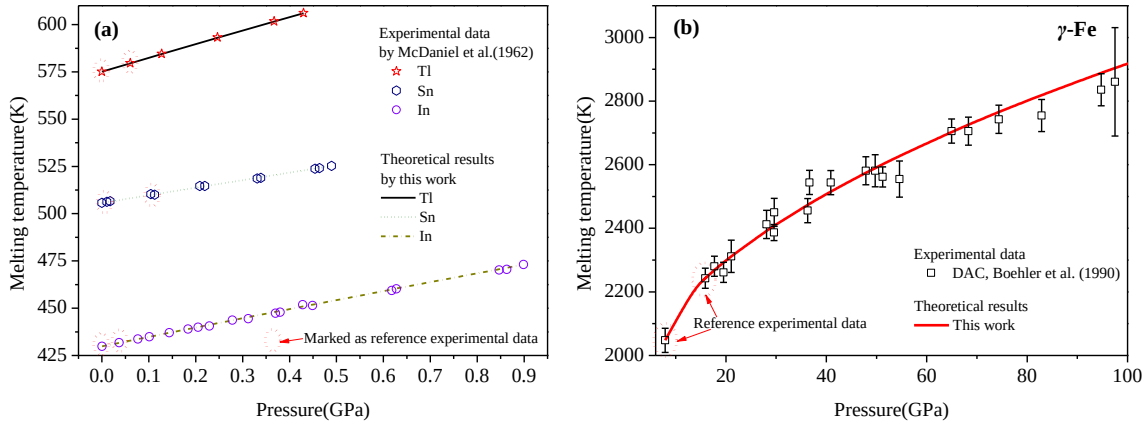


Figure 7. Comparison of pressure dependence of melting temperature of Tl, Sn, In and γ-Fe predicted by our model with the experimental data.

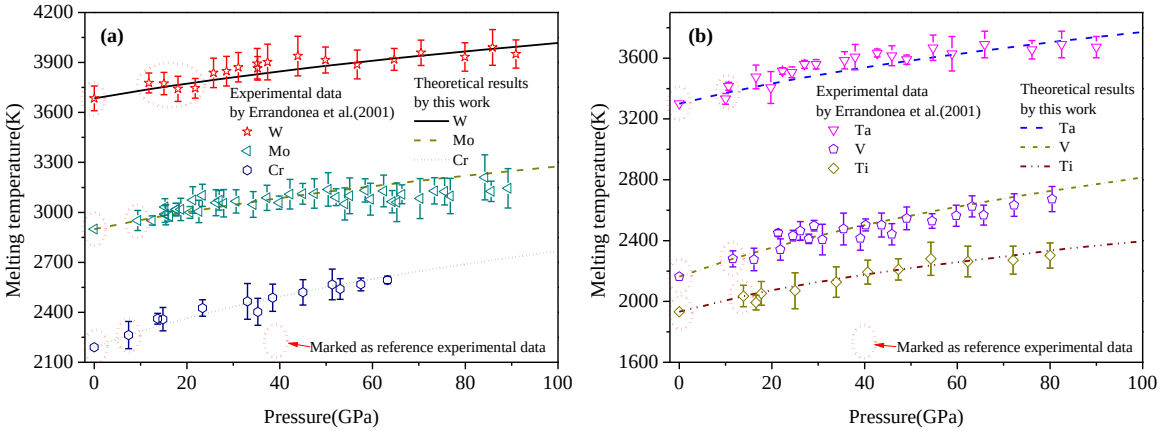


Figure 8. Comparison of pressure dependence of melting temperature of W, Mo, Cr, Ta, V and Ti predicted by our model with the experimental data.

4 Conclusions

A pressure-dependent melting temperature model without any adjustable parameter for metals is developed in this study based on the Force-Heat Equivalence Energy Density Principle. The model uncovers the interrelationship between the melting temperature at different pressures, the bulk modulus and its first pressure derivative at zero pressure. The predicted pressure-dependent melting curves of metals by the proposed model are highly consistent with the available experimental data. Moreover, the model is more convenient to apply than the existing theoretical and simulation methods. The proposed model can easily predict the melting curve of metals to very high pressure only using two melting points at low pressures. The study develops a theoretical approach to predicting the melting curve of metals to very high pressure.

Acknowledgments

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