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The universal equation of state applied to analysis of EOS data for solid molybdenum and tungsten

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Abstract The universal equation of state of solids (UEOS) proposed by Vinet is applied to analysis of EOS data for Mo and W in literature obtained experimentally and by ab initio theoretical calculations reported by different groups. It is demonstrated that the experimental measurements and theoretical calculations are consistent with each other and UEOS is a good analytical expression of EOS for solid Mo and W. The bulk modulus and thermo-expansion coefficients calculated from EOS analysis for Mo and W are in agreement with values obtained by direct measurements with other techniques with high accuracy.

Introduction

Equation of state (EOS) for solids is of fundamental importance in theory of solids and in practical applications, especially for refractory metals such as Mo and W, which are often used at high temperatures or under high-pressure conditions. It is important to predict their mechanical properties at high temperatures. A lot of works have been done to determine EOS either by direct experiments or by first principle theoretical calculation [1–7]. It is valuable to analyze and make comparison of these data obtained with quite different approaches by different groups to find the analytical expression of EOS suitable for these metals. In this paper, we shall collect as possible so far all the EOS data reported obtained by experiments and first-principle theoretical calculation by different groups for Mo and W, and demonstrate that all the results either obtained by experiments or by first-principle theoretical calculation are well consistent and in accord with the universal equation of state (UEOS) proposed by Vinet et al. [8–10].

A short review of EOS investigation methods for solid molybdenum and tungsten

The EOS for one-component system is a functional $f(P, V, T) = 0$ representing a curved surface in P–V–T space. The isotherms and Hugoniots are particular curves on this surface. Along the Hugoniots, the energy is known while the pressure and volume vary. The static experimental study of EOS is evident, but it is limited to low pressure and small temperature change. The Hugoniots are often obtained by shock-wave compression produced often by two-stage light gas gun. The dynamic Hugoniot method can cover a large range of pressure and volume change, but the temperature is missing, which is inconvenient in use and in understanding EOS in usual sense.

A static measurement of the pressure-dependent change of volume of Mo was reported by Mao et al. [1]. On calibrating the wave length shift with the pressure of the ruby R_1 flourescence line in the Diamond-window pressure cell from 0.06 to 1 Mbar (100 GPa), these authors measured simultaneously the fluorescence line shift of ruby and specific volume of four metals (including Mo) by measuring the X-ray diffraction lines and assuming the ratio of inter atomic distances d/d_0 to be equal to $(V/V_0)^{1/3}$, where V_0 is the atomic volume at 1 bar. The pressure was

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determined from the pressure volume function of Carter et al. [11] related to the ruby R_1 wavelength.

For measuring Hugoniot, people used to carry out shock-wave compression test and transform the kinematic variables into thermodynamic variables as follows [12, 13]. Due to the laws of conservation of mass, momentum and energy during the test of shock-wave compression across the shock-wave front, we have

$$\rho_0 u_s = \rho_H (u_s - u_p), \tag{1}$$

$$P_H - P_0 = \rho_0 u_s u_p, \tag{2}$$

$$\left(E_H - E_0 + u_p^2/2\right)^2 \rho_0 u_s = P_0 u_p \tag{3}$$

where u_s is the shock front velocity, u_p the particle velocity in the compressed region, E_H, P_H, ρ_H, the specific energy, the pressure and the density behind the shock-wave front, respectively. E_0, P_0, and ρ_0 are correspondingly the values of these quantities ahead of the shock-wave front.

If no phase transformation occurs during the test, for many substances, in a wide range of particle velocities, u_s is a linear function of u_p:

$$u_s = c_0 + s u_p. \tag{4}$$

The Hugoniot parameters, the intercept c_0 and the slope s can be obtained by least square statistic fitting of the measured values u_s and u_p. Thus, from Eqs. 1–4, we can have:

$$P_H = P_0 + \frac{\rho_0^2 c_0^2 \eta}{(1 - \eta s)^2}, \tag{5}$$

$$E_H = E_0 + \frac{c_0^2 \eta^2}{2(1 - \eta s)^2} = E_0 + \frac{1}{2}(P_H + P_0)(V_0 - V_H), \tag{6}$$

$$\eta = 1 - \frac{V}{V_0} = 1 - \frac{\rho_0}{\rho}. \tag{7}$$

Having the values of kinematic Hugoniot parameters c_0 and s, one can calculate the thermodynamic quantities E, P for different values of V. The possibility of transformations of kinematic variables into thermodynamic quantities is based on the assumption that the material in the compressed region is isotropic and in thermodynamic equilibrium state, which, as it is well known, is generally related only to thermostatic state in thermodynamic limit. As in Eqs. 5–7, the effect of temperature and the caloric terms are missing, so it is difficult to get entirely EOS in terms of $P(V, T)$ in analytic form merely from the shock-wave compression test data. To circumvent this circumstance, it is necessary to resort to some physical models such as Gruneisen model of solids and Debye model of specific heat. Hixon et al. [2] assumed the Gruneisen function $\gamma = V\left(\frac{\partial P}{\partial E}\right)_V$ to be dependent only on volume and further validity of the approximation $\rho\gamma = \text{constant}$. Taking advantage of Debye theory, these authors derived a set of equations and used the experimentally measured Hugoniot parameters c_0 and s to calculate the Hugoniots and isotherms of EOS for different temperature for Mo and W and presented the numerical results in tables.

The first-principle theoretical calculation of P–V relation was conducted by Christensen et al. [3] for Mo, and Ruoff et al. [6] for W. These authors used a full-potential linear muffin-tin orbital (FP-LMTO) method and obtained $P\left(\frac{V}{V_0}\right)$ relation at 0 K up to $\frac{V}{V_0} = 0.4$, where V_0 is the volume at zero pressure. Later, Wang et al. [5] reported their results of ab initio calculation of Hugoniots and 293 K isotherm up to 1,000 GPa for Al, Cu, Ta, Mo, W. These authors used the classical mean-field approximation and derived the cold and the thermal parts of the Helmholtz free energy entirely from the 0 K total energies and the electronic density of states calculated with the full-potential linearized augmented plane wave method. This approach permitted them to do efficient computation without involving empirical parameters except for atomic volumes. They reported the Hugoniots in form of figures and presented their 293 K isotherms of P–V relation in form of tables. To the authors knowledge, neither the theoretical works of Wang et al. [5], Christensen et al. [3], Ruoff et al. [6] nor the experimental studies of Hixon et al. [2] and Mao et al. [1] have explicitly given the analytical expression of EOS for Mo and W in terms of P–V–T variables.

Analysis of EOS data for Mo and W using UEOS proposed by Vinet et al. [8–10]

We are interested in analytical expression of EOS for Mo and W in terms of P–V–T variables, but as we have seen in previous sections, most of the present EOS data for them were given in Hugoniots, where the T variable is lacking.

Based on the discovery of universal features of scaled-bonding energy versus scaled-atomic separation in many solids, Vinet et al. [8–10] proposed a UEOS, which was demonstrated to be valid for many solids with different bonding nature. In our calculation of the total energy by LMTO method, we found that several metallic diborides also follow UEOS [14, 15]. It came to us that the UEOS proposed by Vinet et al. might be the most appropriate analytical expression of EOS for solid Mo and W.

The UEOS for solids proposed by Vinet et al. [8–10] reads:

$$P(T, x) = \frac{3B_0(T_R)}{x^2}(1 - x)\exp(b(T_R)(1 - x)) + \Delta P_{th} \tag{8}$$

where

$$x = \left(\frac{V}{V_0(T_R)}\right)^{1/3}. \tag{9}$$

$V_0(T_R)$ is the volume at zero pressure and the reference temperature T_R.

ΔP_{th} is the difference of thermal pressure between temperature T and T_R

$$\Delta P_{th} = \alpha_0(T_R)B_0(T_R)(T - T_R) \tag{10}$$

where $B_0(T_R)$ is the bulk modulus at T_R and $\alpha_0(T_R)$ the thermal expansion coefficients.

$$b(T_R) = \frac{3}{2}[B'(T_R) - 1] \tag{11}$$

where $B'(T_R)$ is the pressure derivative of the bulk modulus at T_R.

From Eq. 8, it can be seen that

$$\text{Let} \quad H \equiv \frac{P(T,x) - \Delta P_{th}}{3(1-x)} x^2 \tag{12}$$

$$\text{Then} \quad \ln H = \ln B_0(T_R) + b(T_R)(1-x) \tag{13}$$

that is, on the isotherm at T, ln H will be a linear function of $(1 - x)$ or $1 - \left(\frac{V}{V_0}\right)^{1/3}$.

The intercept on the ordinate will give $\ln B_0(T_R)$ and the value of the slope of the straight line of linear fitting b will give the pressure derivative of the bulk modulus $B_0'(T_R) = \frac{2}{3}b + 1$. Vinet et al. claimed that from UEOS Eq. 8, the EOS for solids can be determined by four parameters: V_0, B_0, B'_0, α_0.

On the other hand, if EOS of solids can be really described by UEOS proposed by Vinet et al., there must be linear relation between ln H and $(1 - x)$, and from the intercept and slope of the fitted line, we can calculate the bulk modulus $B_0(T_R)$ and its pressure derivative. Further, if the thermal pressure is a linear function of T, then from Eq. 10 and the known value of B_0 obtained by Eq. 13, we can calculate the thermal expansion coefficient α_0 in order to compare these values with that obtained by other techniques.

Using the EOS data available in literature for Mo and W, we did calculations of ln H as function of $1 - x$ and presented the results for different isotherms in Tables 1–6.

Table 1 0 K isotherms of ln H as function of $1 - x$ for Mo and W

P (GPa)	0 K isotherm for Mo			0 K isotherm for W		
	ρ (g/cm^3)	$1 - x$	ln H	ρ	$1 - x$	ln H
0	10.243			19.307		
10	10.604	0.0115	5.646	19.895	0.00995	5.794
20	10.933	0.0215	5.693	20.438	0.01880	5.833
30	11.238	0.0304	5.734	20.943	0.02675	5.861
40	11.523	0.0385	5.769	21.418	0.03400	5.903
50	11.792	0.0459	5.801	21.868	0.04067	5.933
60	12.046	0.0526	5.833	22.296	0.04685	5.961
70	12.289	0.0589	5.86	22.704	0.05259	5.987
80	12.521	0.0647	5.888	23.096	0.05798	6.012
90	12.743	0.0702	5.912	23.472	0.06304	6.035
100	12.958	0.0754	5.935	23.835	0.06782	6.057
150	13.928	0.0974	6.036	25.487	0.08841	6.153
200	14.772	0.1149	6.119	26.932	0.10502	6.232
250	15.526	0.1297	6.188	28.227	0.11892	6.298
300	16.207	0.1418	6.253	29.403	0.13082	6.359

In Tables 1 and 2, 0, 200, 600 and 1,000 K isotherms of ln H vs. $1 - x$ derived from Hixon et al.'s [2] experimental work are presented. Since their shock-wave compression test was conducted at the ambient temperature, the reference temperature should be taken equal to the ambient. In Table 2, the $P(\eta, T)$ denotes the pressure for η and T, here $\eta = 1 - \frac{V}{V_0}$, V_0 is the volume for the reference state (at the ambient temperature and atmospheric pressure). The calculated 293 K isotherms of ln H as function of $1 - x$ from shockwave experimental work of Hixon et al. for Mo and W and static experimented work of Mao et al. [1] are presented in Tables 3 and 4. The theoretical 293 K isotherm due to Wang et al. are presented in Table 5 and the 0 K isotherm for Mo by Christensen et al. and that for W by Ruoff et al. are given in Table 6.

All results of our calculated ln H as function of $1 - x$ are plotted in Figs. 1–7, where the solid lines are the least square linear fitting of the dots. For simplicity, we only plotted the 1,000 K isotherms in Fig. 2, it is because the numerical data of ln H for 200, 600 and 1,000 K are essentially identical either for Mo or for W. It can be clearly seen that linearity of the solid lines in Figs. 1–7 is very good, which indicates that UEOS proposed by Vinet et al. is quite appropriate to be used as analytical expression of EOS for solid Mo. As we see in Tables 1–3, 5, 7 and in corresponding figures (Figs. 1–3, 5, 7) the linearity of the fitting lines of ln H versus $1 - x$, either for the experimental results or for the theoretically calculated isotherms is also very good for W, which indicates that Vinet equation of UEOS applies also quite well for solid W.

From the intercept on the ordinate and the slope of the fitting straight line in Figs. 1–7, we can calculate the B_0 and B_0' values as shown in each figure. The average values of B_0 for 0, 200, 600 and 1,000 K isotherms are 265.2 GPa for Mo while that obtained solely from 293 K isotherm equal 266.2 GPa. B_0 obtained from Mao et al's static experiment at the ambient temperature is 266.3 GPa which is almost identical with the value of B_0 obtained from Hixon's work. The B_0' values obtained with Hixon's results and with Mao et al.'s results are, respectively, 4.00 and 3.96. The difference between them is 1%. The bulk modulus B_0 obtained from Hixon et al.'s data equals to 308.8

Table 2 200, 600 and 1,000 K isotherms of ln H as function of $1 - x$ using data of $P(\eta, T)$ for Mo and W reported by Hixon et al. [2]

η	$1 - x$	Isotherm for Mo						Isotherm for W					
		200 K		600 K		1,000 K		200 K		600 K		1,000 K	
		$p(\eta, T)$	ln H	$p(\eta, T)$	ln H	$p(\eta, T)$	ln H	$p(\eta, T)$	ln H	$p(\eta, T)$	ln H	$p(\eta, T)$	ln H
0.000		−0.36		1.29		3.02		−0.38		1.32		3.08	
0.020	0.0067	5.25	5.618	6.88	5.616	8.61	5.615	6.14	5.767	7.83	5.765	9.59	5.765
0.040	0.0135	11.44	5.647	13.06	5.645	14.79	5.645	13.35	5.799	15.03	5.797	16.79	5.797
0.060	0.0204	18.27	5.678	19.89	5.675	21.62	5.675	21.32	5.663	23.00	5.662	24.76	5.662
0.080	0.0274	25.83	5.708	27.44	5.706	29.16	5.706	30.14	5.861	31.81	5.86	33.57	5.86
0.100	0.0345	34.18	5.74	35.78	5.738	37.51	5.738	39.90	5.893	41.56	5.892	43.32	5.892
0.120	0.0417	43.42	5.772	45.01	5.771	46.73	5.771	50.70	5.926	52.36	5.926	54.11	5.926
0.140	0.0491	53.64	5.805	55.22	5.804	56.94	5.804	62.66	5.96	64.31	5.959	66.06	5.959
0.160	0.0565	64.96	5.838	56.53	5.837	68.25	5.837	75.92	5.994	77.56	5.993	79.31	5.993
0.180	0.064	77.51	5.873	79.01	5.872	80.78	5.872	90.63	6.028	92.27	6.028	94.02	6.028
0.200	0.0717	91.43	5.907	92.99	5.906	94.7	5.906	106.98	6.064	108.61	6.064	110.35	6.064
0.220	0.0795	106.92	5.943	108.46	5.942	110.17	5.942	125.17	6.10	126.79	6.1	128.53	6.100
0.240	0.0874	124.17	5.98	125.69	5.979	127.4	5.979	145.45	6.138	147.06	6.137	148.8	6.137
0.260	0.0955	143.41	6.017	144.92	6.017	146.62	6.016	168.10	6.176	169.70	6.176	171.44	6.173
0.280	0.1037	164.93	6.056	166.43	6.055	168.13	6.055	193.45	6.215	195.04	6.215	196.78	6.215
0.300	0.1121	189.06	6.096	190.55	6.095	192.24	6.095	221.91	6.256	223.49	6.255	225.22	6.255
0.320	0.1206	216.2	6.137	217.67	6.137	219.36	6.136	253.95	6.298	255.51	6.297	257.24	6.297
0.340	0.1293	246.82	6.18	248.28	6.179	249.97	6.179	290.14	6.341	291.69	6.341	293.42	6.341
0.360	0.1382	281.5	6.224	282.94	6.224	284.63	6.223	331.19	6.386	332.72	6.386	334.45	6.386
0.380	0.1473	320.95	6.27	322.37	6.27	324.05	6.27						

Table 3 293 K isotherms of ln H as function of $1 - x$ using data for Mo and W reported by Hixon et al. [2]

P (GPa)	293-K isotherm for Mo			293-K isotherm for W		
	ρ	$1 - x$	ln H	ρ	$1 - x$	ln H
0.0	10.215			19.256		
10.0	10.579	0.0116	5.637	19.850	0.01007	5.782
20.0	10.911	0.0262	5.684	20.397	0.01901	5.821
30.0	11.218	0.0307	5.724	20.906	0.02703	5.859
40.0	11.505	0.0389	5.76	21.384	0.03434	5.892
50.0	11.775	0.0463	5.791	21.835	0.04103	5.923
60.0	12.031	0.0531	5.822	22.265	0.04724	5.951
70.0	12.274	0.0594	5.851	22.675	0.05302	5.98
80.0	12.507	0.0653	5.877	23.069	0.05845	6.002
90.0	12.731	0.0708	5.902	23.447	0.06353	6.026
100.0	12.945	0.0759	5.927	23.811	0.06833	6.048
150.0	13.918	0.0980	6.029	25.465	0.08895	6.145
200.0	14.764	0.1155	6.113	26.916	0.10563	6.224
250.0	15.519	0.1301	6.183	28.213	0.11955	6.292
300.0	16.201	0.1425	6.246	29.390	0.13146	6.352

Table 4 293 K isotherms of ln H as function of $1 - x$ using experimental data for Mo reported by Mao et al. [1]

$x = d/d_0$	P (GPa)	$1 - x$	ln H
0.991	7.4	0.0087	5.630
0.9884	10	0.0116	5.637
0.9856	12.6	0.0144	5.647
0.9805	17.7	0.0195	5.673
0.9806	17.6	0.0194	5.676
0.9781	20.1	0.0219	5.679
0.9718	27	0.0282	5.708
0.9625	38.2	0.0375	5.751
0.9493	56.8	0.0507	5.81
0.948	58.1	0.0520	5.813
0.9364	76.9	0.0636	5.868
0.9327	83.2	0.0673	5.882
0.9319	84.7	0.0681	5.886
0.9295	89.2	0.0705	5.898
0.9283	91.3	0.0717	5.902
0.9264	95	0.0736	5.911
0.92622	95.4	0.0738	5.9125

and that obtained from Wang et al.'s theoretically calculated 293 K isotherm equals to 298.6 GPa and from Ruoff's theoretical work equals to 305.0 GPa and the handbook value of B_0 equals to 311 GPa [16]. The average B_0' value from Hixon's work equals 4.12 and that from Wang et al.'s 293 K isotherm equals to 4.25. They differ from each other by 3%.

Table 5 293 K isotherms of ln H versus $1 - x$ for Mo and W calculated using data reported by Wang et al. [5]

P (GPa)	For Mo			For W		
	V/V_0	$1 - x$	ln H	V/V_0	$1 - x$	ln H
0.000	1			1		
2.512	0.9902	0.0033	5.53	0.9918	0.002741	5.716
5.012	0.9809	0.0064	5.552	0.9839	0.005396	5.725
10.000	0.9629	0.0125	5.563	0.9642	0.010374	5.752
15.850	0.9435	0.0192	5.579	0.9532	0.015850	5.777
25.120	0.917	0.0285	5.625	0.9303	0.023795	5.815
39.810	0.8825	0.0408	5.701	0.8989	0.034904	5.87
50.120	0.8617	0.0484	5.745	0.8796	0.041861	5.904
63.100	0.8383	0.0571	5.791	0.8578	0.049843	5.943
79.430	0.8124	0.0669	5.842	0.8335	0.058901	5.987
100.000	0.7841	0.0779	5.897	0.8066	0.069136	6.035
125.900	0.7536	0.09	5.956	0.7775	0.080468	6.089
158.500	0.7215	0.1031	6.022	0.7468	0.092734	6.151
199.500	0.688	0.1172	6.092	0.7143	0.106091	6.216
251.200	0.6534	0.1323	6.167	0.6804	0.120462	6.287
316.200	0.618	0.1482	6.246	0.6459	0.135586	6.365
398.100	0.5824	0.1649	6.33	0.6114	0.151586	6.449
501.200	0.5467	0.1823	6.418	0.5763	0.167822	6.536
631.000	0.5117	0.2002	6.51	0.5414	0.184972	6.627
794.300	0.4779	0.2182	6.609	0.5075	0.202351	6.724
1000.000	0.4431	0.2376	6.704	0.474	0.220305	6.824

In Table 7 are the values for $P(\eta, T)$ cited from Hixon's work [2] for Mo and W under the condition $\eta = 0$ for different temperature where $\eta = 1 - \frac{V}{V_0}$ denotes the volume reduction.

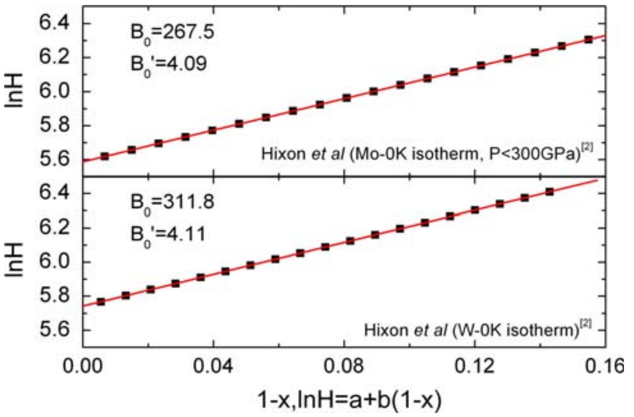

Fig. 1 0 K isotherm of ln H versus $1 - x$ for Mo and W derived from Hixon et al.'s shock-wave experiment

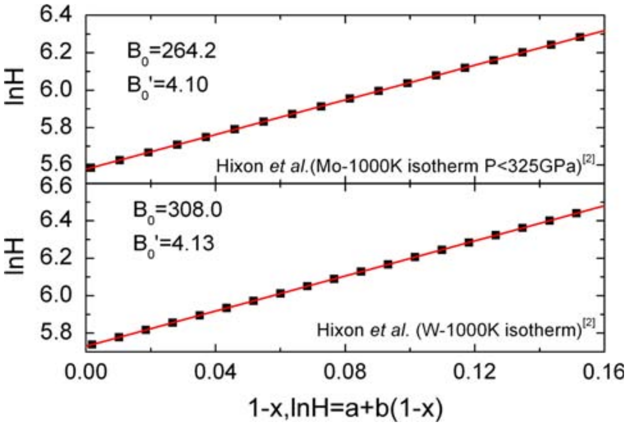

Fig. 2 1,000 K isotherm of ln H versus $1 - x$ for Mo and W derived from Hixon et al.'s shock-wave experiment

Table 6 0 K isotherm of ln H versus $1 - x$ calculated using original data for Mo and W reported by Christensen and Ruoff et al. [3, 6]

V/V_0	$1 - x$	0 K isotherm for Mo [3]			0 K isotherm for W [6]		
		P (100 GPa)	$P - P_0$ (100 GPa)	ln H	P (100 GPa)	$P - P_0$ (100 GPa)	ln H
1	0	−0.033	0		−0.033	0	
0.95	0.0171	0.141	0.174	5.792	0.141	0.174	5.792
0.9	0.0348	0.366	0.399	5.875	0.366	0.399	5.875
0.85	0.0528	0.655	0.688	5.965	0.655	0.688	5.965
0.8	0.0717	1.028	1.061	6.052	1.028	1.061	6.052
0.75	0.0916	1.51	1.543	6.138	1.51	1.543	6.138
0.7	0.1122	2.137	2.17	6.23	2.137	2.17	6.23
0.65	0.134	2.962	2.995	6.326	2.962	2.995	6.326
0.6	0.1567	4.062	4.095	6.429	4.062	4.095	6.429
0.55	0.1807	5.562	5.595	6.541	5.562	5.595	6.541
0.5	0.2063	7.662	7.695	6.663	7.662	7.695	6.663
0.45	0.2338	10.71	10.743	6.801	10.71	10.743	6.801
0.4	0.2632	15.3	15.333	6.96	15.3	15.333	6.96

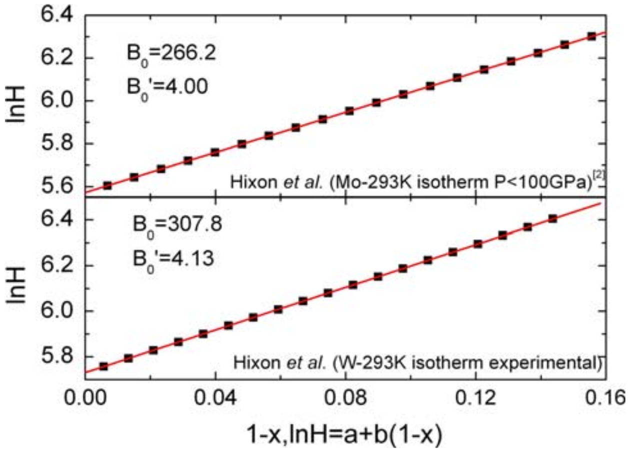

Fig. 3 293 K isotherm of ln H versus $1 - x$ for Mo and W derived from Hixon et al.'s shock-wave experiment

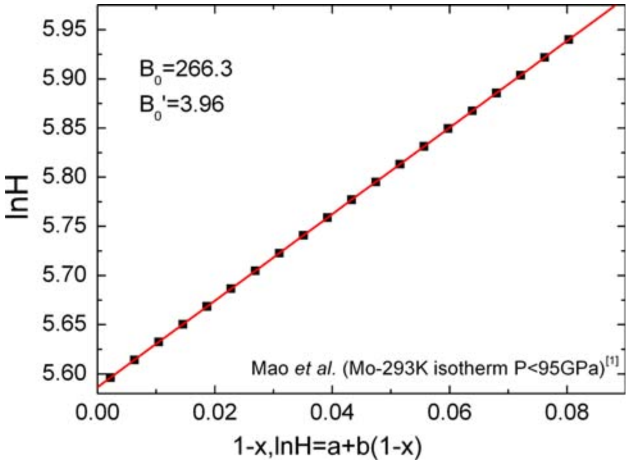

Fig. 4 293 K isotherm of ln H versus $1 - x$ for Mo derived from Mao et al.'s static experiment

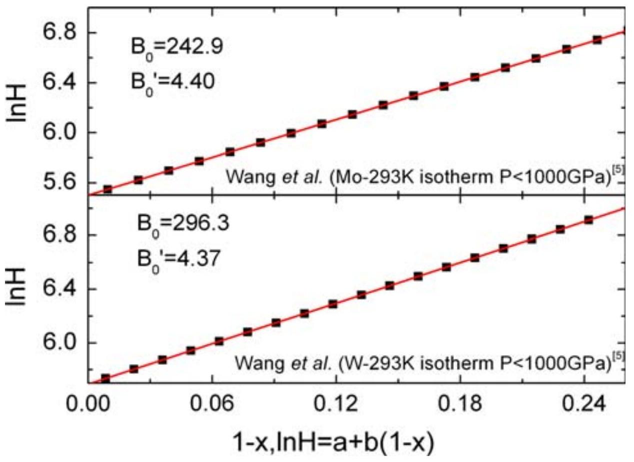

Fig. 5 293 K isotherm of ln H versus $1 - x$ for Mo and W derived from Wang et al.'s theoretical calculation

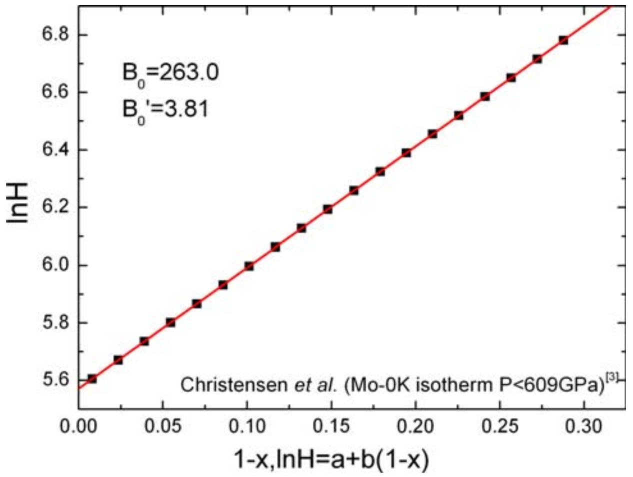

Fig. 6 0 K isotherm of ln H versus $1 - x$ for Mo derived from Christensen et al.'s theoretical calculation

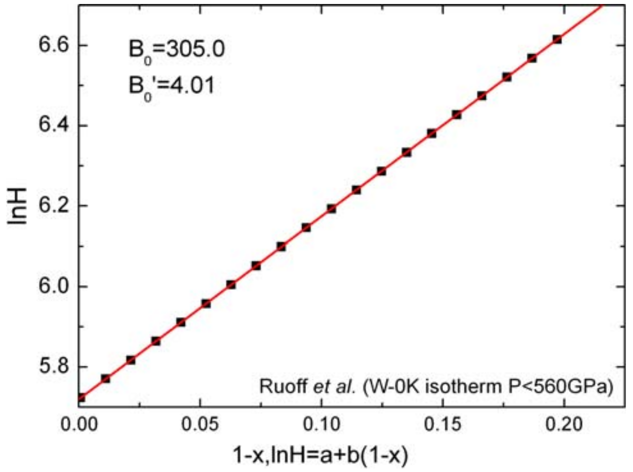

Fig. 7 0 K isotherm of ln H versus $1 - x$ for W derived from Ruoff et al.'s theoretical calculation

Since Hixon et al. carried out their shock-wave compression test at the ambient temperature, V_0 should be taken as the volume for the standard state, i.e. for the room temperature and at the pressure of atmosphere, so the negative signs in Table 7 for the temperatures lower than the ambient are understandable. From the data in Table 7, we can calculate the thermal pressure difference between T and the reference temperature T_R, $\Delta p_{th}(T - T_R)$ ($T_R = 293$ K), which is shown in Fig. 8 for molybdenum and Tungsten. The solid lines in Fig. 8 are the linear fitting lines. It is apparent that ΔP_{th} is linearly dependent on $T - T_R$ in both the figures. From the slope of the line equal to 0.00427 (GPa/K), and the B_0 value 266.2 Gpa using Eq. 10, we calculated the linear thermal expansion coefficient $\alpha_0 = 5.35 \times 10^{-6}$ for Mo, which is in quite good agreement with the handbook value $5.2–5.7 \times 10^{-6}$ for temperatures range from 100 to 1,000 °C [16].

Table 7 $P(\eta, T)$ at $\eta = 0$ for Mo and W cited from Hixon et al.'s work [2]

	T (K)										
$P(0, T)$ (GPa)		100	200	300	400	500	600	700	800	900	1000
	Mo	−0.66	−0.36	0.03	0.44	0.86	1.29	1.72	2.15	2.58	3.02
	W	−0.72	−0.38	0.03	0.45	0.89	1.32	1.76	2.2	2.64	3.08

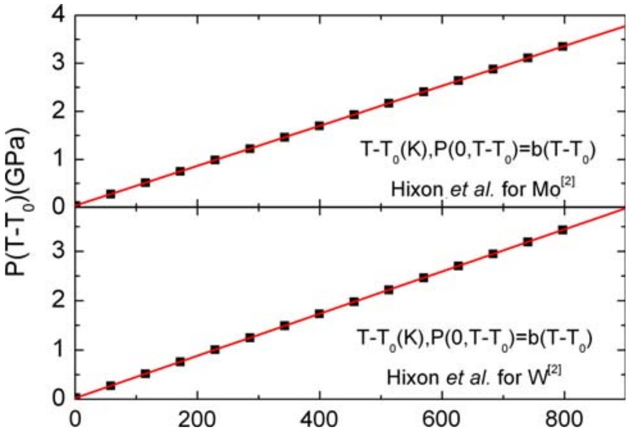

Fig. 8 Linear fitting of thermopressure difference between T and the reference temperature $T_0 = T_R$ for Mo and W calculated with data cited from Hixon et al.'s work [2]

The $P(\eta, T)$ for $\eta = 0$ for W are also presented in Table 7 from which we can see that ΔP_{th} is also a linear function of $T - T_R$. The calculated thermal expansion coefficient equals to 4.6×10^{-6} K, which is almost identical with the handbook value $4.5–4.6 \times 10^{-6}$ K [16].

Concluding remarks

Form our analysis of all available EDS data obtained either experimentally or by first principle calculation by checking validity of UEOS, we see that

- The dynamic experimental work of Hixon on Mo is consistent with the static experimental result of Mao for Mo.
- The experimental determination of EOS for Mo and W is consistent with first-principle calculation with high accurately.
- UEOS proposed by Vinet et al. can be quite well used as the analytical expression of EOS for solid W and Mo in terms of P, V, T variables. Further refinement seems unnecessary.
- The bulk modulus and the thermal expansion coefficients value obtained form EOS analysis agree very well with the handbook values.

We believe that UEOS can be applied to more materials just like the prediction by Vinet et al.'s work in this direction is still under way.

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