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LETTER TO THE EDITOR

A modified Lennard-Jones-type equation of state for solids strictly satisfying the spinodal condition

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Abstract
In this letter, it is pointed out that an ideal universal equation of state (EOS) of solids should have four merits. The EOS corresponding to the generalized Lennard-Jones (GLJ) potential is derived. It is pointed out that the GLJ EOS is not volume analytic, as the exponents contained in the potential function take arbitrary values. On making the exponents satisfy a relationship, the GLJ EOS becomes volume analytic with two parameters (mGLJ EOS), and has all four merits. By applying six EOSs in investigating 50 materials, it is shown that the mGLJ EOS gives the best results.

The equation of state (EOS) of a system describes the relationships among thermodynamic variables such as pressure, temperature, and volume. It provides numerous pieces of information relating to the non-linear compression of a material at high pressure, and has been widely applied in engineering and other scientific research. Recently, rapid advances in computational capabilities and accurate high pressure experimental techniques have given a strong impetus to theoretical work. Significant progress has been achieved over the past few years as regards describing the properties of condensed matter in terms of universal relationships involving a small number of parameters—especially since the 1986 Rose *et al* [1] proposal that there is a universal EOS (UEOS) valid for all kinds of solids that can be obtained through analysing the energy band data; a lot of forms of UEOSs have been proposed, with varying success [2–17].

Among these EOSs, the Vinet EOS [2] has been shown to have fairly high precision [7]. The Vinet EOS can provide a simple analytic expression for the cohesive energy, an important merit. Recently, Baonza *et al* [8–13] proposed another EOS from a pseudospinodal hypothesis; they claimed that the EOS has high precision, equivalent to that of the Vinet EOS. But Brosh *et al* [15] pointed out that the pseudospinodal hypothesis is not necessary for deriving the Baonza EOS, and the EOS cannot even meet the strict spinodal condition. Holzapfel *et al* [16, 17] pointed out that the limiting condition for an EOS at high pressure should be the Thomas–Fermi (TF) model [18–20]. Since most existing EOSs cannot satisfy the limiting condition, they modified the Vinet EOS to satisfy the TF limitation [16, 17] (the Holzapfel EOS). However,

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recently, we proposed two Murnaghan-type EOSs [21], and compared the precision of the five EOSs mentioned above by fitting the experimental compression data for 50 solids. The results show that EOSs satisfying the TF limitation give worse results than other EOSs not satisfying the TF limitation. For practical applications, the TF limiting condition is not important, for it only operates as the volume tends to zero.

We consider that, except for the TF limiting condition, for practical applications, an ideal universal EOS should have the following four merits. The first one is that the energy should be analytic, $U = U(V)$. The second one is that the EOS should be both pressure analytic, $P = P(V)$, and volume analytic, $V = V(P)$. The third one is that it should satisfy the following spinodal condition [15]:

$$B \propto (P - P_{\mathrm{sp}})^{1/2}, \quad \text{with } B(P = P_{\mathrm{sp}}) = 0, \tag{1}$$

have the correct limit as volume tends to infinity, $P(V \to \infty) = 0$, and be applicable to expanded materials, including expanded liquids and solids. The fourth one is that it should have high enough precision with a simple form and a small number of parameters, and allow one to predict the compression curve for materials at high pressure using only the parameters determined from experimental data at low pressure.

Now we explain in more detail what is practical value of the spinodal condition is and why the volume analyticity is a valuable property. First of all, we should point out that, in recent years, the universal EOSs have not been limited solely to just solids or just liquids. This means that an EOS initially proposed for solids might be applied by some researchers to compressed liquids, and vice versa. For example, the Vinet, KD, and Baonza EOSs have been applied both to solids [1, 2, 4, 7, 11–13] and liquids [5, 8–10, 22]. Brosh *et al* [15] explained the physical meaning of the spinodal condition for liquids. They pointed out that the EOS for expanded fluids has been less studied and the general form of the EOS is not well established. The spinodal is a locus in the P–V diagram of compressed liquids, which is the limit of metastability of a substance with respect to a phase transition. In principle, the spinodal can be detected by experiments in the metastable region, but in practice such experiments are extremely difficult. Instead, efforts have been made to locate the spinodal by extrapolation from the stable region of the phase diagram. So an EOS satisfying the spinodal condition is useful to the research on expanded liquids. As for solids, in recent years, researchers have been very interested in porous materials [23–32]. These materials were usually studied using shock wave experiments. In such conditions, we consider very wide density ranges, varying from expanded regions to high compression regions. In many theories for porous materials, the thermodynamic equations of a bulk material are necessary, and an EOS satisfying the spinodal condition may have some advantages [23–32].

We also consider that volume analyticity is a valuable property. For liquids, the direct determination of EOS at high pressure is very difficult for the compression experiment and is far more difficult for a liquid than for a solid. So researchers would normally determine the EOS of a liquid by using other methods. Because the variation of the sound velocity versus pressure in liquids can be easily measured with high precision, many researchers have developed an EOS for liquids in terms of the sound velocity [33–41]. For example, Vinet and KD EOSs have been used on this basis [5, 22]. However, the Vinet EOS is not volume analytic, so in order to apply the Vinet EOS for liquid metals, Schlosser *et al* have separately developed V–P and B–P equations [22]. We consider such an approach is not consistent. However, if one uses volume analytic EOSs to do such research, the inconsistency can be naturally avoided [5]. And for solids, in the research on porous materials, researchers found it more convenient to use the pressure variable than the volume [23–32], and some theories have been developed. For example, the Wu–Jing equation [24–28] has been shown to have the ability to describe properties of porous materials over the wide pressure and temperature ranges. For these theories, the volume analytic EOS of a bulk solid is the foundation [23–32].

Up to now, we have not found an EOS having all four merits. Most present EOSs have various disadvantages. For example, although the Vinet EOS is energy and pressure analytic, it is not volume analytic, and its precision is lower than that of the Baonza EOS [21]. Although the Baonza EOS is pressure and volume analytic, it is not energy analytic, and cannot satisfy the spinodal condition [8–13, 15] as it has been derived by integrating the following relationship rather than equation (1), $B \propto (P - P_{\mathrm{sp}})^{0.85}$, and is inapplicable to expanded materials. The Holzapfel EOS is just pressure analytic, and is not energy and volume analytic, and its precision is the worst [21]. The precision of the two-parameter Murnaghan EOS proposed by us (designated the SMnh EOS) is equivalent to that of the Vinet EOS; it is energy, pressure and volume analytic, but it cannot satisfy the spinodal condition. Midha and Nanda [42] have used an EOS based on the LJ 12–6 potential to study the properties of metals at zero pressure. But the LJ 12–6 EOS only contains one parameter and it cannot be applied to materials at high pressure, although it is energy and pressure analytic; it has all disadvantages corresponding to other merits mentioned above [42].

In this letter, we propose a two-parameter EOS based on the generalized Lennard-Jones (GLJ) potential, which can have all the merits mentioned above, except fulfilling the TF limitation condition. The GLJ potential is as follows [43–45]:

$$\varepsilon(r) = \frac{\varepsilon_0}{m_1 - n_1}\left[n_1\left(\frac{r_e}{r}\right)^{m_1} - m_1\left(\frac{r_e}{r}\right)^{n_1}\right]. \tag{2}$$

If we adopt the nearest neighbour assumption, the total energy of a solid is

$$\begin{aligned} U &= \frac{N\delta\varepsilon_0}{2(m_1 - n_1)}\left[n_1\left(\frac{r_e}{a}\right)^{m_1} - m_1\left(\frac{r_e}{a}\right)^{n_1}\right] \\ &= \frac{9B_0V_0}{m_1n_1(m_1 - n_1)}\left[n_1\left(\frac{V_0}{V}\right)^{m_1/3} - m_1\left(\frac{V_0}{V}\right)^{n_1/3}\right] \end{aligned} \tag{3}$$

where a is the nearest neighbour distance, $V = a^3/\gamma$, $V_0 = (r_e)^3/\gamma$, and δ and γ are structure constants [44, 45]. B_0 and B_0' are the bulk modulus and its first-order pressure derivative at zero pressure, $B_0 = (m_1n_1N\delta\varepsilon_0)/(18V_0)$.

It should be pointed out that in equation (3) one could use an all-neighbour model to replace the nearest neighbour model, and the Madelung factor accounting for the sum of all distant neighbour particles could be used here without changing the analytic form of the energy. However, we can introduce new parameters V_0 and B_0, and the form of the final equations is completely the same as in the nearest neighbour model. So we just use the nearest neighbour model without loss of generality. The EOS can be derived by the differentiation of equation (3) with respect to volume. The result is

$$P = \frac{3B_0}{(m_1 - n_1)}\left[\left(\frac{V_0}{V}\right)^{m_1/3+1} - \left(\frac{V_0}{V}\right)^{n_1/3+1}\right]. \tag{4}$$

It should be pointed out that equation (4) is energy and pressure analytic, but it is not volume analytic for arbitrary values of exponents m_1 and n_1, even for the case of the LJ 12–6 potential [42] with $m_1 = 12$ and $n_1 = 6$. In order to obtain an EOS that is volume analytic, we consider that the exponents in equation (4) should satisfy the condition $m_1/3+1 = 2(n_1/3+1)$, and we should take

$$n_1/3 + 1 = n, \qquad m_1/3 + 1 = 2n. \tag{5}$$

Equation (5) gives the volume analytic condition. It decreases the number of independent parameters in equation (4) from three to two. This may reduce the potential accuracy of fits to the isothermal data. However, the precision of an EOS is not always in proportion to the number of parameters contained in the EOS. For example, the KD EOS is a three-parameter EOS but its precision is just equivalent to that of the two-parameter Baonza EOS and lower than that of the mGLJ EOS developed in this letter. And we have made some comparative calculations using the three-parameter LJ-type EOS; the results show little improvement as compared with using the two-parameter mGLJ EOS.

Substitution of equation (5) into equations (3) and (4) yields

$$U = \frac{B_0 V_0}{n}\left(\frac{V_0}{V}\right)^{n-1}\left[(2n-1)^{-1}\left(\frac{V_0}{V}\right)^{n} - (n-1)^{-1}\right] \tag{6}$$

$$P = \frac{B_0}{n}\left(\frac{V_0}{V}\right)^{n}\left[\left(\frac{V_0}{V}\right)^{n} - 1\right] \tag{7}$$

$$n = \tfrac{1}{3}B_0'. \tag{8}$$

Equation (7) is just the two-parameter EOS we proposed (mGLJ EOS). It can be shown to have almost all of the merits mentioned above, and the precision is higher than those for several popular EOSs. Equation (7) can be easily converted to the volume analytic form

$$\left(\frac{V_0}{V}\right)^{n} = \frac{1}{2}\left(1 + \sqrt{1 + \frac{4nP}{B_0}}\right). \tag{9}$$

The bulk modulus is

$$B = -V\frac{\partial P}{\partial V} = B_0\left(\frac{V_0}{V}\right)^{n}\left[2\left(\frac{V_0}{V}\right)^{n} - 1\right]. \tag{10}$$

We notice that equations (7), (9) and (10) are simpler than most EOSs in the literature [2–17], including Vinet, Baonza, and KD EOSs; they are fairly convenient for practical applications.

We can verify that equation (7) satisfies the spinodal condition of equation (1). The spinodal volume V_{sp} can be determined from the equation $B(V = V_{sp}) = 0$; the spinodal pressure P_{sp} can be determined by substituting V_{sp} into equation (7). We have

$$\left(\frac{V_0}{V_{sp}}\right)^{n} = \frac{1}{2}, \qquad P_{sp} = -\frac{B_0}{4n} \tag{11}$$

substituting equation (9) into (10), and using equation (11), equation (10) changes to

$$B = 2n[(-P_{sp})^{1/2} + (P - P_{sp})^{1/2}](P - P_{sp})^{1/2}. \tag{12}$$

Thus it has been shown that equation (7) strictly satisfies the spinodal condition. It is interesting to note that Hama and Suito [7] divided all EOSs into three types: the derivative form, the volume integral form, and the pressure integral form. However, equation (7) belongs to all three types. Also, equation (12) can be generalized to the following form:

$$B = f((P - P_{sp})^{1/2})(P - P_{sp})^{1/2} \tag{13}$$

where $f(x)$ is an analytic function. The integration of equation (13) in terms of the definition of the bulk modulus in equation (10) yields

$$\frac{V_0}{V} = \int_0^P \frac{\mathrm{d}P}{f((P - P_{sp})^{1/2})(P - P_{sp})^{1/2}} = 2\int_{\sqrt{-P_{sp}}}^{\sqrt{P-P_{sp}}} \frac{\mathrm{d}x}{f(x)}. \tag{14}$$

By using equation (14), we can develop EOSs with other forms and strictly satisfying the spinodal condition.

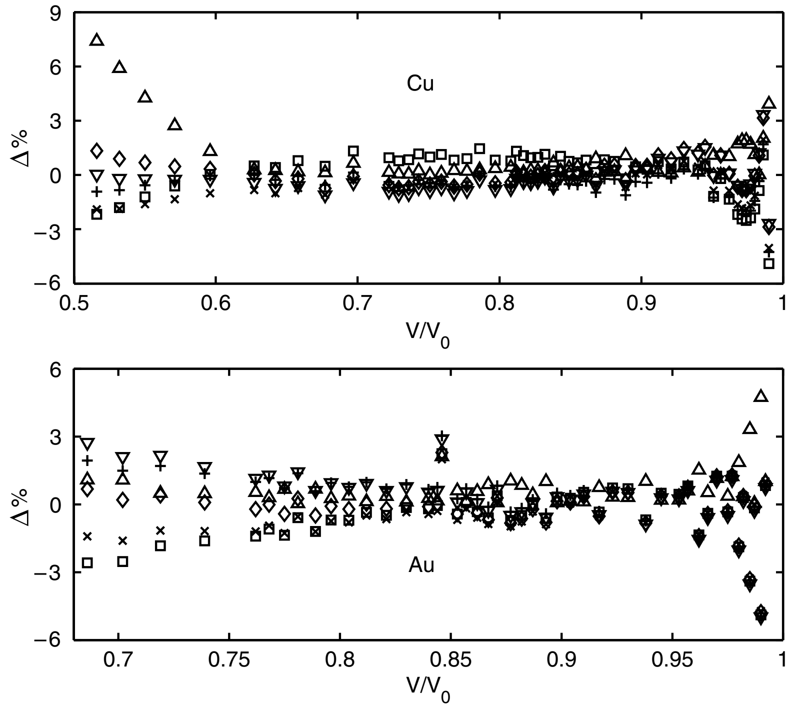

Figure 1. Relative error ($\Delta\% = (P_{\mathrm{cal}} - P_{\mathrm{exp}})/P_{\mathrm{exp}} \times 100\%$) comparison of six EOSs for Cu and Au. □: Vinet; ×: Holzapfel; +: Baonza; △: KD; ▽: SMnh; ◇: mGLJ.

In this letter we investigate six EOSs: the Vinet [2], Holzapfel [16, 17], Baonza [8–13], KD [4, 5], SMnh [21] EOSs and the mGLJ EOS in equation (7). The KD EOS is a three-parameter equation, while the other EOSs are two-parameter equations. We have applied the six EOSs to investigate 50 materials. All experimental data for $V(P, T_0)/V(0, T_0)$ are taken from Kennedy and Keeler [46], except for W [47] and NaCl [48]. The average fitting errors for the pressure ($P = f(V)$) have been listed in table 1. The experimental data for V_0 and the fitted parameters B_0, B_0' for the mGLJ EOS have been listed in table 2. The values of B_0, B_0' for the KD EOS are from [49]; for other EOSs we refer to [21].

Table 1 shows that the mGLJ EOS gives the best results, with the average error 0.603%; the Baonza and KD EOSs give slightly inferior results with average errors of 0.681% and 0.679%, respectively. Although the Holzapfel EOS strictly satisfies the limiting condition at high pressure, the average fitting error reaches 0.851%, which is the worst one. The Vinet and SMnh EOSs give equivalent results with average errors of 0.756% and 0.755%, respectively. In figures 1 and 2, we give the error comparison of the six EOSs for four typical materials, Cu, Au, Al, and Tl. It can be seen that the mGLJ EOS gives the best results for Cu, Au, and Tl, the Vinet EOS gives the best results for Al, and the mGLJ EOS gives the second worst results. The trend is in agreement with the results on total average errors in table 1.

It should be pointed out that researchers usually consider that inverse power potentials are typically too stiff for fitting real compressed solids, but we consider that the situation may change for some cases. This is because inverse power potentials also have many different forms. We consider that we have three typical cases. The first case is that of the potential corresponding to the Murnaghan EOS:

Table 1. Average fitting errors for the pressure (Δ_p%) when using six universal equations of state: Vinet [2], Holzapfel (designated Hlzpf) [16, 17], Baonza [8–13], KD [4, 5], two-parameter Murnaghan-type, proposed by us [43] (designated SMnh), and mGLJ, from equation (7).

No	Solids	Pressure GPa	Vinet Δ_p (%)	Hlzpf Δ_p (%)	Baonza Δ_p (%)	KD Δ_p (%)	SMnh Δ_p (%)	mGLJ Δ_p (%)
1	Cu	0–450	1.050	0.743	0.676	0.90	0.664	0.603
2	Mo	0–350	1.468	1.510	1.507	1.44	1.220	1.039
3	W	0–270	0.239	0.406	0.483	0.26	0.318	0.248
4	Zn	0–250	1.147	0.937	0.670	0.68	0.398	0.323
5	Ag	0–200	0.821	0.660	0.617	0.79	0.503	0.409
6	Pt	0–200	1.046	1.003	1.053	1.00	0.872	0.704
7	Ti	0–200	0.590	1.001	0.763	0.82	1.091	0.811
8	Ta	0–180	0.932	0.972	0.838	0.81	0.918	0.718
9	Au	0–180	0.938	0.890	0.957	0.98	0.949	0.648
10	Pd	0–160	1.059	1.057	1.111	1.14	0.896	0.723
11	Zr	0–140	0.689	1.314	0.620	0.62	0.869	0.653
12	Cr	0–120	1.586	1.645	1.655	1.62	1.650	1.108
13	Co	0–120	0.951	1.107	0.957	0.95	0.968	0.757
14	Ni	0–120	0.870	0.867	0.860	0.95	0.854	0.603
15	$A1_2O_3$	0–120	1.132	1.153	1.158	1.15	1.173	0.778
16	Nb	0–100	2.885	2.808	2.945	2.73	2.925	1.849
17	Cd	0–100	0.824	0.630	0.462	0.33	0.291	0.265
18	Al	0–100	0.787	0.886	1.059	0.64	1.207	1.118
19	Th	0–100	0.383	0.894	0.473	0.62	0.728	0.535
20	V	0–100	0.811	0.721	0.691	0.79	0.687	0.564
21	In	0–90	1.020	0.771	0.784	0.97	0.806	0.675
22	MgO	0–90	0.481	0.482	0.546	0.58	0.553	0.416
23	*Brass	0–85	0.601	0.518	0.516	0.57	0.582	0.417
24	Be	0–80	0.629	0.655	0.597	0.66	0.582	0.454
25	LiF	0–80	0.571	0.482	0.380	0.45	0.350	0.337
26	Pb	0–75	0.559	0.340	0.392	0.53	0.397	0.332
27	Sn	0–60	0.637	0.492	0.410	0.33	0.339	0.307
28	Mg	0–55	0.258	0.349	0.363	0.40	0.579	0.432
29	CsBr	0–55	0.442	0.920	0.386	0.50	0.756	0.591
30	Ca	0–36	0.481	2.593	0.850	0.37	1.325	0.924
31	Tl	0–34	0.501	0.321	0.348	0.50	0.342	0.285
32	NaCl	0–31	0.296	0.124	0.131	0.22	0.292	0.238
33	LiI	0–28	0.378	1.085	0.433	0.38	0.572	0.428
34	LiBr	0–24	0.340	0.316	0.354	0.39	0.354	0.324
35	NaBr	0–24	0.372	0.416	0.351	0.35	0.427	0.375
36	NaI	0–24	0.219	0.624	0.376	0.27	0.565	0.393
37	KF	0–24	1.276	1.175	0.965	0.53	0.775	0.585
38	RbF	0–24	0.347	0.229	0.219	0.24	0.333	0.294
39	LiCl	0–22	0.478	0.388	0.338	0.52	0.307	0.307
40	Li	0–20	0.386	0.412	0.361	0.35	0.650	0.46
41	Na	0–20	0.356	0.830	0.298	0.40	0.850	0.628
42	KI	0–18	0.489	0.355	0.289	0.36	0.363	0.345
43	RbI	0–18	0.389	0.397	0.194	0.19	0.423	0.36
44	RbBr	0–16	0.682	0.327	0.385	0.33	0.314	0.33
45	K	0–14	0.228	1.714	0.365	0.50	1.099	0.838
46	Rb	0–14	0.299	2.467	0.293	0.86	1.181	1.015
47	NaF	0–14	0.604	0.576	0.569	0.61	0.547	0.501
48	RbCl	0–12	0.493	0.338	0.319	0.23	0.242	0.249
49	As	0–10	1.737	1.788	1.710	1.62	1.735	1.676
50	Nd	0–10	1.493	1.544	1.569	1.23	1.584	1.206
	Total average error		0.756	0.851	0.681	0.679	0.755	0.603

Table 2. The experimental data for V_0 and fitted parameters B_0 and B_0' for the mGLJ EOS of equation (7). The values of the fitted parameters for KD EOS are from [49]; for other EOSs we refer to [21].

No	Solids	V_0 ($cm^3\ mol^{-1}$)	mGLJ B_0 (GPa)	mGLJ B_0'	No	Solids	V_0 ($cm^3\ mol^{-1}$)	mGLJ B_0 (GPa)	mGLJ B_0'
1	Cu	7.115	141.6	4.6521	26	Pb	18.27	44.431	5.0287
2	Mo	9.387	268.41	3.8482	27	Sn	16.32	43.896	5.2321
3	W	9.550	314.54	3.7284	28	Mg	14.00	34.982	3.7713
4	Zn	9.166	60.636	5.5094	29	CsBr	47.93	22.371	3.7133
5	Ag	10.27	106.15	5.5119	30	Ca	26.13	19.724	2.2963
6	Pt	9.098	281.98	5.0083	31	Tl	17.23	35.598	5.4247
7	Ti	12.01	99.829	3.3042	32	NaCl	27.00	23.836	4.766
8	Ta	10.80	199.67	3.5864	33	LiI	32.80	33.248	2.29
9	Au	10.22	184.82	4.9877	34	LiBr	25.07	22.254	4.3014
10	Pd	8.896	196.13	5.0336	35	NaBr	32.15	21.191	4.0509
11	Zr	14.02	95.48	2.6273	36	NaI	40.84	20.11	3.6335
12	Cr	7.231	190	4.8214	37	KF	23.43	12.03	5.5064
13	Co	6.689	197.8	4.1116	38	RbF	37.44	15.246	4.4735
14	Ni	6.592	188.68	4.665	39	LiCl	20.60	32.97	3.9019
15	$A1_2O_3$	26.62	250.9	3.8631	40	Li	13.02	10.838	3.2958
16	Nb	10.83	170.17	3.761	41	Na	23.71	6.1984	3.5806
17	Cd	13.00	50.58	5.5586	42	KI	53.29	9.5911	4.2419
18	Al	10.00	77.283	4.3861	43	RbI	59.82	9.5964	4.2867
19	Th	19.79	52.997	3.8543	44	RbBr	49.36	7.791	4.6503
20	V	8.365	159.4	3.6001	45	K	45.62	3.1967	3.2691
21	In	15.73	40.155	5.068	46	Rb	56.08	2.1716	3.3866
22	MgO	8.465	148.15	5.671	47	NaF	15.10	46.648	3.8545
23	*Brass	37.82	118.09	4.578	48	RbCl	43.81	5.9335	5.3173
24	Be	4.890	120.88	3.3834	49	As	12.96	37.666	11.569
25	LiF	9.789	63.36	4.5877	50	Nd	20.60	31.801	4.4802

$$P = \frac{B_0}{B_0'}\left[\left(\frac{V_0}{V}\right)^{B_0'} - 1\right]. \qquad (15)$$

It can be seen from equation (15) that the Murnaghan EOS just contains a single inverse power term; such a case is indeed too stiff for most materials, and this can just be applied to low pressure regions. The second case is that of the Birch EOS:

$$P = \frac{3B_0}{2}\left[\left(\frac{V_0}{V}\right)^{7/3} - \left(\frac{V_0}{V}\right)^{5/3}\right]\left[1 + \frac{3}{4}(B_0' - 4)\left(\left(\frac{V_0}{V}\right)^{2/3} - 1\right)\right]. \qquad (16)$$

The Birch EOS contains several inverse power terms, its stiffness is far less than that of the Murnaghan EOS, and it has been widely used in geophysics and high pressure physics. The limit of the Birch EOS at high pressure is as follows:

$$P = \frac{9}{8}(B_0' - 4)B_0\left(\frac{V_0}{V}\right)^3, \qquad (V \to 0). \qquad (17)$$

The third case is that of the GLJ potential. For simplicity, we only consider our modified mGLJ EOS. First of all, we know that the exponent of the repulsive term in the mGLJ EOS (7) is $2n = 2B_0'/3$, smaller than that for the Murnaghan EOS (which is B_0'), and the attractive term in equation (7) is far stronger than the Murnaghan EOS one (15). So the mGLJ EOS is also far

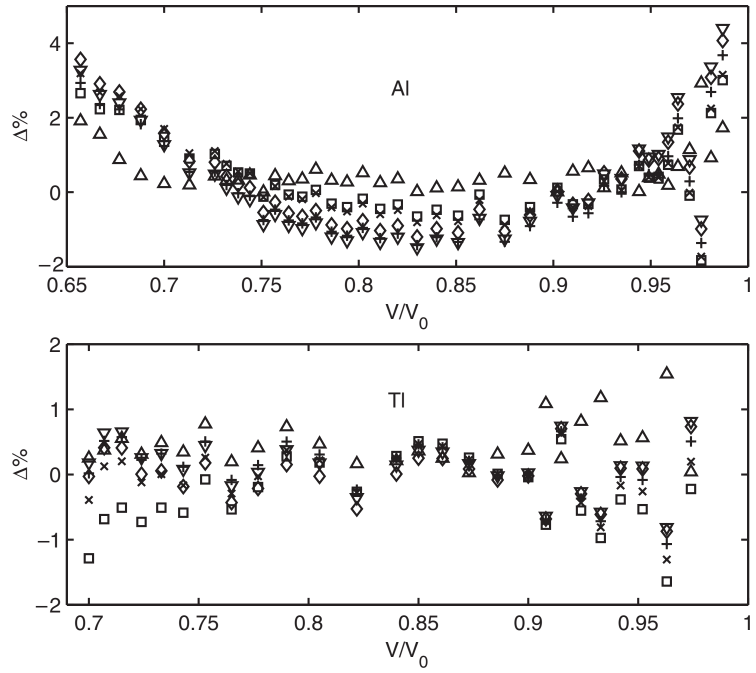

Figure 2. As for figure 1, but for Al and Tl.

softer than the Murnaghan EOS. Also, from table 2, we know that for most materials the value of B_0' is approximately 3–5, and the average value is about 4, so $2n \leqslant 3$ is satisfied for most materials. This is just the typical value of the mGLJ exponents in the fits to the experimental data. And the stiffness of the mGLJ EOS (7) is equivalent to that of equation (16) or even less. Thus we postulate that the applicable compression ranges for the mGLJ EOS should at least be equivalent to those for the Birch EOS. Otherwise, equation (17) shows that the Birch EOS (16) gives an incorrect trend for materials with $B_0' \leqslant 4$, P tends to $-\infty$ as V tends to 0, but the mGLJ EOS (7) has no such disadvantage. Considering its other merits, the mGLJ EOS is attractive for many applications.

It should be pointed out that equation (7) is an isothermal equation; after including the thermal effects in equation (7) as is done in [2, 5, 13–17], one can easily derive all thermodynamic quantities analytically, and can analytically investigate the variations of these quantities with temperature, volume or pressure conveniently both for solids and liquids. For example, Kuchhal *et al* [5] have used the complicated three-parameter KD EOS [4, 5] to study the variations of the sound velocity and volume with temperature and pressure. Baonza *et al* [8–10] also applied their EOS in studying compressed liquids. Since the Baonza EOS cannot satisfy the spinodal condition [15], it cannot be used to describe the transition from compressed liquid to expanded liquid (the same is true for the KD EOS). However, the mGLJ EOS in equation (7) can overcome this shortcoming. We can replace the KD and Baonza EOSs by using the two-parameter mGLJ EOS, and all equations in [5, 8–10] can be simplified. In summary, it is shown that the mGLJ EOS proposed in this letter has almost all four merits of an ideal EOS, and it is fairly convenient for practical applications.

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