

Draft

A new equation of state for high compression *

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A new equation of state for metals is developed. The starting point for this development is a realistic expression for the free energy, allowance being made not only for the lattice energy but also for the Fermi energy, the exchange and correlation energies of the electrons. This expression is extended by means of three free parameters. The equation of state is successfully transformed in such a way that only macrophysical material parameters occur in it. In this way, the equation can be applied both to experimental high-pressure physics and to geophysics, its advantage resting in the fact that the bonding structure has been taken into account better than in other equations of state.

The new equation, along with two other well-proven equations of state, was tried out on isothermal and Hugoniot data of 40 materials. Good agreement with the measured data was found not only for metallic elements, but also for halides and some oxides of geophysical importance. This agreement even proved to be better for most of the materials than that obtained with the other two equations of state.

1. Introduction

To be able to infer from the distribution of density in the interior of the Earth or other planets to the distribution of chemical elements and compounds, it is necessary (albeit not sufficient) to possess reliable equations of state for such high pressures. The original object of this investigation was to deduce from solid-state physics a new isothermal equation of state which, for the metallic core of the Earth, would give a better approximation to measured values. It was found, however, that the new equation is equally suitable for halides, for MgO and Al₂O₃, and that the relevant curves in the pressure–volume plot approximate the observational data more closely. Therefore, the new equation can also be used for the inversion of the data of the entire Earth. Whereas most equations of state commonly used in geophysics have been derived from thermodynamics and the mechanics

of continua or simply constitute empirical expressions, this paper attempts to analyze the bonding forces in such a manner that the result does not become too complicated, i.e. will still be applicable to geophysics.

2. Preliminary physical considerations on the development of the new equation of state

As is well known, solids can be classified into various groups, depending on the type of bonding, which are distinguished by the interaction of neighbouring atoms or molecules: rare-gas solids, ionic crystals, valence crystals with covalent bonding, metals and crystals with hydrogen bond. The various bondings are expressed mathematically by different interatomic potentials from which through derivation, different expressions are obtained for the equations of state of the types of solids. Thus, unified equations of state for all solids may be regarded as a first approximation

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only. Certainly, a unification fully suitable for solid-state physics could be achieved by a theory of mixed bondings. This, however, is very difficult. Phillips and Van Vechten (1969), e.g., suggested a semi-empirical theory involving a partly ionic and partly covalent bonding. In any case, it can be expected that better equations of state will be obtained if the bonding forces are taken into account in a more precise manner. And this is exactly the primary objective of this study. At present, semi-empirical set-ups are used in most cases for the interatomic potentials, which differ for the various types of bonding. In 1907, Mie suggested, for rare-gas solids, the following interatomic potential, mostly designated as the Lennard-Jones potential today

$$\Phi(r) = A_1/r^m - B_1/r^n, \quad \text{where } m > n \quad (1)$$

Since this set-up is an empirical one

$$\Phi(r) = A_2 e^{-r/r_0} - B_2/r^6 \quad (2)$$

is frequently used in place of it (Lidiard, 1974). This set-up lends itself better to an explanation in physical terms. The first term describes the shell-shell interaction by means of the Born-Mayer form, the second one represents the attractive Van der Waals forces. Equation 1 has already been used for expressing the ionic bonding, the electrostatic attractive force resulting from the second term with $n = 1$. For the covalent bonding, on the other hand, a simple inverse power law has, so far never been used, sometimes a Morse potential was employed.

The bonding conditions for metals are even more complex. But it is precisely these conditions in which interest is centred, not only to obtain a more realistic equation of state, but also a better melting temperature-pressure relation. The latter would be of special significance in further discussion of the core paradox (Kennedy and Higgins, 1973; Ullmann and Walzer, 1980a,b). Matsuda and Hiwatari (1973) suggest the following pair potential:

$$\Phi(r) = \epsilon(\sigma/r)^n - \alpha\gamma^3 \exp(-\gamma r) \quad (3)$$

In all three formulas mentioned, r is the distance between the atoms, the other quantities are constants. The theoretical curves of the dependence of

the triple-point temperature, critical-point temperature, fractional volume change on melting and other quantities of n , as derived from eq. 3, however, show compatibility with the observed data only for alkali metals and rare-gas solids, while set-up (3) is a complete failure for transition metals and noble metals. This clearly indicates that more use must be made of the electron theory of metals in a new set-up. It is well known that metallic bonding is very complex. Free mobility for the conduction electrons results in great uncertainty of the space coordinates. According to Heisenberg's uncertainty principle, the uncertainty of the generalized momentums is low in this case, however. The mean kinetic energy of the conduction electrons is low, and their interaction with the atomic trunks (i.e. atoms without conduction electrons) effects a large proportion of the metal bonding. Transition metals have, in addition, incomplete d-shells so that for iron, for instance, the inner electron shells considerably contribute to bonding. As with the rare-gas solid Ar (Keeler and Batchelder, 1970), the Cauchy relation $c_{12} = c_{44}$ is also not satisfied for the elastic constants of most transition and noble metals (see Tables 4.2.-4.4. of Leibfried and Breuer, 1978). This indicates that it would be appropriate to take non-central forces into account here, too. As is well known, there is a great variety of approximation methods for solving Schrödinger equation for metals. However, interest is only in solutions which can be applied to the parameters of the Earth's interior known in geophysics. Two notable attempts have been made to make equations of state derived from the Thomas-Fermi (TF) atom model applicable to geophysics (Gilvarry, 1969; Boschi and Caputo, 1970). The pressures of at most 363.24 GPa (3.6324 Mbars) achieved in the Earth are still so low, however, that shell structure of the atoms is still significant. A number of improvements have been made in the TF model, which succeeded in making it more suitable for application. As is well known, the model was extended by Dirac (1930), who added a term stemming from the exchange energy of the electrons. Von Weizsäcker (1935) made a further improvement by adding a term for the kinetic-energy density that is proportional to the square of the gradient of electron density. This

idea was systematically enhanced by Hohenberg and Kohn (1964), who substituted the von Weizsäcker term by an expansion after the gradient of electron density. But all these extensions do not suffice to make allowance for the radial oscillations of the electron density in the atom, i.e. the shell structure of the atom. This is, however, necessary for applications in planetary physics, because the shell structure still exists up to the highest pressures present there (~ 3000 GPa in the centre of Jupiter). Lee and Thorsos (1978) attempted to take shell structure into account in an extended TF-model for elements having atomic numbers between 5 and 30. However, there is little promise in calculating the mass density-pressure plot for iron for geophysical purposes. Interesting papers have been published recently, in which the TF approach is used for diatomic and triatomic molecules (Jacob et al., 1978; Dreizler et al., 1979; Gross and Dreizler, 1979; Shih, 1979). Perrot (1979a) described in a very clear way how density is calculated as a function of pressure and temperature for the TF-model and some extensions of the model. The solution of a differential equation of fourth order for the determination of local electron density constitutes the core of these calculations. While the calculations are too extensive to be used as an equation of state suited for geophysical purposes, they, as well as the previously mentioned papers, gave important suggestions for the calculation of the equation of state developed in the next section. In addition, the aforesaid modifications of the TF model apply only to compressions higher than those occurring in the Earth. Thus, for instance, the TF Dirac model is probably applicable only to $x \leq 0.02$ in Li, $x \leq 0.05$ in Be and Al and $x \leq 0.1$ in Cu, where $x = \rho_0/\rho$, ρ is the mass density and ρ_0 is the mass density at zero pressure (Perrot, 1979b).

3. Development of the new equation of state

Let the free energy of a metal be represented as the following sum

$$\Phi = \Phi_1 + \Phi_0 + \Phi_i + \Phi_e \quad (4)$$

where

$$\Phi_1 = \frac{1}{2}NZ\epsilon^* \left[A(v/v^*)^{-4} - 2B(v/v^*)^{-2} \right] \quad (5)$$

the interaction free energy, assuming a Lennard-Jones potential

$$\Phi_0 = \frac{1}{2} \sum_{i=1}^{3N} h\nu_i \quad (6)$$

the zero-point free energy

$$\Phi_i = kT \sum_{i=1}^{3N} \ln[1 - \exp(-h\nu_i/kT)] \quad (7)$$

the thermal free energy and Φ_e the free energy of the free electrons. Many authors (e.g. Midha and Nanda, 1975; Mulargia and Boschi, 1979) have used such a representation or a similar one. Hirschfelder et al. (1954), assuming three shells from neighbouring atoms around a mean atom, found, for a f.c.c. lattice, $A = 1.0110$ and $B = 1.2045$. Moreover, the quantities are: T temperature, h Planck's constant, k Boltzmann's constant, ν_i frequency, v atomic volume, N number of atoms, Z coordination number, ϵ^* and v^* are energy and volume constants. From now on, the dependence on temperature is neglected, thus restricting the problem to isothermal equations of state. There are several possibilities for calculating the electronic proportions of free energy (March, 1974). Employ the Hartree-Fock energy E_{HF}

$$E_{\text{HF}} = N(2.21/r_s^2 - 0.916/r_s) \quad (8)$$

The first term on the right-hand side (Fermi term) represents the mean kinetic energy of the electrons, the second term (exchange term) defines the mutual repulsion of electrons having the same spin. To fully allow for the interaction of the conduction electrons, use, additionally, Wigner's (1938) interpolation formula for the correlation energy E_{corr}

$$E_{\text{corr}} = N[-0.88/(r_s + 7.8)] \quad (9)$$

where r_s is the mean interelectronic spacing measured in Bohr units. Only the valence electrons are taken into account. The energies in eqs. 8 and 9 are expressed in Ryd. It is found through simple consideration that x defined above can also be expressed by $x = r_s^3/r_{s0}^3$, r_{s0} being the r_s for zero pressure. r_s lies between 2 and 6 Bohr units for metals. To simplify the formulas, introduce heuristically, though somewhat forcedly, $r_{s0} = 4$ Bohr

units into the formulas. A well-substantiated expression for the free energy of the metals results from the substitution of eqs. 5–9 in eq. 4.

This expression is now generalized through the introduction of free parameters a , b and n . At the same time, it becomes thus possible to introduce macrophysical quantities into the formulas. This makes it possible to compare the formula with high-compression data and with data from the Earth's interior. The physically well-substantiated set-up for free energy is

$$\Phi = a(A/x^{2n/3} - 2B/x^{n/3}) + b[C/x^{2/3} - D/x^{1/3} - E/(x^{1/3} + F)] \quad (10)$$

The terms on the right-hand side mean, respectively, repulsive and attractive lattice term, Fermi free energy of the electrons, exchange and correlation term of the electrons. The quantities A–F are fixed and are well substantiated in physical terms: A = 1.0110; B = 1.2045; C = 0.138 Ryd; D = 0.229 Ryd; E = 0.220 Ryd; F = 1.95. Contrary to this, the quantities a , b and n are fixed only for one material each and will be expressed below by better-known quantities. Using the thermodynamic relation $P = -(\partial\Phi/\partial x)_T$, the following new equation of state from eq. 10 is obtained

$$P = (2n/3)a(A/x^{2n/3+1} - B/x^{n/3+1}) + \frac{2}{3}b\left\{C/x^{5/3} - D/2x^{4/3} - E/\left[2(x^{1/3} + F)^2 x^{2/3}\right]\right\} \quad (11)$$

From pressure P , calculate the bulk modulus κ by means of $\kappa = -x\partial P/\partial x$ and obtain

$$\kappa = \frac{2n}{3}a\left[\frac{(2n/3+1)A}{x^{2n/3+1}} - \frac{(n/3+1)B}{x^{n/3+1}}\right] + \frac{2}{9}b \times \left[5Cx^{-5/3} - 2Dx^{-4/3} - E\frac{2 + Fx^{-1/3}}{(x^{1/3} + F)^3 x^{1/3}}\right] \quad (12)$$

Furthermore

$$-x\partial\kappa/\partial x = \frac{2n}{3}a\left[\frac{(2n/3+1)^2 A}{x^{2n/3+1}} - \frac{(n/3+1)^2 B}{x^{n/3+1}}\right] + \frac{2}{27}b\left\{25Cx^{-5/3} - 8Dx^{-4/3} - E\frac{2 + Fx^{-1/3}}{(x^{1/3} + F)^3 x^{1/3}}\right\}$$

$$-E(x^{1/3} + F)^{-4}\left[Fx^{-1/3}(1 + Fx^{-1/3}) + (2 + Fx^{-1/3})(4 + Fx^{-1/3})\right] \quad (13)$$

Denote the bulk modulus at vanishing pressure by κ_0 , its pressure derivative at vanishing pressure by κ_1 . Thus $\kappa_0 \equiv \kappa|_{x=1}$ and $\kappa_1 \equiv \partial\kappa/\partial P|_{x=1}$. Moreover, $\partial\kappa/\partial P = (-x\partial\kappa/\partial x)\kappa^{-1}$. In this way it is possible, using eqs. 11–13 specialized for the case $x = 1$, to determine the quantities a , b and n as functions of the constants κ_0 and κ_1 known for many materials, and of the material-independent constants A–F. This is necessary for the numerical determination of the quantities Φ , P and κ as a function of $x (= \rho_0/\rho)$. As a result

$$n = (L\kappa_1 - K)/2 + \left\{[(L\kappa_1 - K)/2]^2 - M + N\kappa_1\right\}^{1/2} \quad (14)$$

$$a = (3/2)\kappa_0 n^{-1}[(2n/3 + 1)A - (n/3 + 1)B + GH]^{-1} \quad (15)$$

$$b = Gna \quad (16)$$

where

$$G \equiv (B - A)\left\{C - [D + E/(1 + F)^2]/2\right\}^{-1}$$

$$H \equiv [5C - 2D - E(2 + F)(1 + F)^{-3}]/3$$

$$I \equiv \left\{25C - 8D - E(1 + F)^{-4} \times [F(1 + F) + (2 + F)(4 + F)]\right\}/9$$

$$J \equiv (4A - B)/9$$

$$K \equiv (4A - 2B)/3J$$

$$L \equiv (2A - B)/3J$$

$$M \equiv (A - B + GI)/J$$

$$N \equiv (A - B + GH)/J$$

The new equation of state, eq. 11, which must be used together with eqs. 14–16 and the constants A–N, contains a more precise analysis of the bonding forces, and it is desired to demonstrate that it is also more suited than other equations of state when applied to high-pressure data. The constants A–N are identical for all materials, however κ_0 and κ_1 must be specifically chosen for the material concerned. Consequently, eq. 11 is easily applicable to practical high-pressure studies and to

geophysics. The author hopes that the new equation of state constitutes a sound compromise between a deeper theoretical-physical penetration of the problem and the requirements of simplicity and agreement with measured data existing in practical high-pressure research and geophysical modelling.

4. Other equations of state

When the new equation of state was used, it was found that it showed very good agreement with high-pressure data for geophysically relevant oxides and for halides also, although it had originally been designed for metals only. This induced the use of other equations of state for comparison purposes also, only two very realistic ones having been used for comparison in the illustrations. These two other equations of state are developed below.

As is well known (see, e.g. Gupta and Shanker, 1979), an interatomic potential of the following form is frequently used for materials with ionic bond (e.g. for alkali halides)

$$\Phi = -\alpha_m e^2/r + \beta e^{-r/r_0} - \delta_1/r^6 - \delta_2/r^8 \quad (17)$$

where α_m is the Madelung constant, β and r_0 are the constants of the Born-Mayer repulsive term and δ_1 and δ_2 are the van der Waals dipole-dipole and dipole-quadrupole interaction constants. To substitute the macrophysical quantities κ_0 and κ_1 for the constants, using the approach taken in the previous section, neglect the last two terms on the right-hand side of eq. 17, because the higher pressure derivatives of the bulk modulus are unknown or uncertain for most materials. Here again r is the interatomic spacing. Thus, substitute eq. 18 for eq. 17, where c_1 - c_3 are constants that are expressed below by functions of κ_0 and κ_1

$$\Phi = -c_1 x^{-1/3} + c_2 \exp(-x^{1/3}/c_3) \quad (18)$$

From this it follows that

$$P = [3\kappa_0/(D_2 - 2)] \times \{x^{-2/3} \exp[D_2(1 - x^{1/3})] - x^{-4/3}\} \quad (19)$$

where

$$D_2 = (3/2)(\kappa_1 - 1) + (1/2)[(3\kappa_1 - 7)^2 + 8]^{1/2} \quad (20)$$

Equation 19 constitutes the Born-Mayer equation of state (see also Zharkov and Kalinin, 1971; Pan'kov and Ullmann, 1979).

If the Lennard-Jones potential of eq. 1 is specialized to the case $m = 2n$,

$$\Phi = A_1/x^{2n/3} - B_1/x^{n/3} \quad (21)$$

If A_1 , B_1 and n are eliminated according to the approach used in the previous section, from eq. 21

$$P = [3\kappa_0/(\kappa_1 - 2)](x^{(1-2\kappa_1)/3} - x^{-(1+\kappa_1)/3}) \quad (22)$$

This is the equation of state M1 by Ullmann and Pan'kov (1976) that was developed by these authors primarily on the basis of thermodynamic considerations. The practical use of this equation of state was proven by the two authors themselves and by Walzer et al. (1979). On the other hand, from eq. 2

$$P = [3\kappa_0/(D_1 - 7)] \times \{x^{-2/3} \exp[D_1(1 - x^{1/3})] - x^{-3}\} \quad (23)$$

where

$$D_1 = (3/2)(\kappa_1 - 1) + (1/2)[(3\kappa_1 - 17)^2 + 28]^{1/2} \quad (24)$$

The equation of state, eq. 23, is not used here for a comparison. It is surely significant for rare-gas solids.

5. Comparison of the three equations of state with experimental data

In the comparison of the equations of state with measured data experimental compression data from volumetric measurements, shock-wave data and X-ray studies were used. Room isotherm data taken from experimental Hugoniot data were used amongst others. Ullmann and Pan'kov (1976) collected these values from literature and reduced them to room isotherms, using the common approach. Estimation of the Hugoniot pressure by means of the Mie-Grüneisen equation and Rankine-Hugoniot conservation laws is shown, for instance, by Walzer et al. (1979). The same input data as listed in Table I were used for the room isotherms of the three models employed. Each of the three curves was plotted in P - x plots

TABLE I
Material parameters employed *

Material	κ_0 (kbar)	κ_1	Figure	Reference
Elements				
4th period				
K	31.2	3.85	1A	Smith and Smith (1965)
Ca	183	2.78	1B	Polynomial fitting after Vaidya and Kennedy (1970)
V	1537	3.5	1C	Guinan and Steinberg (1974), Bolef (1961)
Fe(ϵ)	2060	4.0	1D	Takahashi et al. (1968)
Ni	1790	6.2	1E	Guinan and Steinberg (1974)
Cu	1330	5.65	1F	Barsch and Chang (1967)
Zn	638	6.40	1G and 1H	Ullmann and Pan'kov (1976), Fig. 18
Ge	724.3	4.35	1I	Anderson (1966)
5th period				
Rb	26.2	3.39	1J	Grover (1971)
Nb	1690	6.9	1K	Guinan and Steinberg (1974)
Ag	1015	5.53	1L	Daniels and Smith (1958), Vaidya and Kennedy (1970)
Cd	457.9	6.77	1M	Anderson (1966)
In	392	6.0	1N	Voronov and Goncharova (1972)
Sn(w)	532	6.01	1O	Guinan and Steinberg (1974)
Sn(w)	532	4.9	1P	Guinan and Steinberg (1974), Ullmann and Pan'kov (1976), Fig. 25
I	83.7	6.0	1Q	Vaidya and Kennedy (1972)
6th period				
Au	1664	6.51	1R	Barsch and Chang (1967)
Pb	419	5.72	1S and 1T	Miller and Schulle (1969)
2nd period				
Li	115	3.56	1U	Day and Ruoff (1974)
3rd period				
Na	61.8	3.59	1V	Anderson (1966), Ho and Ruoff (1968)
Mg	344.2	4.16	1W	Anderson (1966)
Al	729.1	4.7	1X	Ahrens and Thomsen (1972), Thomas (1968)
Si	970.8	4.16	1Y	Anderson (1966)
S	88.4	6.55	1Z	Vaidya and Kennedy (1972)
Halides				
NH ₄ Cl	176.7	8.21	2A	Garland and Renard (1966)
NH ₄ Br	158.6	7.66	2B	Garland and Yarnell (1966)
AgCl	417.4	7.00	2C	Loje and Schuele (1970)
AgBr	377.7	7.49	2D	Loje and Schuele (1970)
LiF	665.7	5.24	2E	Anderson (1966)
NaCl	237.5	5.35	2F	Roberts and Smith (1970), Spetzler et al. (1972)
NaBr	192.0	5.3	2G	Barsch and Chang (1967), Roberts and Smith (1970)
NaI	162.2	5.48	2H	Barsch and Schull (1971)
CsCl	167.4	5.98	2I	Barsch and Chang (1971)
CsBr	143.4	5.95	2J	Barsch and Chang (1971)
CsI	118.9	5.93	2K	Barsch and Chang (1971)
Oxides				
MgO	1599	4.25	3A	Anderson et al. (1968)
Al ₂ O ₃	2505	3.99	3B	Anderson et al. (1968)
FeO	1740	4.0	3C	Mao et al. (1969), Ullmann and Pan'kov (1976), Fig. 49
Fe ₂ O ₃	2027	4.5	3D	Anderson et al. (1968)
CaO	1049	5.26	3E	Anderson et al. (1968)
Stishovite	3460	3.5	3F	Chung (1974), Ullmann and Pan'kov (1976), Fig. 51

* These data have been compiled by Ullmann and Pan'kov (1976). The origin of the data is given in the fifth column.

TABLE II

References from which the observational results have been taken

Material	Figures	Symbol	Reference
Alkali metals	1A, 1J, 1U, 1V	●	Room isotherm based on Hugoniot data reduction (Grover et al., 1969)
		○	Static data (Vaidya et al., 1971)
		X	Rice (1965), Bakanova et al. (1965), Carter et al. (1971), Grover et al. (1969)
		△	Bridgman's data (quoted by Birch, 1966)
		●	Bridgman's data (quoted by Birch, 1966)
Cu, Ag, Au, Mg, Ca	1F, 1L, 1R, 1W, 1B	△	Bridgman's data (quoted by Birch, 1966)
Zn, Cd, Al, Si, Ge, Sn, Pb, V, Ni	1G, 1H, 1M, 1X, 1Y, 1I, 1O, 1P, 1S, 1C, 1E	●	Room isotherm based on Hugoniot data reduction (Carter et al., 1971)
		⊕	Zero isotherm (Al'tshuler et al., 1962)
		○	Static data (Vaidya and Kennedy, 1970)
		X	Hugoniot data (Carter et al., 1971)
		▽	Bridgman's data (quoted by Vaidya and Kennedy, 1970; Kennedy, 1972)
In, Nb, S	1N, 1K, 1Z	△	Bridgman's data (quoted by Birch, 1966)
		X	Hugoniot (McQueen and Marsh, 1960; Al'tshuler et al., 1960)
		●	Room isotherm (McQueen and Marsh, 1960)
		○	Static data (Vaidya and Kennedy, 1970, 1972)
		○	Static data (Vaidya and Kennedy, 1970, 1972)
Pb	1S, 1T	X	Hugoniot data (Rice et al., 1958)
		●	Room isotherm based on the Hugoniot data mentioned above
		△	Bridgman's data (quoted by Birch, 1966)
I	1Q	+	Hugoniot data (Al'tshuler et al., 1962)
		⊕	Room isotherm based on the Hugoniot data mentioned above
Fe	1D	○	Static data (Vaidya and Kennedy, 1972)
		X	Hugoniot data (Duvall and Fowles, 1963)
		●	Hugoniot data (Keeler, 1972)
		●	Isotherms from Hugoniot data (Takeuchi and Kanamori, 1966)
		▲	Isotherms (McQueen and Marsh, 1960; Pan'kov and Kalinin 1974)
		●	Isotherms (Zharkov et al., 1975)
NaCl, NaBr	2F, 2G	○	X-ray data (Takahashi et al., 1968)
		□	Shock-wave data (Bancroft et al., 1956)
		X	Smoothed Hugoniot data (Takeuchi and Kanamori, 1966)
		+	Smoothed Hugoniot data (Takeuchi and Kanamori, 1966)
		○	Static data (Vaidya and Kennedy, 1971)
		△	Bridgman's data (Birch, 1966)
NaCl, NaBr	2F, 2G	X	Hugoniot (Van Thiel, 1966; Fritz et al., 1971; Weaver, 1971)
		●	Room isotherm based on the Hugoniot data mentioned above
		○	Static data (Vaidya and Kennedy, 1971)
		□	X-ray data (Perez-Albuerne and Drickamer, 1965)

TABLE II (continued)

Material	Figures	Symbol	Reference
NaI, LiF	2H, 2E, 2C,	⊙	Static data (Vaidya and Kennedy, 1971)
AgCl, AgBr,	2D, 2A, 2B,	△	Bridgman's data (Birch, 1966)
NH ₄ Cl,	2I, 2J, 2K	●	Isotherm from Hugoniot data (Keeler, 1972)
NH ₄ Br,		X	Hugoniot data (Van Thiel, 1966)
CsCl, CsBr,		+	Hugoniot data (Al'tshuler et al., 1963; Kormer et al., 1964)
CsI		▽	Bridgman's data (Vaidya and Kennedy, 1971)
		□	X-ray data (Perez-Albuerno and Drickamer, 1965; Hammond's data quoted by Mao, 1970)
		⊙	Isotherm from the equation of state by Decker (1971)
MgO, Al ₂ O ₃	3A, 3B	X	Smoothed Hugoniot data (Carter et al., 1971)
		●	Room isotherm from Hugoniot data (Carter et al., 1971)
		▲	Room isotherm from Hugoniot data (Pan'kov and Kalinin, 1974)
		□	X-ray data (Drickamer et al., 1966)
		+	Hugoniot data (Al'tshuler, 1965) and ceramic sample. Hugoniot data by McQueen and Marsh (Birch, 1966)
		⊙	Data by Zharkov et al. (1975)
		⊕	Hugoniot data after McQueen and Marsh (Birch, 1966)
FeO, CaO	3C, 3E	□	X-ray data (Drickamer et al., 1966)
		⊕	Room isotherm computed by Al'tshuler and Sharipdzhanov (1971)
		▲	Room isotherm from Hugoniot data (Pan'kov and Kalinin, 1974)
		⊙	X-ray data (Mao et al., 1969)
		⊙	Data by Zharkov et al. (1975)
Fe ₂ O ₃	3D	□	X-ray data (Drickamer et al., 1966)
		X	Hugoniot data after McQueen and Marsh (Birch, 1966; D.L. Anderson and Kanamori, 1968)
		⊕	Hugoniot data (Syono et al., 1974)
		⊙	Data by Zharkov et al. (1975)
Stishovite	3F	□	X-ray data (Liu et al., 1974)

along with the experimental results that had been reduced to isothermal conditions. In this way, it can quickly be found which equation of state is best suited for which materials. The curve taken from the new equation of state, eq. 11, has been designated by MX, the Born-Mayer equation of state, eq. 19, by BM and eq. 22, i.e. model 1 by Ullmann and Pan'kov (1976), by M1. To ensure a

fair comparison of the equations of state, the author has consciously confined himself to the materials selected by Ullmann and Pan'kov (1976) and also adopted the representation of the experimental data in the $P-x$ plots. The origin of the observational results is given in Table II. The Hugoniot adiabatic data are marked by crosses, while the isotherm data have been marked by

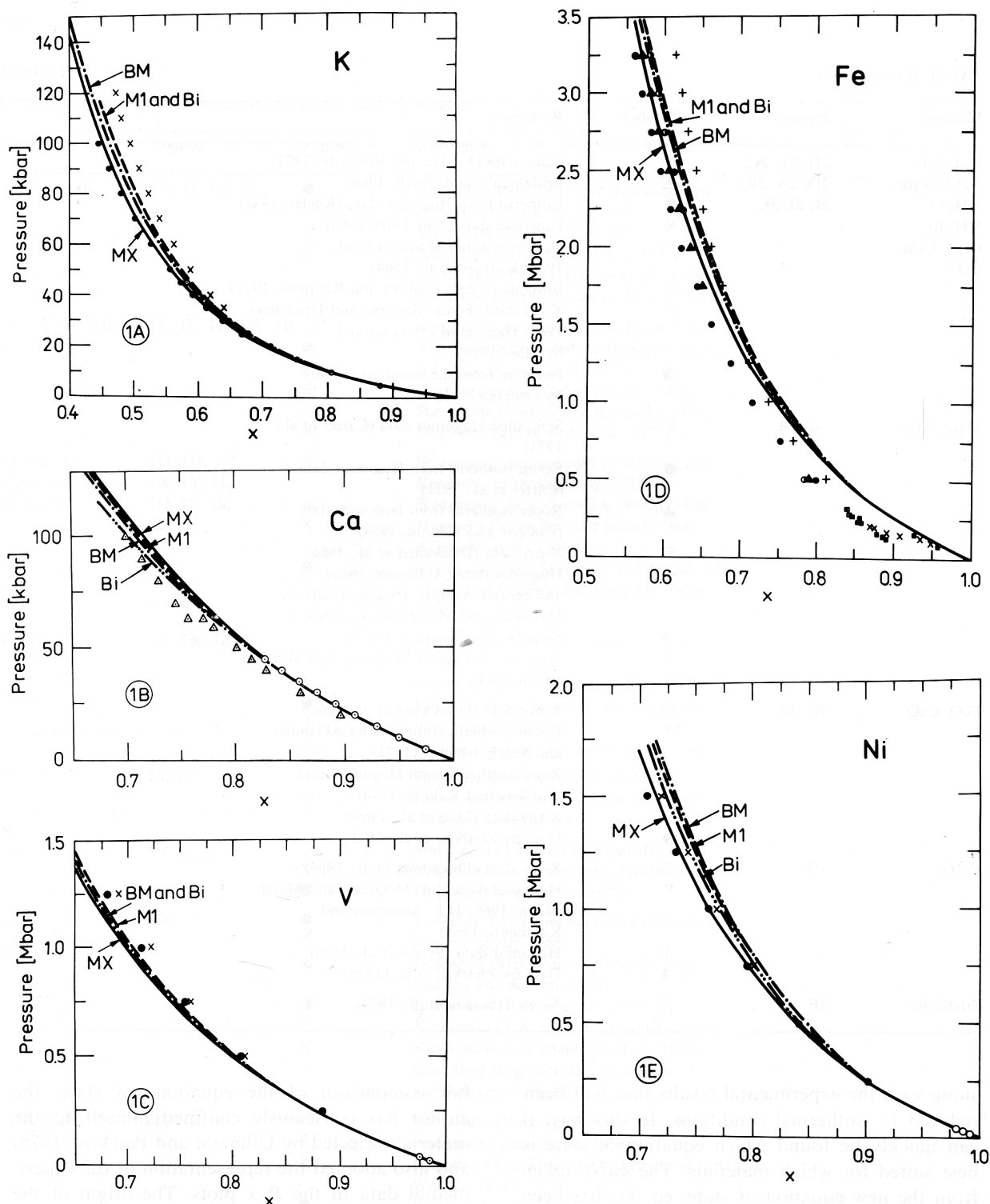
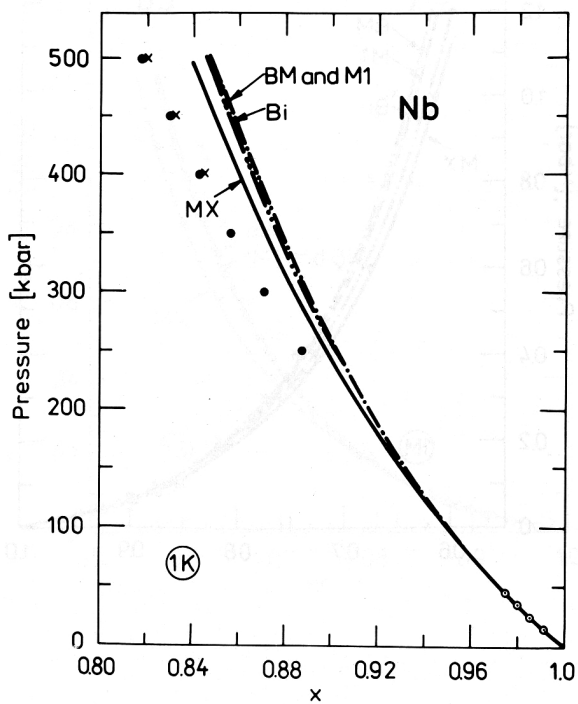
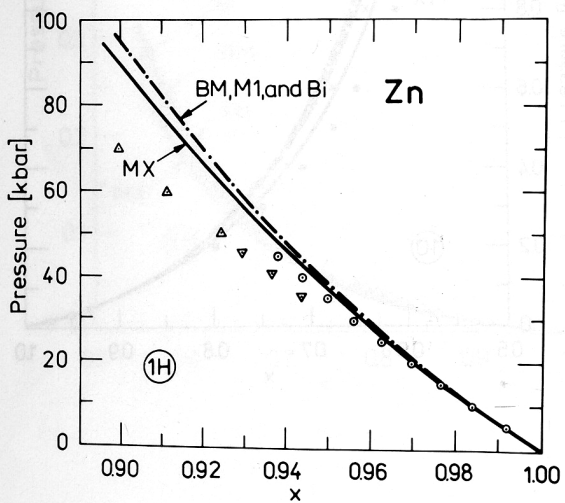
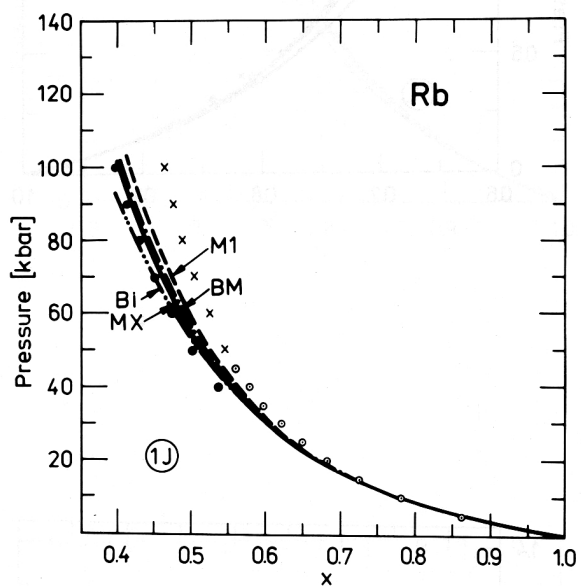
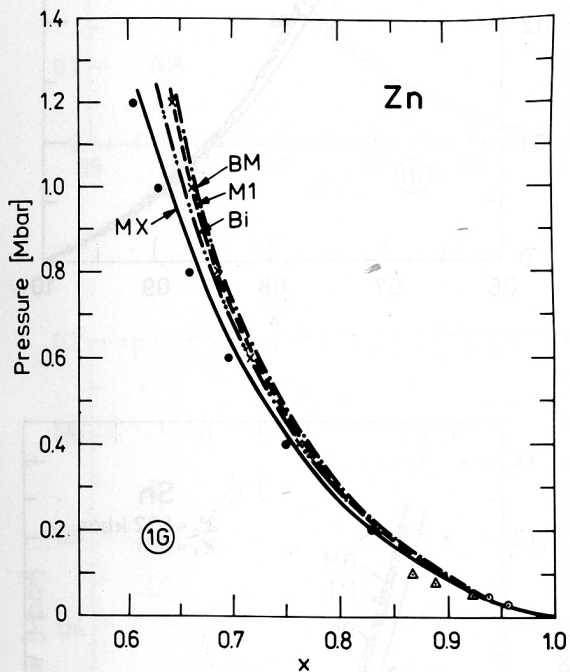
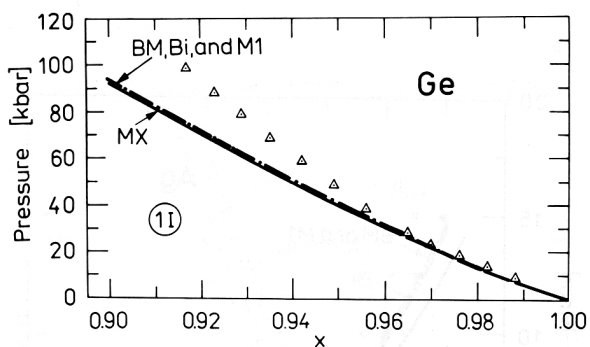
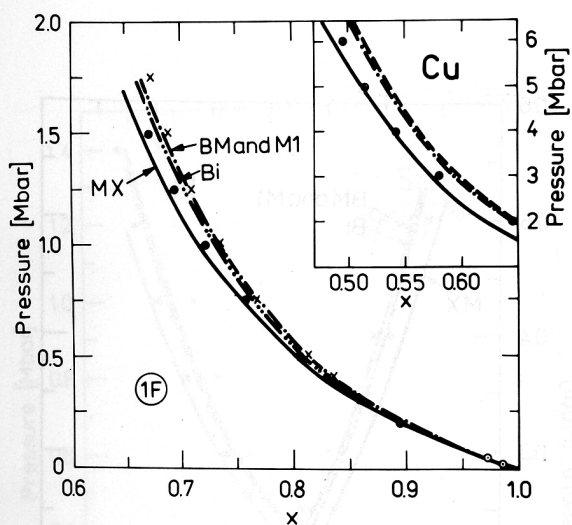
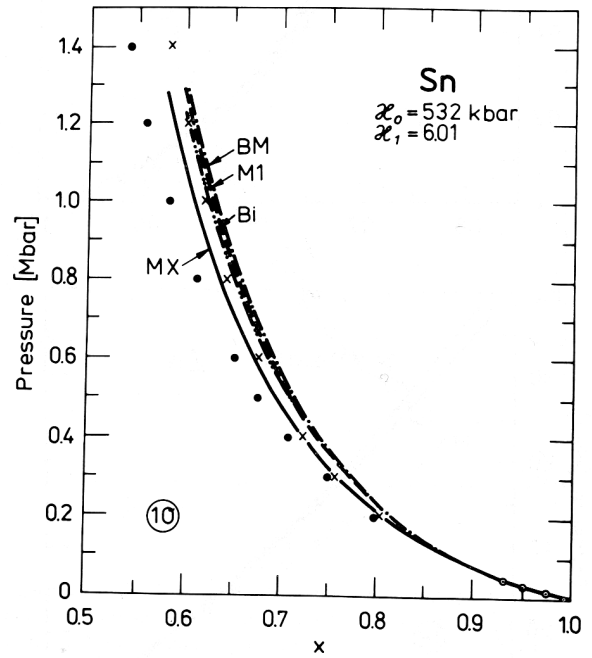
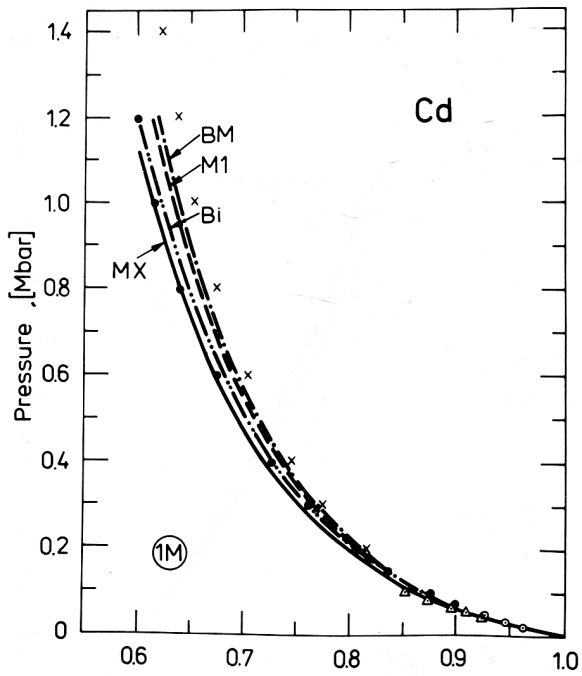
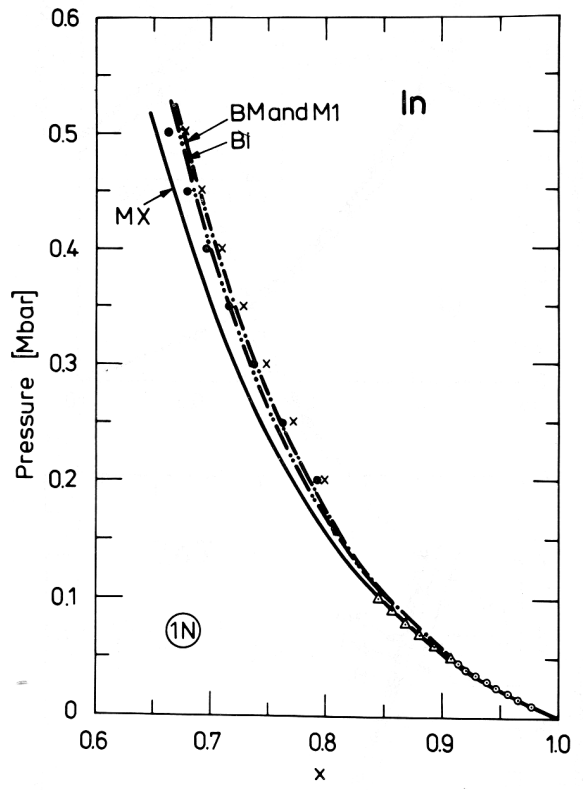
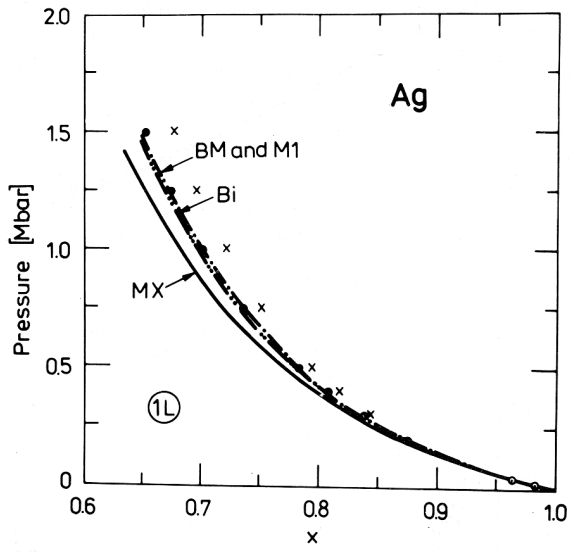
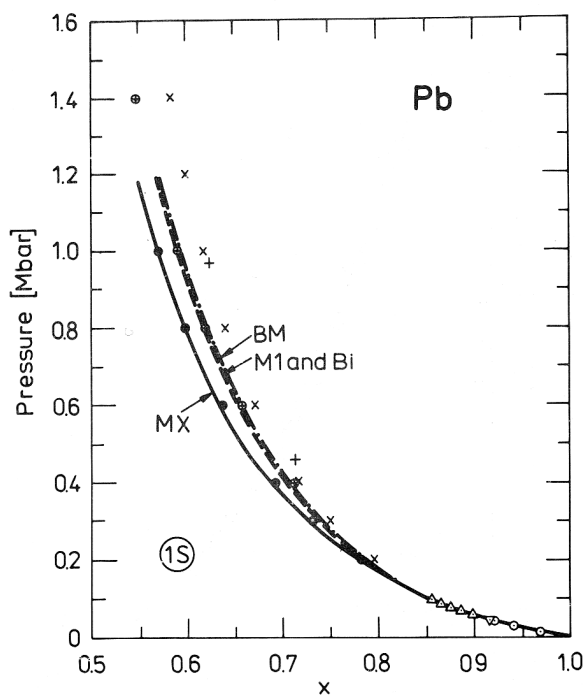
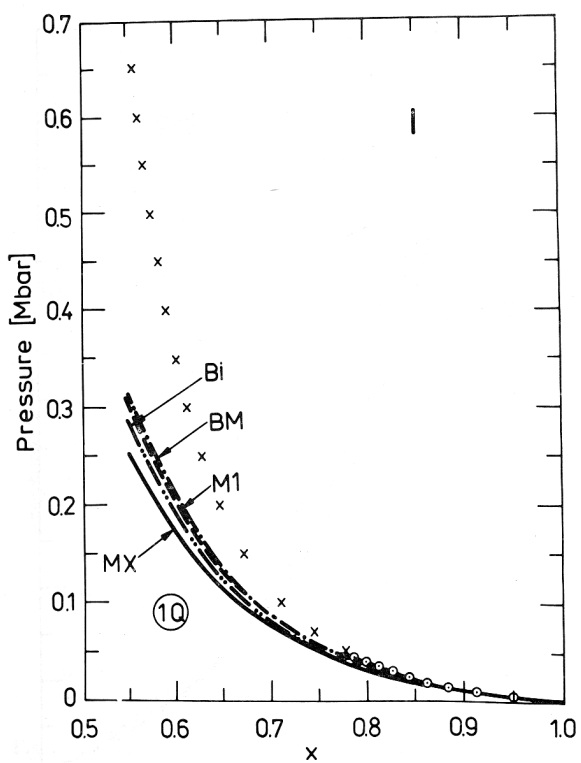
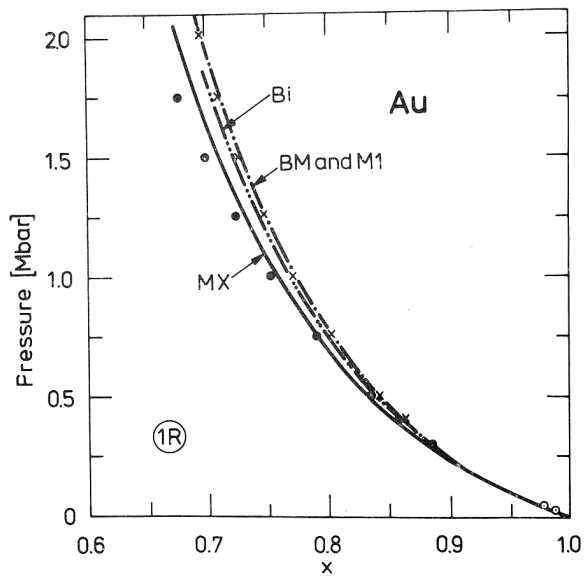
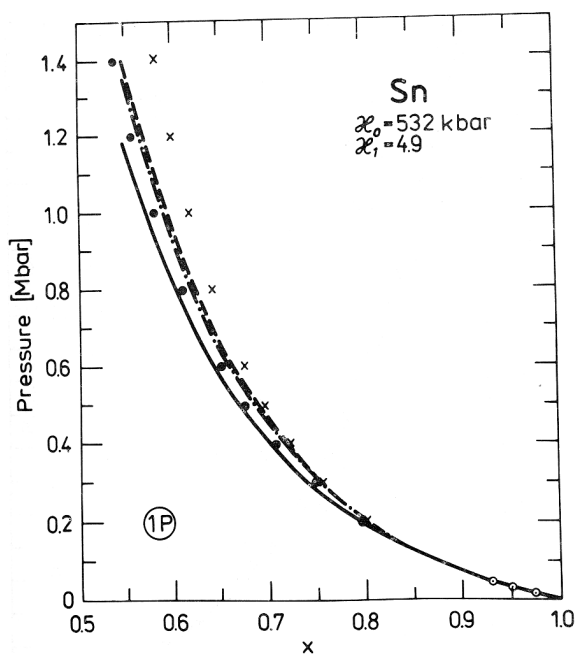


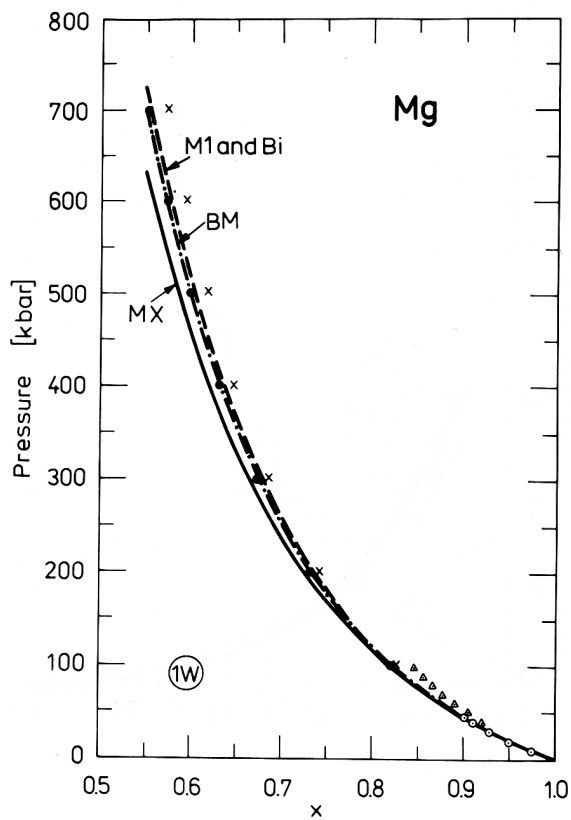
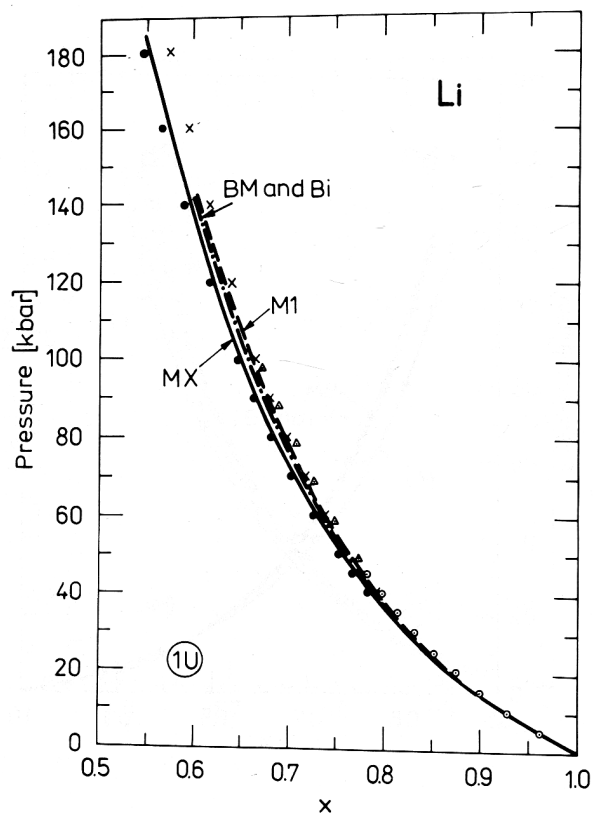
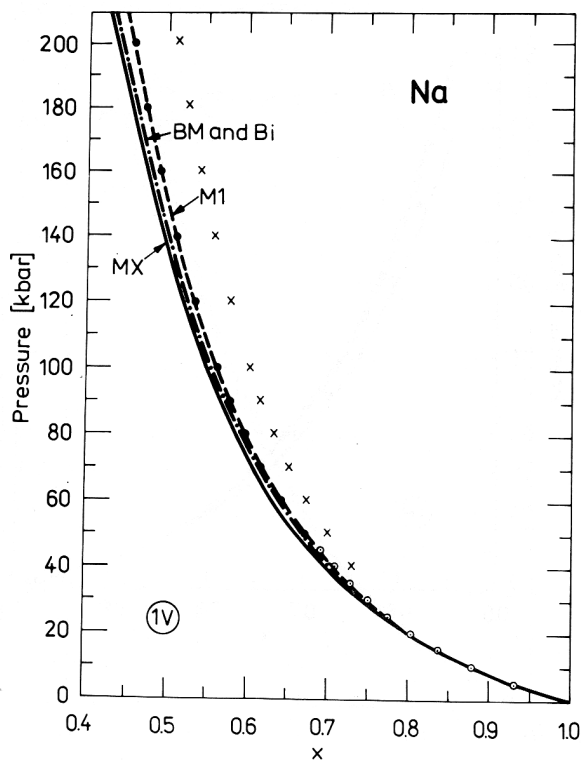
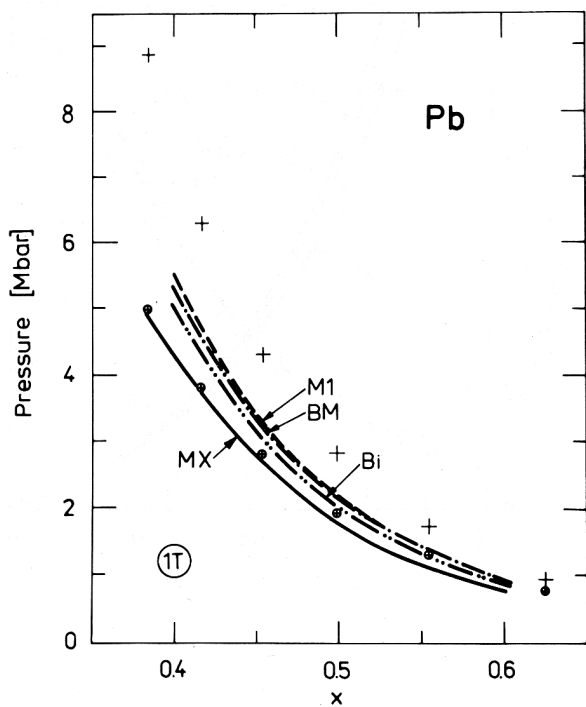
Fig. 1. Pressure versus the zero-pressure density to density ratio. These figures are valid for the elements that are arranged according to the periods of the Periodic Table. All curves are isotherms. The continuous curve (MX) was calculated according to the new equation of state, eq. 11, the dot-point-dot curve (BM) according to the Born-Mayer equation, eq. 19, and the dotted curve (M1) according to eq. 22 that has been developed on the basis of a thermodynamic approach by Ullmann and Pan'kov (1976). The experimental values are often reduced to such an extent that they can be compared to the theoretical curves. Further details of the figures, in particular on the origin of the experimental high-compression data, can be found in Table II.



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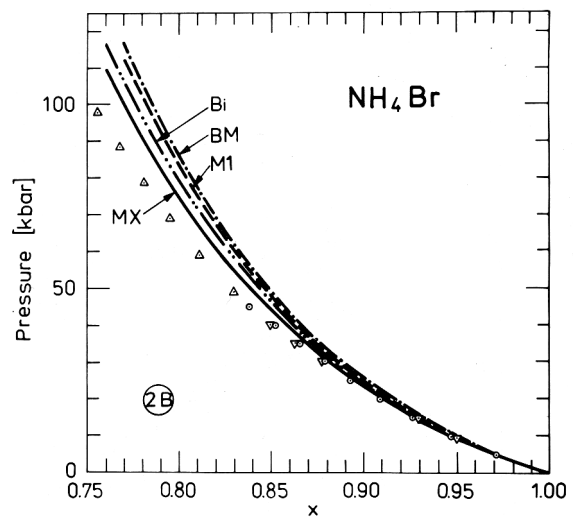
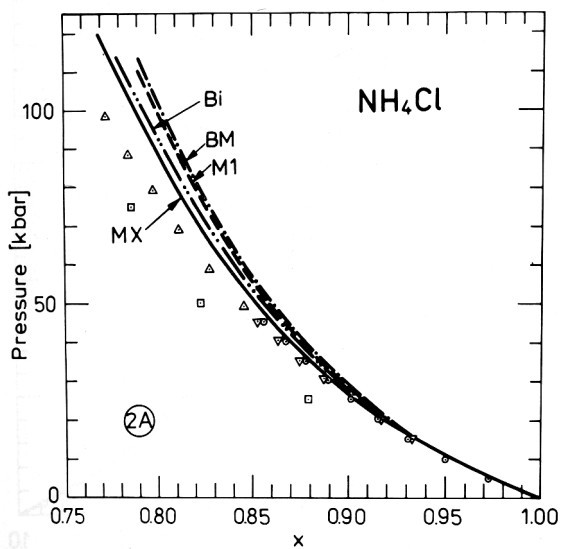
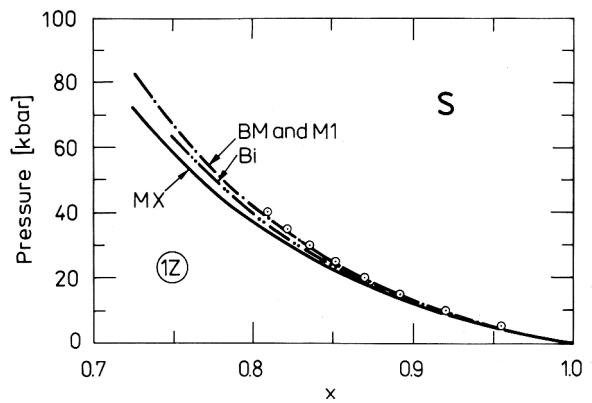
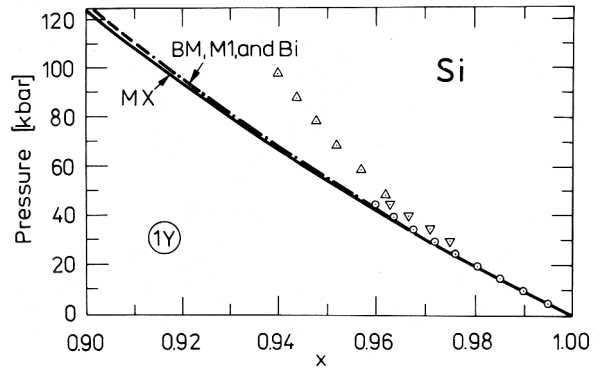
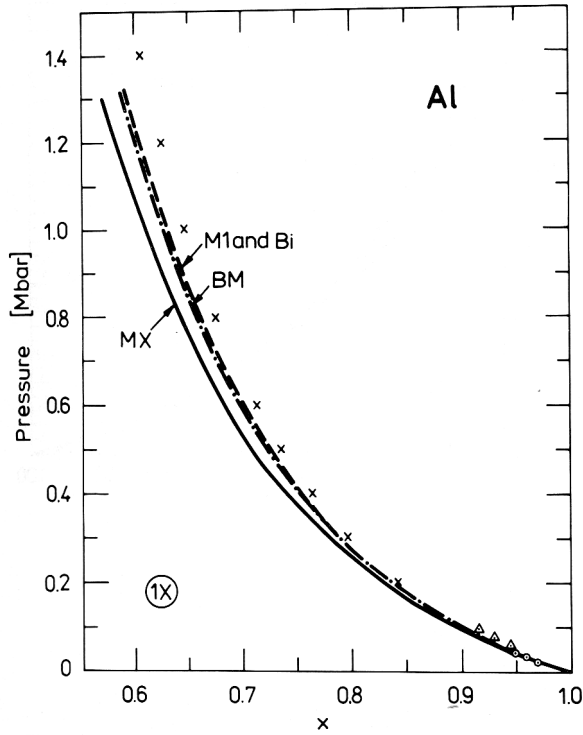
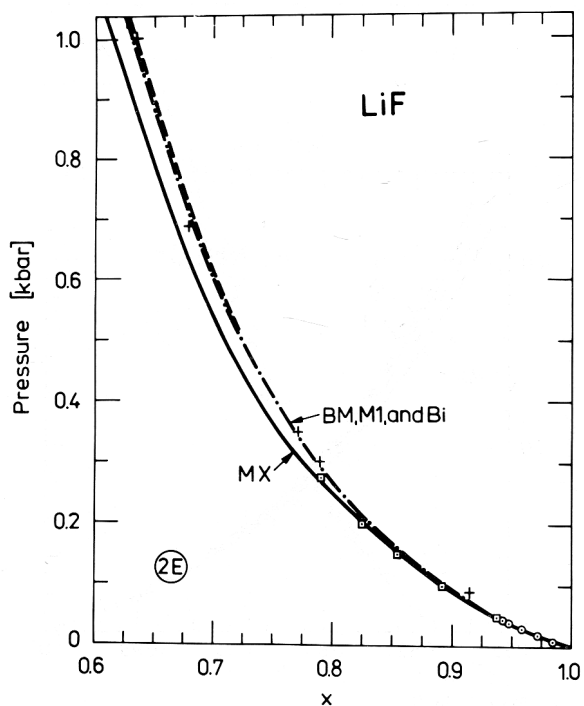
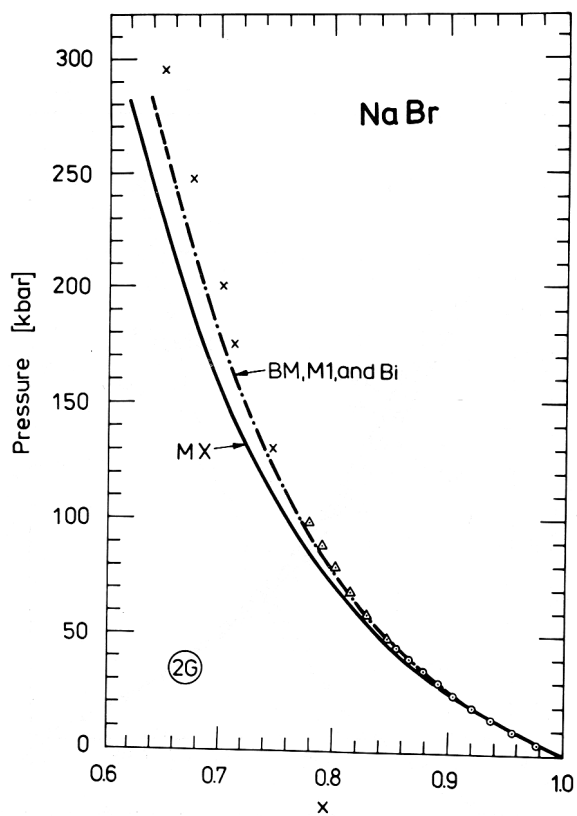
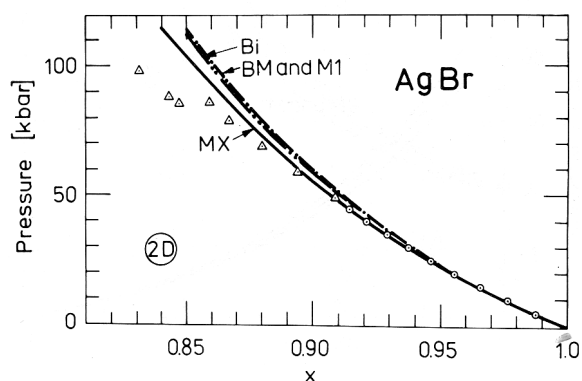
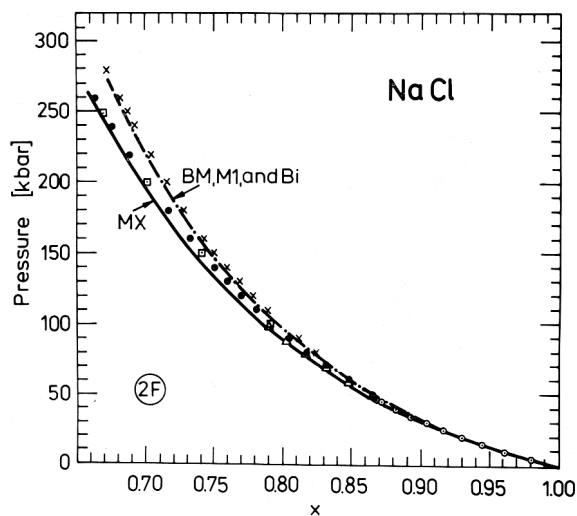
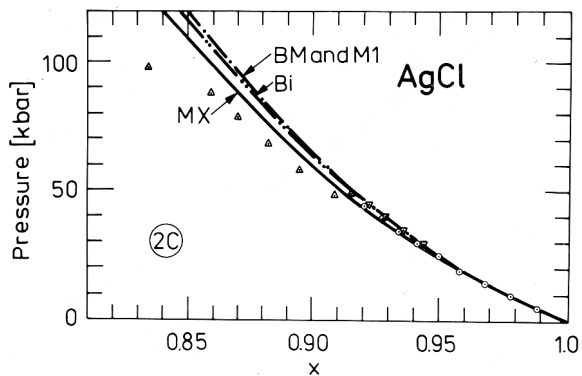


Fig. 2. Pressure versus the zero-pressure density to density ratio for halides. Data as in Fig. 1.



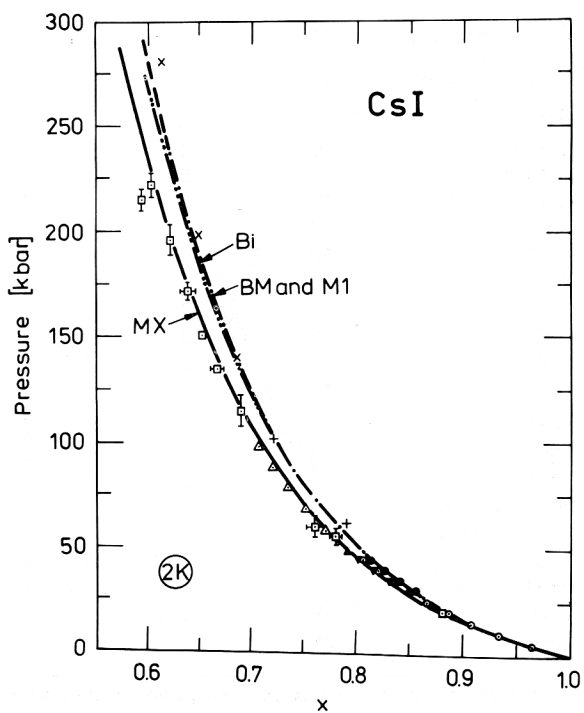
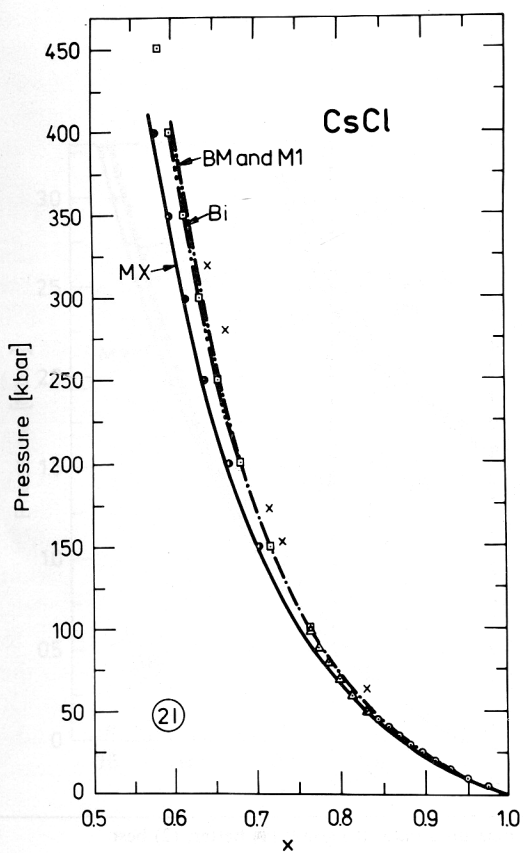
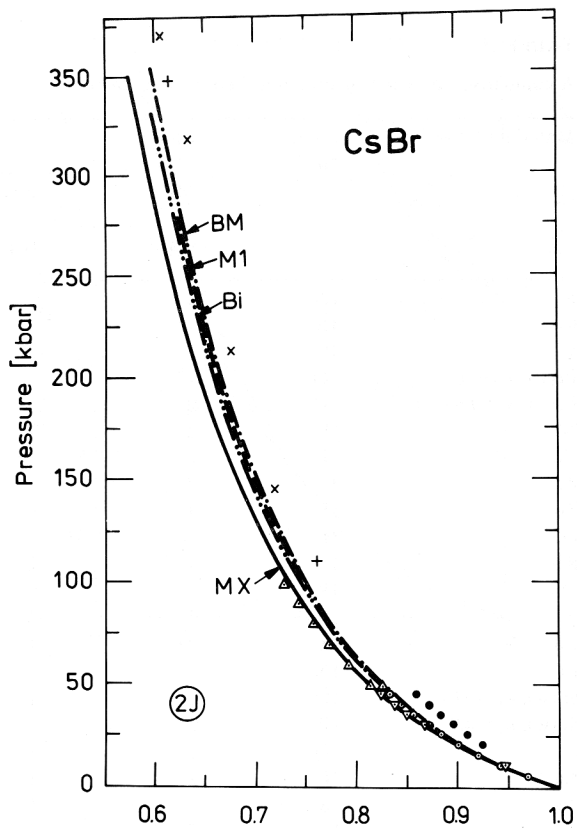
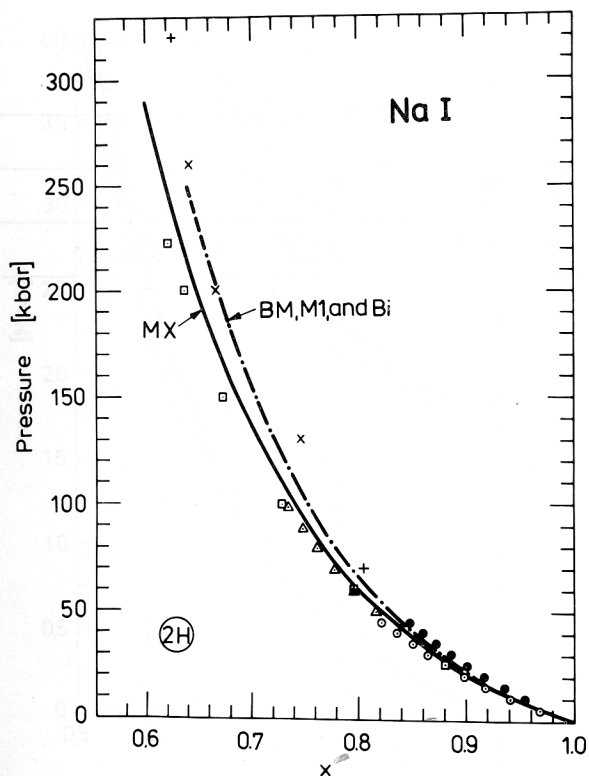
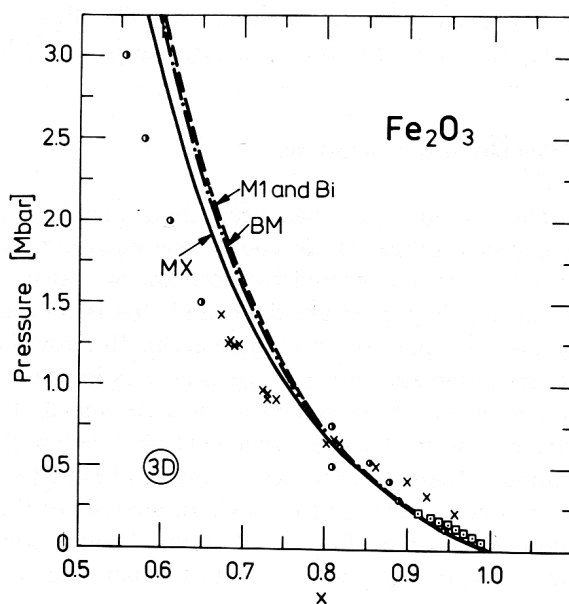
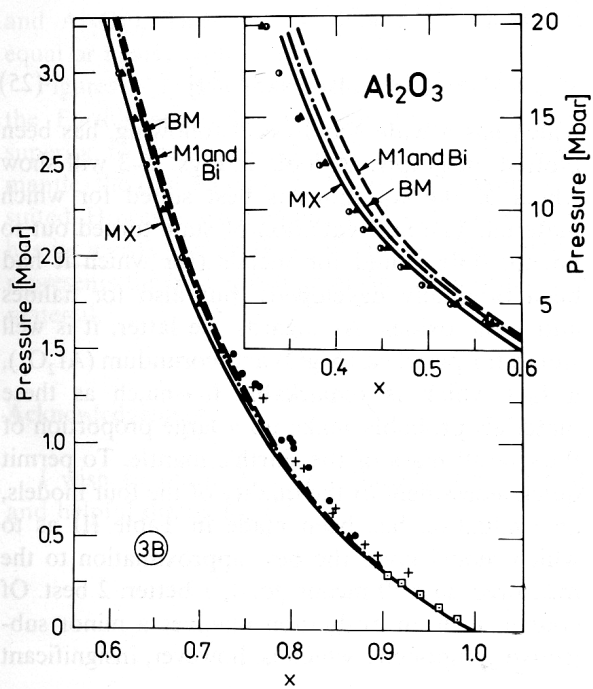
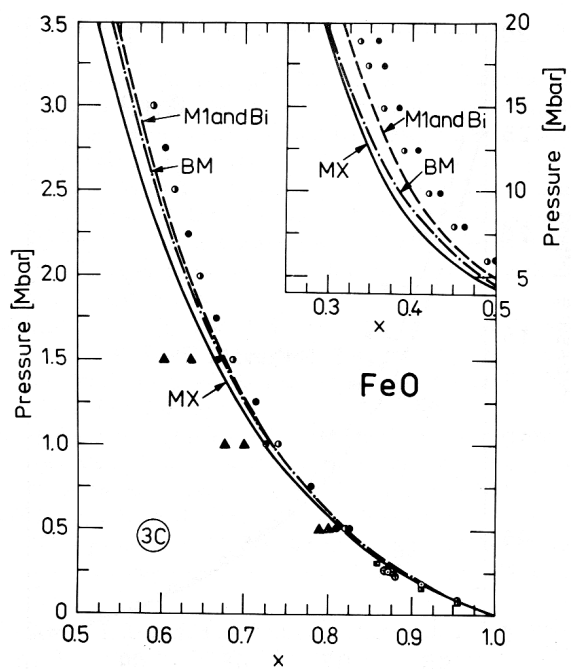
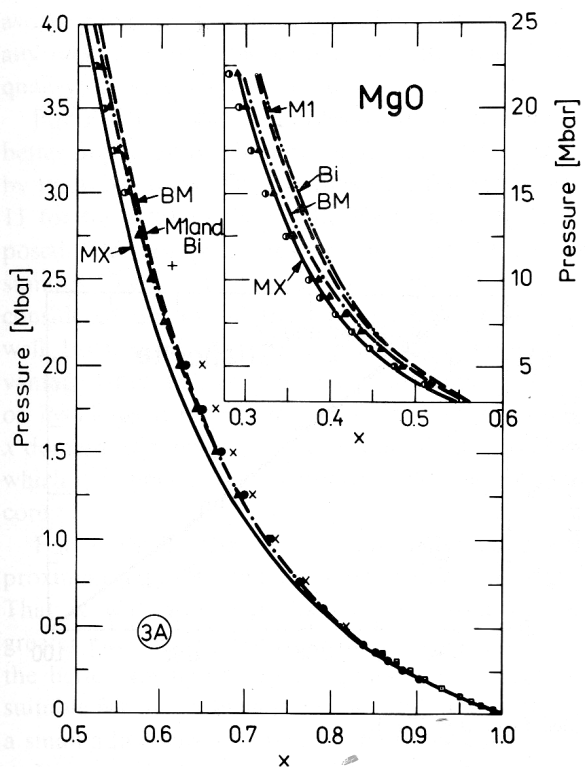


TABLE III
A comparison of experimental and theoretical data ^a

Material	Figure No.	Model			
		MX	BM	M1	Bi
		(eq. 11)	(eq. 19)	(eq. 22)	(eq. 25)
K	1A	2	1	1	1
Ca	1B	1	1	1	2
V	1C	1	1	1	2
Fe(ϵ), $x > 0.65$	1D	1	1	1	1
Fe(ϵ), $x < 0.65$	1D	2	1	1	1
Ni	1E	2	1	1	1
Cu	1F	2	1	1	1
Zn	1G	2	1	1	1
Zn	1H	1	0	0	0
Ge	1I	1	1	1	1
Rb	1J	2	2	1	1
Nb	1K	1	0	0	0
Ag	1L	1	2	2	2
Cd	1M	2	1	1	2
In	1N	1	1	1	2
Sn(w), $\kappa_1 = 6.01$	1O	2	1	1	1
Sn(w), $\kappa_1 = 4.9$	1P	2	1	1	1
I	1Q	1	1	1	1
Au	1R	2	1	1	2
Pb	1S	2	1	1	1
Pb	1T	2	1	1	1
Li	1U	2	1	1	1
Na	1V	1	1	2	1
Mg	1W	1	2	1	1
Al	1X	1	1	1	1
Si, $x > 0.96$	1Y	2	2	2	2
Si, $x < 0.96$	1Y	0	0	0	0
S	1Z	1	2	2	2
NH ₄ Cl	2A	2	1	1	2
NH ₄ Br	2B	2	1	1	1
AgCl	2C	2	1	1	1
AgBr	2D	2	1	1	1
LiF	2E	2	2	2	2
NaCl	2F	2	1	1	1
NaBr	2G	1	2	2	2
NaI	2H	2	1	1	2
CsCl	2I	2	2	2	2
CsBr	2J	2	1	1	1
CsI	2K	2	1	1	1
MgO, $x > 0.75$	3A	2	2	2	2
MgO, $0.55 < x < 0.75$	3A	1	2	2	2
MgO, $x < 0.55$	3A	2	1	1	1
Al ₂ O ₃ , $x > 0.65$	3B	2	2	2	2
Al ₂ O ₃ , $x < 0.65$	3B	2	1	1	1
FeO	3C	1	1	2	1
Fe ₂ O ₃	3D	1	1	1	1
CaO	3E	1	2	2	2
Stishovite	3F	2	2	2	2

^a Numbers indicate that the respective equation of state approximates the measured data: (0) good; (1) better; (2) best



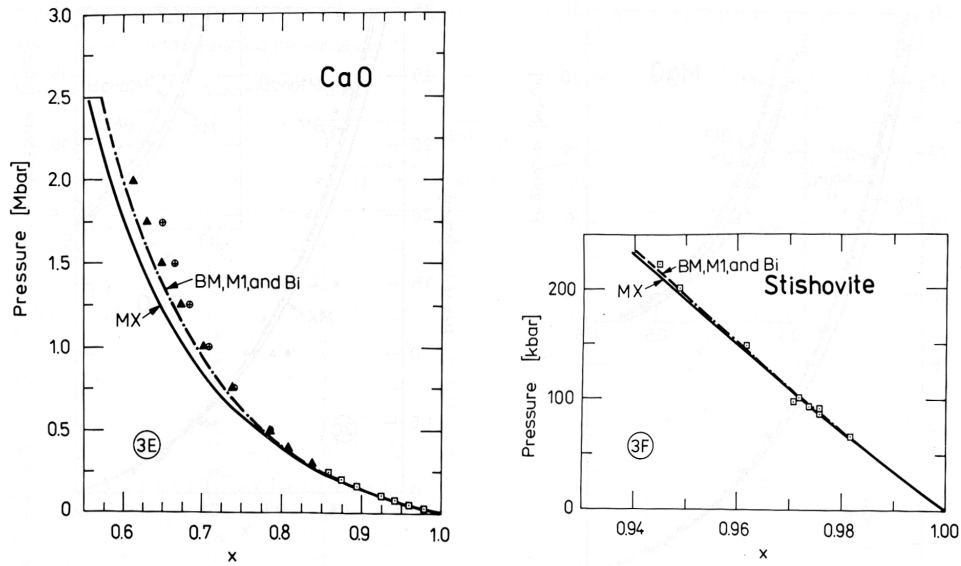


Fig. 3. Pressure versus the zero-pressure density to density ratio for oxides. Data as in Fig. 1.

circles, squares, triangles and other more conspicuous symbols. It goes without saying that it is primarily the agreement of the isothermal measured data with the theoretical curves which is decisive for the quality of the theory. The illustrations are arranged in the same order as in Table I.

6. Geophysical conclusions

The present work has been done mainly for geophysical purposes. Of course, the equations of state have to be verified by comparison with experimental high-pressure data, and this is indeed an essential part of this publication. But for an extrapolation to the very high pressures in planetary interiors, those equations of state appear to have prospects of success which are physically well founded. Therefore, the new equation of state (eq. 11) has been developed through an analysis of the interatomic forces. For an additional comparison, the x - P curves of the Birch-Murnaghan equation

of state (represented in the figures as Bi)

$$P = \frac{3}{2}\kappa_0(x^{-7/3} - x^{-5/3}) \times \left[1 + \frac{3}{4}(4 - \kappa_1)(1 - x^{-2/3})\right] \quad (25)$$

which has a wide geophysical following, has been plotted on graphs. A look at Figs. 1-3 will show which of the equations is best suited for which material. The new equation of state turned out to be not only suited for metals (for which it had been originally developed), but also for halides and some oxides. As regards the latter, it is well suited for periclase (MgO) and corundum (Al₂O₃), a fact which is remarkable inasmuch as these materials probably make up a large proportion of the overall mass of the Earth's mantle. To permit quick assessment of the quality of the four models, an evaluation has been made in Table III as to which model gives the best approximation to the measured data: 0 means good, 1 better, 2 best. Of course, such an evaluation involves a minor subjective component, which is, however, insignificant

as can be shown by an independent repetition. In any case, it is possible to get a rough idea of the quality of the equations of state.

For $x < 0.65$, the compression of h.c.p. iron is better predicted by the new equation of state than by the other ones. This implies that the use of eq. 11 for the whole core of the Earth must be proposed. The computations are not very time-consuming. For $x > 0.65$, the four equations of state considered do not fit the experimental data very well, because of phase changes. This is no disadvantage since in geophysics the equation of state on iron is used mainly for $x < 0.65$. For the whole x domain, the new equation is a good fit to nickel, which is believed to be a minor constituent of the core.

For $x > 0.75$, the four equations of state approximate equally well the compression of MgO. That is why they can likewise be used in the greater part of the mantle. For $x < 0.55$, eq. 11 is the better approximation. Equation 11 would be suitable for an investigation into the possibility of a small admixture of MgO in the outer core.

For $\kappa_1 = 4$, the equation by Birch–Murnaghan and the equation by Ullmann–Pan'kov are identical. A lot of geophysically relevant materials, e.g. Fe and FeO, have values of $\kappa_1 = 4$, or the κ_1 values deviate less than 0.25 from that value (e.g. MgO and Al_2O_3). That is why their x - P curves are equal or nearly equal, respectively.

Figures 1–3 show that, for the high pressures of the Earth's core, the new equation of state is superior to the other equations. For the Earth's mantle, the four equations of state are equally well suited. However, each equation of state considered has its merits; Table III summarizes which model represents the best approximation to the respective material.

Acknowledgement

I wish to thank Dr. W. Ullmann for interest and helpful discussions.

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