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Predicting Characteristics of NdFeB towards 140 GPa

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Abstract

The equation of state and the shear modulus data of sintered $Nd_2Fe_{14}B$ were investigated up to 140 GPa by the Gruneisen's model, the volume superposition principle and the Hugoniot's relations. Then, the results were compared to the prior experiments with a standard deviation of 0.125% from 18 GPa to 78 GP; and then, the loading pressure was extended to higher. Meanwhile, the softening feature has not been observed both in adiabat and shear modulus throughout the interested range.

Keywords

Gruneisen's Model, $Nd_2Fe_{14}B$, Volume Superposition Principle, Hugoniot, Shear Modulus

1. Introduction

Creating a simple, usable and reliable computing model of a complex mixture, such as NdFeB, is quite stubborn theoretically under high pressure and high temperature, but is really significant in aerospace engineering and defense industry [1]. In recent years, some of shock and FEM experimental data of NdFeB had been already published in lower pressure range [2]-[5]; we have reached at the top of pressure, 78 GPa, experimentally so far, and the satisfactory result will allow us confidently to predict the characteristics of NdFeB in a higher pressure region.

For the sake of simplifying our calculation, the anisotropic $Nd_2Fe_{14}B$ was chosen, because of its principle application in modern society with its high magnetic energy product, remanence ratios and coercive force, and we ignored the existence of B in the model.

2. Methods

2.1. Gruneisen's Model

Based on the shock experimental inertia of $Nd_2Fe_{14}B$ within 18 GPa - 78 GPa [3], as a linear mixed substance, it

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is suitable for calculating [6] by

$$p - p_x = \frac{\gamma}{V}\left(E - E_x\right) \tag{1}$$

where P, V, E, γ, P_x and E_x are, respectively, total pressure, volume, energy, Gruneisen's coefficient, cold pressure and energy. Among of them, P_x and E_x can be specifically represented by the Born-Meyer's potential [6],

$$P_X = Q\delta^{2/3} \cdot \left\{\exp\left[q\left(1-\delta^{-1/3}\right) - \delta^{2/3}\right]\right\} \tag{2}$$

$$E_X = \frac{3Q}{\rho_{0K}}\left\{\frac{1}{q}\cdot\exp\left[q\left(1-\delta^{-1/3}\right)\right] - \delta^{1/3} - \left(\frac{1}{q} - 1\right)\right\} \tag{3}$$

where Q, q, ρ_0 and α_v are, respectively, the parameters of cold energy, the initial density and the volume dilatation, $\delta = \rho/\rho_{0k}$ and $\rho_{0k} = \rho_0$ (1 + 300 a_v).

2.2. Volume Superposition Principle

Instead of computing this intermetallic compound, each component, Nd, Fe and B will be allowed to be treated separately, according to their proportion by weight, 26.68%, 72.32% and 0.99% due to the chemical stability of the compound under high pressure and high temperature, as mentioned above. The average formulae are listed below,

$$V(p) = \sum_{i=1}^{n}\alpha_i V_i(p) \tag{4}$$

$$E(p) = \sum_{i=1}^{n}\alpha_i E_i(p) \tag{5}$$

where α_i denotes weight percentage of each component.

2.3. Hugoniot's Relation

The interaction of particles in $Nd_2Fe_{14}B$ will be ignored if the compound is actually treated as an ideal mixture. The compressibility of $Nd_2Fe_{14}B$, therefore, can be evaluated by the Hugoniot of each component itself [6], as follows,

$$p_H = \frac{\eta\rho_0^2 c_0^2}{\left(1-\lambda_0\eta\right)^2} \tag{6}$$

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

where c_0 and λ_0 are, respectively, the wave velocity and the characteristic parameter of $Nd_2Fe_{14}B$. At the initial state, they are,

$$c_0 = \frac{\sum_n m_i c_{0i}}{n} \tag{8}$$

$$\lambda_0 = \frac{\sum_n m_i \lambda_i}{n} \tag{9}$$

where m_i stands for the mass of each independent component in mixture. Sequentially, we take c_0 = 3.686 and λ_0 = 1.059, at the same pressures in literature [6]. Then we can get $Q \approx 55.7$ and $q \approx 6.85$ by the following formulae [6],

$$c_0^2 = \frac{Q\left(q-2\right)}{3\rho_{0k}} \tag{10}$$

$$\lambda_0 = \frac{q^2 + 6q - 18}{12(q-2)} \tag{11}$$

It must be emphasized that c_0 and λ_0 in Equations (8)-(11) should be demarcated to the absolute zero from the room temperature in calculation by the linear mixed rule [3].

$$c_0' = c_0\left[1+\left(2\lambda_0 - \frac{\gamma_0^2}{4} - 1\right)\alpha_v T_0\right] \tag{12}$$

$$\lambda' = \lambda_0\left[1+\left(\frac{\lambda_0}{2} - \frac{\gamma_0^2}{8\lambda_0} - 1\right)\alpha_v T_0\right] \tag{13}$$

where γ_0 is the initial Grunasen's coefficient of $Nd_2Fe_{14}B$, which is taken as 1.492, and ρ_{0k} as 7.451 g/cm^3 [3]. While the boron has to be erased from processing queue due to lack of its Hugoniot and trivial weight, which is also reasonable in common senses.

2.4. Shear Modulus

The effective shear modulus, G, can be deduced from the SCG model [7], based on the quasi-elasticity as unloading along with the shock adiabat [6], as follows,

$$G = \frac{3}{4}\rho_0\left(c_l^2 - c_b^2\right) \tag{14}$$

where c_l and c_b are, respectively, the Euler's longitudinal and bulk wave velocity, and given by,

$$c_b^2 = \frac{\gamma V p_H}{2} - V^2\frac{\mathrm{d}p_H}{\mathrm{d}V}\left[1 - \frac{\gamma\eta V_0}{2V}\right] \tag{15}$$

$$\frac{\mathrm{d}p_H}{\mathrm{d}V} = -\rho_0^2 c_0^2 \frac{1+\lambda\eta}{(1-\lambda\eta)^3} \tag{16}$$

$$c_l = \sqrt{\frac{3-3\nu}{1+\nu}}c_b \tag{17}$$

where ν, the Poisson's ratio, is taken as 0.24, and γ is supposed to depend on volume V only. Then we have,

$$\gamma = \gamma_0\left(\frac{\rho_0}{\rho}\right)^q \tag{18}$$

where ρ is density at final state, and a = 0.822 nm is the lattice constant of $Nd_2Fe_{14}B$.

For convenience reasons in the following calculation and discussion, part of initial parameters of Nd and Fe are listed in **Table 1**.

Compare with prior experiments, the calculated results have been listed in **Table 2**.

3. Results and Discussion

By using Equations (1)-(16), a new D-u relation, D = 3.476 + 1.203 u, of $Nd_2Fe_{14}B$ can be obtained, as shown in **Figure 1** together with a series of experiments and literature data of Nd and Fe. It is apparently, these points are well fitted between species with a deviation of ±0.125% throughout the given pressures range, and the result, the D-u line located between lines of Nd and Fe, and more closed to the latter, is just because of the volume superposition principle. That is, the pressure properties of linear mixtures will strongly depend on their components' volume or weight, if only their inertia being kept during loading process. Therefore, the same distribution can be seen on a corresponding group of adiabats P vs. V of **Figure 2**, which are fitted by polynomial with standard deviation of ±2.30% as loading $Nd_2Fe_{14}B$ up to 140 GPa.

Considering the accordance between calculations and experiments below 78 GPa in **Figure 1** and **Figure 2**,

Table 1. Part of initial parameters of Nd and Fe.

Elements	C_0/km/S	λ_0	γ_0	$\alpha_v/10^{-5}$/K	α_i/%	ρ_0/g/cm^3	C_0'/km/S	λ_0'
Nd	2.2	1.015	0.57	2.994	26.68	7.003	2.219	1.010
Fe	3.955	1.30	1.78	3.51	72.32	7.856	3.989	1.291

Table 2. Comparison of calculations vs. experiments.

*p/GPa	p/GPa	*D/km/s	D/km/s	*u/km/s	u/km/s	*ρ/g/cm^3	ρ/g/cm^3
77.84	78	5.695	5.64	1.861	1.80	11.034	10.944
50.99	53.32	5.040	5.18	1.377	1.40	10.222	10.211
41.10	39.58	4.929	4.68	1.135	1.00	9.653	9.476
27.75	26.4	4.609	4.44	0.820	0.80	9.036	9.089
19.23	18.23	4.302	4.20	0.608	0.60	8.653	8.693

*Cited from literature [3].

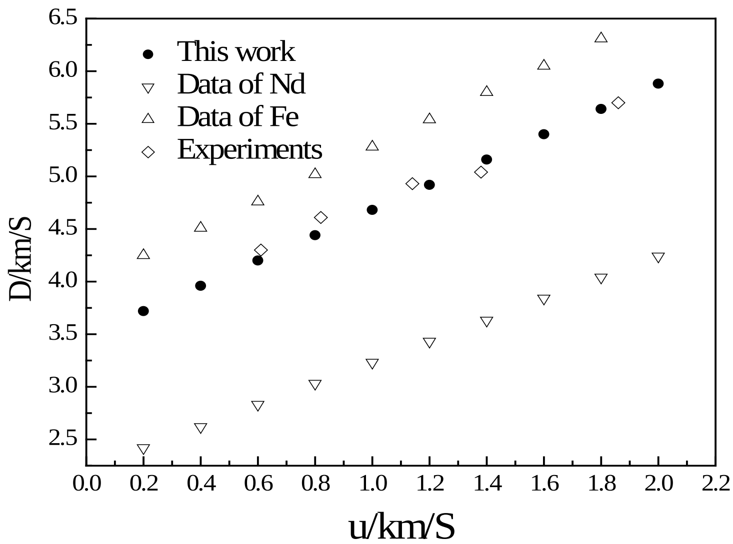

Figure 1. Theoretical D-u vs. experimental one of $Nd_2Fe_{14}B$.

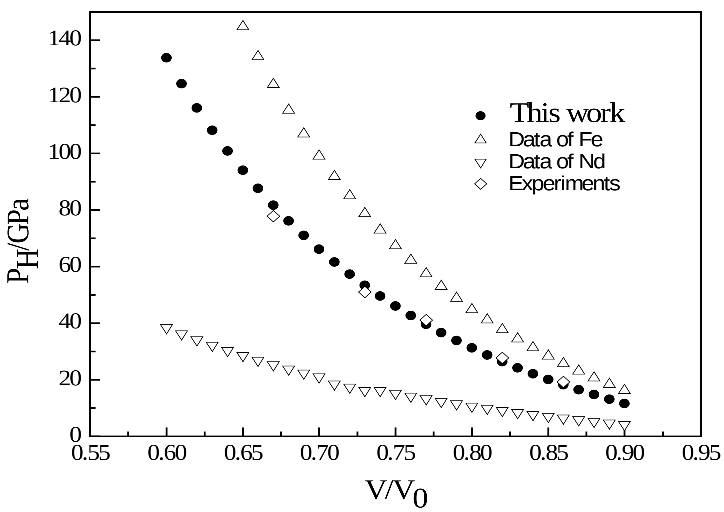

Figure 2. Theoretical adiabat vs. experimental one of $Nd_2Fe_{14}B$.

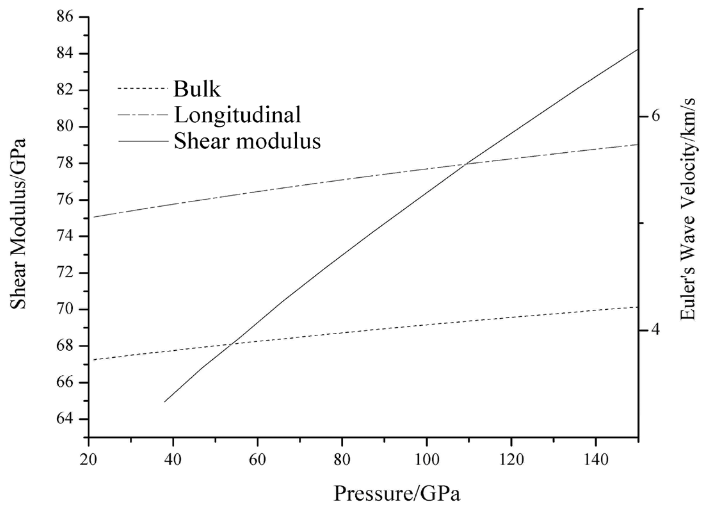

Figure 3. Euler's bulk and longitudinal wave velocity and the Shear modulus vs. axial stress of $Nd_2Fe_{14}B$.

the segments are also reasonable from 78 GPa to 140 GPa based on the prior assumption of the stability chemically as loading pressure on $Nd_2Fe_{14}B$.

On the basis of above discussion, the longitudinal, bulk wave velocities and the shear modulus of $Nd_2Fe_{14}B$ can be estimated by Equations (14)-(18) as shown together in **Figure 3**. A pair of quasi-parallel curves and a monotonous line very distinctly proved that the organization inside $Nd_2Fe_{14}B$ were unchanged with such rising pressure, which meant no shock softening meanwhile, or no melting occurred from the lowest to the highest pressure region once again.

4. Conclusions

A simple and effective algorithm for evaluating $Nd_2Fe_{14}B$ has been developed via comparing experiments below 78 GPa and predicted towards 140 GPa together with the shear modulus, even no corresponded experimental data accompanied. We believe the deviation in calculation can be further reduced by carefully adjusting parameters in the equations listed above; and the processing method can be consequentially extended to other inert mixtures under high pressure and high temperature. But two rules should be followed:

1) Each component of solid mixture should be inert during shock compression, and

2) Each initial parameter of components should be known in advance.

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