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Neutron spectroscopy of magnesium dihydride

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ABSTRACT

Inelastic neutron scattering spectra of α-MgH_2 powder have been measured at $T = 7$ K with an energy resolution better than 1.5% using the time-of-flight direct geometry spectrometer SEQUOIA. Based on these spectra, the density $g(E)$ of phonon states in α-MgH_2 has been experimentally constructed for the first time. Comparing the available experimental data on the heat capacity of α-MgH_2 with those calculated using the obtained $g(E)$ confirmed the good accuracy of its determination.

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1. Introduction

Due to the very large neutron scattering cross-section of H atoms, inelastic neutron scattering (INS) is one of the most direct and powerful means of studying the lattice dynamics of metal hydrides. Under rather realistic simplifying assumptions, the one-phonon scattering contribution can be derived from the INS spectrum of a powder sample and further converted to the phonon density of states, $g(E)$, where E is the phonon energy. The "experimental" $g(E)$ spectra thus obtained can directly be compared with results of computer calculations and are traditionally used to establish the main features of vibrational spectra of the studied hydrides, such as the peaks positions, cut-offs of the vibrational bands, etc.

The $g(E)$ spectrum can also be used to calculate the contribution from lattice vibrations to the heat capacity $C_V(T)$ at constant volume. For dielectric hydrides like those of Mg and Al and many other metals, this spectrum therefore fully determines the heat capacity and, consequently, every standard thermodynamical potential. The $g(E)$ spectrum derived from INS measurements at low temperatures allows, in principle, calculating the $C_V(T)$ dependence up to very high temperatures, much exceeding the temperature of thermal decomposition of the hydride at ambient pressure. This is a definite advantage of applying the INS technique to hydrides because the high-energy modes of H vibrations in hydrides make the standard Debye model inapplicable for the quantitative description and any extrapolations of their $C_V(T)$ dependences. Meanwhile, the thermodynamical properties of hydrides above the decomposition temperature are usually most interesting for applications, e.g., for the hydrogen storage.

Constructing the $C_V(T)$ dependence based on $g(E)$ requires accurate and detailed INS data, and such a dependence was only recently obtained for α-AlH_3 in our work [1] using the INS results of Ref. [2]. The heat capacity of α-AlH_3 was calculated at temperatures 30–1000 K with an accuracy of no worse than few per cent [1] and further used to construct the line of the $Al + (3/2)H_2 = AlH_3$ equilibrium at temperatures up to 900 K and hydrogen pressures up to 9 GPa [3] (a brief description of these results can also be found in the review paper [4] in this issue).

It should be noted, however, that the good accuracy of the $C_V(T)$ determination for α-AlH_3 was partly achieved thanks to the specific shape of its $g(E)$ spectrum divided into three well-separated vibrational bands. To estimate the accuracy of the $C_V(T)$ determination that neutron spectroscopy can provide in the general case of a dielectric hydride with broad bands of lattice and optical vibrations, we have chosen α-MgH_2 for the present investigation. A unique feature of α-MgH_2, which decomposes to Mg and H_2 at ~550 K under ambient pressure, is that its heat capacity has earlier been determined up to a temperature as high as 2000 K [5] using the analogy with a more thermally stable and thoroughly studied MgF_2 compound. A comparison with results of Ref. [5] gave a rare opportunity to check the accuracy of calculation of the heat capacity of α-MgH_2 using the INS data.

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α-MgH_2 with a tetragonal rutile-type structure, space group $P4_2/mnm$, is the most stable modification of magnesium dihydride under ambient conditions [6]. Lattice dynamics of powder samples of α-MgH_2 were earlier studied by INS with the beryllium filter spectrometer IN1-BeF at ILL, France [7] and inverse-geometry spectrometer TOSCA at ISIS, UK [8,9]. These studies revealed the basic features of the α-MgH_2 phonon spectrum, and the origin of these features was well established by *ab initio* calculations supplemented the experiment in Ref. [8]. However, the experimental results of works [7–9] were insufficient to construct $g(E)$ suitable for calculating the heat capacity. The main obstacle was that at energy transfers exceeding 100 meV, the one-phonon scattering intensity could not be reliably isolated from the intense multi-phonon contribution caused by the large neutron momentum transfers Q. Large neutron momentum transfers at high energy transfers are intrinsic to spectrometers with small energy of the registered neutrons, like IN1-BeF and TOSCA.

In the present work, we studied α-MgH_2 powder using a direct-geometry neutron spectrometer SEQUOIA at ORNL, USA. The obtained INS spectra had much smaller contributions from the multiphonon neutron scattering due to the ability of the spectrometer to provide small momentum transfers at large energy transfers. This allowed us to get a more accurate one-phonon INS spectrum than previously and to construct the experimental phonon density of states for α-MgH_2 for the first time. With this $g(E)$, we calculated the dependence $C_V(T)$ of heat capacity of α-MgH_2 at constant volume and further estimated the corrections converting the $C_V(T)$ to $C_P(T)$ at constant pressure at temperatures up to 2000 K by using the literature data on the compressibility of α-MgH_2 [6,10] and the coefficient of thermal expansion determined from our own X-ray diffraction measurements at 11–300 K.

2. Experimental details

Powder of magnesium dihydride was purchased from Sigma–Aldrich. An X-ray examination showed the powder to consist of 98% α-MgH_2 and 2% Mg metal. A one gram sample of this powder was measured at 7 K using the newly constructed fine energy resolution spectrometer SEQUOIA at the Spallation Neutron Source (Oak Ridge National Laboratory) [11]. SEQUOIA is a direct geometry time-of-flight spectrometer with variable energies of incident neutrons, from 10 to 2000 meV. To get the best energy resolution of $\Delta E/E_i = 1$–1.5% at every studied energy transfer, we measured the INS spectra with 5 different incident energies of $E_i = 45$, 115, 220, 350 and 750 meV selected by the Fermi chopper that was rotating at 420 Hz for $E_i = 45$ meV and 600 Hz for other energies. The data were recorded over a wide range of scattering angles, from −30° to +60° in horizontal plane and ±18° in vertical directions. Prior to further treatment, the collected neutron scattering data were transformed from the time-of-flight and instrument coordinates to the dynamical structure factor $S(Q,E)$. The background spectra for the empty container were measured under the same conditions and subtracted from the original data.

To determine the coefficient of thermal expansion of α-MgH_2, X-ray diffraction patterns of the α-MgH_2 powder were collected at temperatures from 11 to 300 K using monochromated synchrotron radiation with a wavelength of λ = 0.10798 Å at beam line 11-ID-C at the Advanced Photon Source, ANL. The patterns were recorded on a Perkin-Elmer 2D detector. Rietveld refinements were performed with the GSAS and EXPGUI [12].

3. Results and discussion

3.1. Inelastic neutron scattering

Fig. 1 shows the $S(Q,E)$ spectrum of α-MgH_2 merged from the spectra measured with the five different energies of the incoming neutrons. The spectrum mostly agrees with results of Refs. [8,9]. According to the *ab initio* calculations in Ref. [8], the phonon density of states of α-MgH_2 is composed of the ranges of lattice modes at $E < 40$ meV and optical vibrations at $40 < E < 190$ meV. The contributions from the Mg atoms to the INS spectrum are small for all vibrations, because the neutron scattering cross-section of H is about 20 times larger than that of Mg [13]. Furthermore, in the case of optical vibrations, the scattering intensity is inversely proportional to the mass of the atom, which is 24 times smaller for H than for Mg. The INS spectrum in Fig. 1 thus well represents vibrations of the H atoms in α-MgH_2.

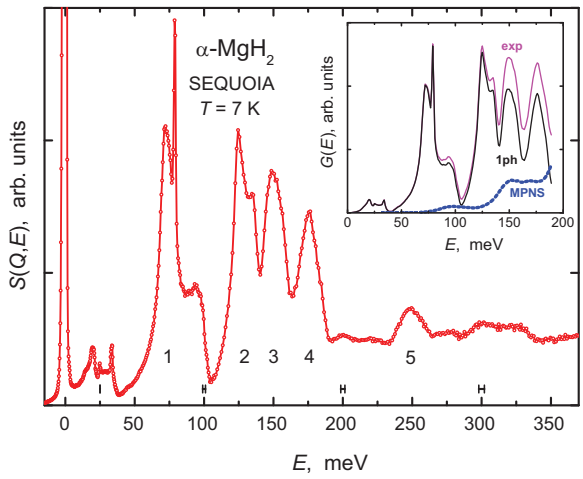

Fig. 1. The dynamical structure factor $S(Q,E)$ of the α-MgH_2 powder sample (open circles) as a function of the energy loss ($E > 0$) or gain ($E < 0$) of the inelastically scattered neutrons measured at 7 K with the SEQUOIA spectrometer at ORNL, USA. The strong peak at $E = 0$ is due to the elastic neutron scattering. The horizontal bars at the bottom of the figure indicate the energy resolution. In the inset, the thick solid line labelled "exp" shows the generalized phonon density of states, $G(E)$, derived from $S(Q,E)$ with subtracted elastic peak; the dashed line "MPNS" represents the multiphonon contribution to $G(E)$ calculated in an isotropic harmonic approximation, and the thin solid line "1ph" is the one-phonon $G(E)^{1ph}$ spectrum of α-MgH_2 obtained from $G(E)$ by subtracting the MPNS contribution.

As seen from Fig. 1, the spectrum of optical H vibrations consists of a band between 40 and 105 meV (two pronounced peaks at 72 and 79 meV, and a shoulder at ≈94 meV) and another band between 105 and 190 meV (a peak at 125 meV with a shoulder at 134 meV, and two peaks at 150 meV and 176 meV). According to the calculations in Ref. [8], the scattering intensity at higher energy transfers, including the peak at 250 meV, could only have resulted from multiphonon neutron scattering. To prove this, we analyzed the momentum transfer dependences of the integral intensities of peaks numbered 1–5 in Fig. 1. These dependences are shown in Fig. 2 and fitted with curves

$$I(Q) = (a \cdot Q^2 + b \cdot Q^4)\exp(-u_H^2 Q^2) \quad (1)$$

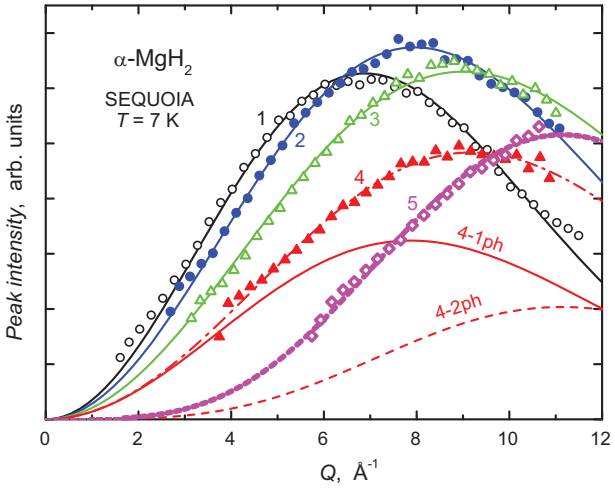

Fig. 2. The integral intensities of peaks 1–5 in Fig. 1 plotted as a function of neutron momentum transfer. The experimental data (symbols) are fitted using Eq. (1). The solid and dashed lines represent, respectively, the one-phonon and two-phonon scattering contributions to the fits (see text).

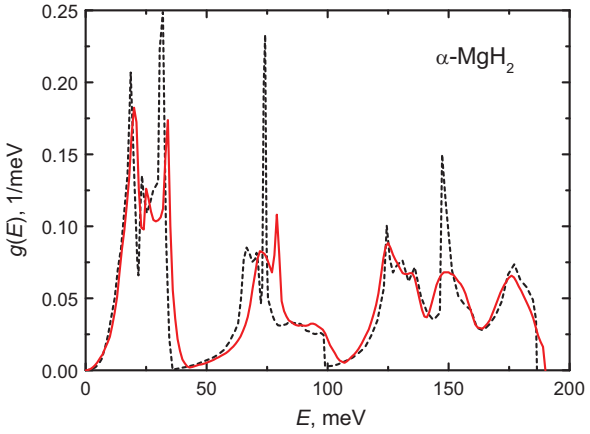

Fig. 3. The densities $g(E)$ of phonon states of α-MgH_2 obtained from the INS data of the present paper (solid curve) and calculated in Ref. [8] (dashed curve).

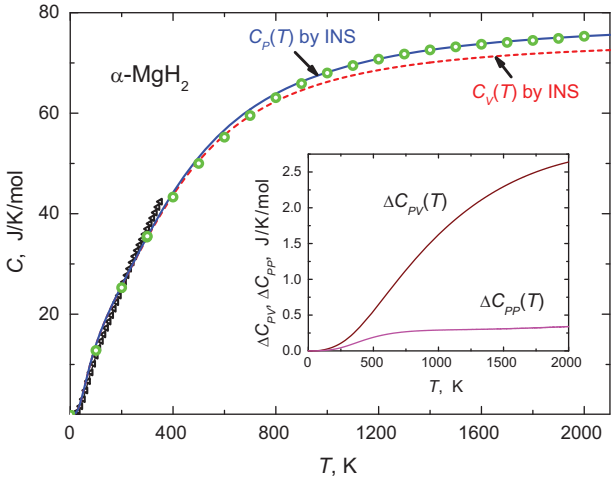

Fig. 4. The heat capacity of α-MgH_2 as a function of temperature. The open left-triangles depict the experimental $C_P(T)$ dependence measured at temperatures from 15 to 360 K in Ref. [15]. The open circles show results of Ref. [5], in which the $C_P(T)$ values at $T \leq 300$ K were taken from the unpublished experimental work [18], and those at higher temperatures were estimated by comparison with the experimental $C_P(T)$ data for MgF_2. The dashed curve represents the $C_V(T)$ dependence for α-MgH_2 calculated by using Eq. (3) and the $g(E)$ spectrum constructed in this work. The solid curve shows $C_P(T) = C_V(T) + \Delta C_{PV}(T) + \Delta C_{PP}(T)$, where $\Delta C_{PV}(T)$ is the adjustment for the difference between $C_P(T)$ and $C_V(T)$ at constant volume and $\Delta C_{PP}(T)$ takes into account changes in $C_P(T)$ due to the volume expansion (see text).

where a, b and u_H^2 are the fitting parameters. The $a{\cdot}Q^2$ and $b{\cdot}Q^4$ factors characterize, respectively, the one- and two-phonon scattering contributions with the same value u_H^2 of the mean squared displacement of hydrogen atoms. As seen from Fig. 2, peaks 1, 2 and 3 can approximately be described by one-phonon neutron scattering alone. Peak 4 originates from both one- and two-phonon scattering. These contributions to its calculated total intensity (thick dash-dotted curve) are shown by the thin solid and dashed curves labelled "4-1ph" and "4-2ph", respectively. Peak 5 can be fully attributed to the two-phonon scattering, all in accord with [8].

Having omitted the elastic peak centred at $E = 0$ from the experimental $S(Q,E)$ spectrum shown in Fig. 1, and approximating the low energy acoustical part of phonon spectrum ($E < 5$ meV) by the Debye dependence $g(E) \sim E^2$, and assuming that the one-phonon part of the resulting spectrum of inelastic neutron scattering is located in the energy range 0–190 meV, we calculated the contribution from multiphonon neutron scattering (MPNS) in an isotropic and harmonic approximation using an iterative technique [14]. These inelastic $S(Q,E)$ spectrum and calculated MPNS spectrum were transformed to the nearly spectrometer-independent, generalized vibrational densities of states according to:

$$G(E) = \frac{S(Q,E)E \cdot \exp(u_H^2 Q^2)}{Q^2[n(E,T)+1]} \quad (2)$$

where $n(E, T) = [\exp(E/k_BT) - 1]^{-1}$ was the population Bose factor and $T = 7$ K was the temperature of the INS measurement. The value of $u_H^2 = 0.019$ Å^2 was taken from fitting the Q-dependences of the integral intensities of peaks 1–3 using Eq. (1). Subtracting the multi-phonon $G(E)$ spectrum from the experimental one gave a one-phonon $G(E)^{1ph}$ spectrum. All three $G(E)$ spectra are shown in the inset of Fig. 1.

The $G(E)^{1ph}$ spectrum thus obtained was further transformed to the phonon density of states, $g(E)$, by renormalization of the integrated area under the $G(E)^{1ph}$ curve to 3 and 6 degrees of freedom for the lattice ($E = 0$–40 meV) and optical ($E = 40$–190 meV) modes, respectively. As seen from Fig. 3, the $g(E)$ spectrum of α-MgH_2 constructed in this way agrees with the *ab initio* calculations of Ref. [8].

3.2. Heat capacity

The heat capacity of α-MgH_2 at constant volume was calculated as:

$$C_V(V_0,T) = R\int \left(\frac{E}{k_BT}\right)^2 g(E)n(E,T)[n(E,T)+1]\,dE \quad (3)$$

where $V_0 = V(7\,K) \approx V(0\,K)$ is the molar volume of α-MgH_2 at a temperature of 7 K of the INS measurement; $R = 8.314$ J mol^{-1} K^{-1} is the universal gas constant and $k_B = 1.381 \times 10^{-23}$ J K^{-1} is the Boltzmann constant. With the $g(E)$ spectrum normalized to 9 states in total, this equation gives $C_V(T) \xrightarrow{T\to\infty} 9R = 3R \times 3$ per gram-mole of α-MgH_2 in accordance with the Dulong and Petit law. The calculated $C_V(V_0,T)$ dependence is shown in Fig. 4 (dashed curve) together with the experimental $C_P(T)$ data available in the literature [5,15] (open symbols).

The calculated $C_V(V_0,T)$ dependence was further converted to the $C_P(V_0,T)$ dependence at constant pressure using the equation [16]:

$$\Delta C_{PV}(T) = C_P - C_V = \frac{\alpha^2 TV}{\beta} \quad (4)$$

where $V(T)$ is the molar volume of α-MgH_2; $\alpha = (1/V)(\partial V/\partial T)_P$ is the coefficient of volume expansion and $\beta = -(1/V)(\partial V/\partial P)_T$ is the isothermal compressibility. The $C_P(V_0,T)$ dependence calculated using Eq. (4) was also corrected for the effect of thermal expansion, $\Delta C_{PP}(T)$.

The $C_P(V,T)$ dependence thus produced is shown in Fig. 4 by the solid line. In a wide temperature interval from 100 to 2000 K, it well agrees with the $C_P(T)$ dependence from Ref. [5] shown by open circles and obtained by rescaling the experimental results for MgF_2. In contrast, the $C_P(T)$ dependence measured in Ref. [15] noticeably departures both from ours and from that constructed in Ref. [5]. As one can see from Fig. 4, its deviation from our dependence exceeds −15% at 100 K and +5% at 360 K and should further increase if smoothly extrapolated to higher temperatures. Most likely, this is a result of a certain systematic error in the measurements of Ref. [15].

Below one can see details of the C_V to C_P conversion carried out in our work. The procedure was very similar to that used in Ref. [1].

Eq. (4) requires knowledge of the $V(T)$ or $\alpha(T)$ dependence for α-MgH_2. We could not find such dependences in the literature and derived these from an X-ray diffraction investigation of α-MgH_2 powder at temperatures 11–300 K. The obtained $V(T)$ dependence is shown in Fig. 5 by open circles (to save space, we did not show the

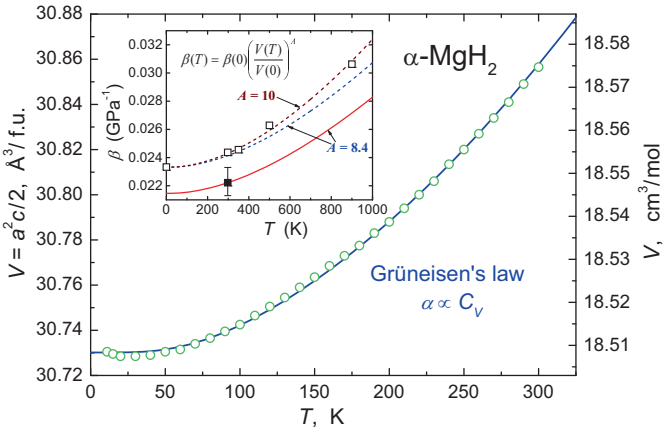

Fig. 5. The experimental temperature dependence of the volume of α-MgH_2 (open circles) fitted using Eq. (5) (solid curve). The inset shows the experimental (solid square) [6] and calculated (open squares) [10] values of compressibility of α-MgH_2 and results of fitting and extrapolating these data using power functions (dashed and solid curves).

temperature dependences of parameters of the tetragonal unit cell α-MgH_2, which varied from $a = 4.51292(4)$ Å and $c = 3.01775(5)$ Å at 11 K to $a = 4.51907(4)$ Å and $c = 3.02188(5)$ Å at 300 K, the ratio of $c/a \approx 0.6687$ remaining virtually unchanged). To extrapolate $V(T)$ outside the experimental temperature interval 11–300 K, we made use of the semi-empirical Grüneisen law saying that the coefficient of thermal expansion is approximately proportional to the heat capacity,

$$\alpha(T) = BCV(T)$$

(see, e.g., [16] for discussion). Correspondingly, we fitted the experimental dependence with an equation

$$V(T) = V(0)\exp\left[B\int_0^T C_V(\tau)\mathrm{d}\tau\right] \quad (5)$$

by varying the B parameter. The resulting fit is shown in Fig. 5 by the solid curve. The optimum $B = 7.40 \times 10^{-7}$ mol/J gave us both $V(T)$ and $\alpha(T)$ dependences.

To get the $\beta(T)$ dependence, which was also necessary for Eq. (4), we exploited one other Grüneisen's semi-empirical relation to say that $(1/\beta)(\partial\beta/\partial T)_P \approx 8.4\alpha$ (see [17] for discussion and references). As seen from the inset to Fig. 5, the resulting equation

$$\beta(T) = \beta(0)\left[\frac{V(T)}{V(0)}\right]^{8.4} \quad (6)$$

satisfactorily described the theoretical $\beta(T)$ dependence for α-MgH_2 [10] shown by open squares (it could be noticed though that the function with a superscript equal to 10 would fit it better). The required $\beta(T)$ dependence (solid curve in the inset to Fig. 5) was obtained by drawing dependence (6) through the experimental point at room temperature [6] shown by the solid square.

The $\Delta C_{PV}(T)$ dependence calculated using Eq. (4) is shown in the inset to Fig. 4. It should however be taken into account that the $C_V(T)$ dependence calculated via Eq. (3) in the present work refers to the molar volume V_0 of α-MgH_2 at $T = 7$ K because the phonon density of states was determined at this temperature. The dependence $C_P(V_0,T) = C_V(V_0,T) + \Delta C_{PV}(T)$ should therefore be corrected for the thermal expansion of the α-MgH_2 compound. As shown in Ref. [1], this correction can be written in the form:

$$\Delta C_{PP}(T) \approx \frac{T(1 - V_0/V)}{\beta}\left(\frac{\partial^2 V}{\partial T^2}\right)_P \quad (7)$$

The $\Delta C_{PP}(T)$ dependence calculated using this equation and the already available $V(T)$ and $\beta(T)$ dependences is presented in the inset to Fig. 4. As one can see, $\Delta C_{PP}(T)$ is much smaller than $\Delta C_{PV}(T)$, but taken together these two corrections give the $C_P(V,T)$ dependence that neatly fits the experimental results at high temperatures.

4. Conclusion

Based on the inelastic neutron scattering spectra measured at 7 K with an energy resolution better than 1.5%, the density $g(E)$ of phonon states in α-MgH_2 has been experimentally constructed for the first time. The $g(E)$ spectrum thus obtained was further used to calculate the temperature dependence of the heat capacity of α-MgH_2 and to compare it with the dependence accurately determined earlier [5] at temperatures from 300 to 2000 K. The difference between the two dependences proved to be less than 2.5% throughout this temperature interval. The investigation of α-MgH_2 thus demonstrated that studies on powder samples of dielectric hydrides using the existing neutron spectrometers can give the phonon densities of states accurate enough for calculating the heat capacity (and therefore every standard thermodynamical potential) in a wide temperature interval including temperatures much exceeding the upper limit of thermal stability of the hydride at ambient pressure.

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