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Anharmonic properties of MgB_2

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ABSTRACT

The higher order elastic constants have been calculated for hexagonal structured material MgB_2 at 300K using Lennard-Jones interaction potential. The orientation dependent three types of acoustic wave velocities and Debye average velocities have been also evaluated using second order elastic constants and related parameters. The behaviour of the orientation dependent acoustic wave velocities of this material has been discussed.

KEYWORDS

Elastic constants;
Gruneisen numbers;
Non-linearity parameters;
Acoustic velocities.

INTRODUCTION

The discovery of superconductivity with a transition temperature of 39K in the intermetallic compound MgB_2 had a strong impact in the superconductor field. Since its discovery, many attempts to search for new superconducting diborides have been performed. MgB_2 has a simple AlB_2-type structure with hexagonal Mg and graphite type B[1,2].

Recently experimental and theoretical results have shown that strong electron-phonon interaction is the relevant mechanism for superconductivity in this compound, and also that MgB_2 is a multiple-gap superconductor. The band structure is dominated by chemical bonding in the hexagonal B sheets in MgB_2. Although the nominal electron count is the same as in graphite (Mg has nominal 2^+ charge), the top of the B derived σ bonding band structure contains holes. The negative charge of the B-layers and the corresponding positive charge of the Mg-layers play a role in raising the in-plane σ orbitals relative to E_F as compared to graphite[3,4].

Therefore in the present paper, we have calculated the three types of acoustic wave velocities for MgB_2 for each direction of propagation of wave using the second order elastic constants that are important for surface and structural study of this material. The six-second order elastic constants (SOEC) and ten-third order elastic constants (TOEC) are calculated using Lenard-Jones Potential that is a many body interaction potential. The results obtained are interesting for the characterization of this material.

Theory

Theory of elastic constants

The second and third order elastic constant of hexagonal structured crystal are given by the following expressions[5,6]:

$$
\begin{array}{ll}
C_{11}=24.1p^4C' & C_{12}=5.918p^4C' \\
C_{13}=1.925p^6C' & C_{33}=3.464p^8C' \\
C_{44}=2.309p^4C' & C_{66}=9.851p^4C' \\
C_{111}=126.9p^4B+8.853p^4C' & C_{112}=19.168p^2B-1.61p^4C' \\
C_{113}=1.924p^4B+1.155p^6C' & C_{123}=1.617p^4B-1.155p^6C' \\
C_{133}=3.695p^6B & C_{155}=1.539p^4B \\
C_{144}=2.309p^4B & C_{344}=3.464p^6B \\
C_{222}=101.039p^2B+9.007p^4C' & C_{333}=5.196p^8B
\end{array}
\qquad (1)
$$

where $p=c/a$: axial ratio; $C'=\chi a/p^5$; $B=\Psi a^3/p^3$ and $\Psi=-\chi/\{6a^2(m+n+6)\}$. Here χ is a parameter, which is calculated using experimental value of any one second order elastic constant (SOEC).

Ultrasonic velocity in hexagonal structured crystal

There are three types of ultrasonic velocities in hcp crystals as one longitudinal and two shear wave velocities, which are given by following expression[5,6].

$$
V_1^2=\{C_{33}\mathrm{Cos}^2\theta+C_{11}\mathrm{Sin}^2\theta+C_{44}+\{[C_{11}\mathrm{Sin}^2\theta-C_{33}\mathrm{Cos}^2\theta+C_{44}(\mathrm{Cos}^2\theta-\mathrm{Sin}^2\theta)]^2+4\,\mathrm{Cos}^2\theta\,\mathrm{Sin}^2\theta\,(C_{13}+C_{44})^2\}^{1/2}\}/2\rho \qquad (2)
$$

$$
V_2^2=\{C_{33}\mathrm{Cos}^2\theta+C_{11}\mathrm{Sin}^2\theta+C_{44}-\{[C_{11}\mathrm{Sin}^2\theta-C_{33}\mathrm{Cos}^2\theta+C_{44}(\mathrm{Cos}^2\theta-\mathrm{Sin}^2\theta)]^2+4\,\mathrm{Cos}^2\theta\,\mathrm{Sin}^2\theta\,(C_{13}+C_{44})^2\}^{1/2}\}/2\rho \qquad (3)
$$

$$
V_3^2=\{C_{44}\mathrm{Cos}^2\theta+C_{66}\mathrm{Sin}^2\theta\}/\rho \qquad (4)
$$

where V_1, V_2 and V_3 are the longitudinal, quasi-shear and shear wave velocities. The ρ and θ are the density of the material and angle with the unique axis of the crystal respectively.

V_D is the Debye average velocity and is calculated from the initial slopes of the three acoustical branches[7].

$$
V_D=\left(\frac{1}{3}\sum_{i=1}^{3}\int\frac{1}{V_i^3}\frac{d\Omega}{4\pi}\right)^{-1/3} \qquad (5)
$$

RESULTS

The unit cell parameters a and p for MgB_2 are 3.073Å and 1.1476 respectively. The harmonic parameter χ and anharmonic parameter Ψ are calculated using one SOEC (C_{33}). The SOEC and TOEC are calculated for MgB_2 using Eqn (1) and are presented in TABLE 1. The value of specific heat per unit volume (C_V) and thermal energy density (E_0) are evaluated using physical constant TABLE and Debye temperature. The values of ρ, C_V and E_0 are presented in TABLE 2.

The three ultrasonic velocities V_1, V_2 and V_3 are calculated using the second order elastic constant values with the Eqns. (2-4) at different temperatures and at different angles with the unique axis (z-axis) of the crystal. The velocities (V_1, V_2, V_3) and Debye average velocity (V_D) at temperature 300K and at different angles with unique axis of crystal are shown in figure 1.

The Gruneisen numbers are calculated with the expressions given by S. Rajgopalan[8] at $\theta=0^0$ in temperature 300K. The Grüneisen numbers and acoustic coupling constants are presented in TABLE 3.

DISCUSSION AND CONCLUSIONS

One of the unique properties of MgB_2, the elastic constants are important since they are related to hardness and therefore of interest in applications where mechanical strength and durability are important. Also, the second and third order elastic constants are used for the determination of the ultrasonic properties.

We have calculated the higher order elastic constants using the potential method following the Keating's approach. Keating's approach essentially the same as the coupling parameter approach, but it has the advantage that the potential energy expansion is automati-

TABLE 1: Second and third order elastic constants in 10^{12} Nm^{-2} of MgB_2 at 300K

T[K]	C_{11}	C_{12}	C_{13}	C_{33}	C_{44}	C_{66}	Ref.
300	3.62	0.89	0.76	2.03	0.46	1.36	Present work
300	3.65	0.98	0.65	2.03	0.25	1.33	[9]

T[K]	C_{111}	C_{112}	C_{113}	C_{123}	C_{133}	C_{144}	C_{155}	C_{222}	C_{333}	C_{344}
300	-27.25	-4.56	-0.34	-0.71	-1.44	-0.69	-0.46	-21.41	-2.67	-1.35

TABLE 2: Density ($10^3 Kgm^{-3}$), specific heat per unit volume C_V ($10^6 Jm^{-3}K^{-1}$), energy density E_0 ($10^8 Jm^{-3}$) of MgB_2 at 300K

Parameters↓	300K
ρ	5.61
C_V	26.57
E_0	46.04

TABLE 3: Average Gruneisen number $<\gamma_i^j>_L$, square of average Gruneisen number $<\gamma_i^j>^2_L$ for longitudinal wave, average square Gruneisen number $<(\gamma_i^j)^2>_L$ and $<(\gamma_i^j)^2>_S$ for longitudinal and shear wave and non-linearity parameters D_L, D_S for longitudinal and shear wave along Z-axis for MgB_2 at 300K

Parameters	300K
$<\gamma_i^j>_L$	0.0494
$<\gamma_i^j>^2_L$	0.0846
$<(\gamma_i^j)^2>_L$	0.0024
$<(\gamma_i^j)^2>_S$	0.0193
D_L	0.7488
D_S	0.1735

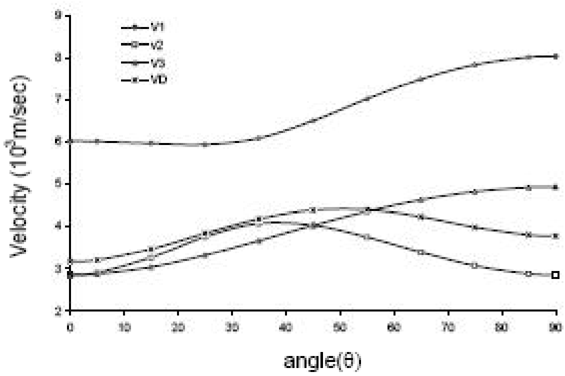

Figure 1: Velocity vs angle for MgB_2 at 300K

cally invariant towards a rigid rotation or translation of the lattice. In the coupling parameter approach these conditions have to be applied separately. A perusal of TABLE 1 indicates that the present values of second order elastic constants (SOEC) at the temperature 300K are in good agreement with the other[9].

However, the third order elastic constants (TOEC) at temperature 300K could not be compared due to lack of reported values in the literature. Thus our method of calculation for temperature dependent SOEC/ TOEC is well justified.

A perusal of figure 1 shows that the orientation dependent velocity(V_1, V_2 and V_3) at certain temperature is mainly affected by combined effect of second order elastic constants and the ultrasonic velocity in MgB_2.

Our results (SOEC and TOEC) should also be useful for estimating relative thermal residual stress variations under different growth conditions of the material. The Debye average velocity (V_D) have characteristic maximum at 55^0 from the z-axis. In the same way the velocity V_2 has characteristic minimum at 35^0 from the z-axis while V_1 and V_3 increases as the angle increases with the unique axis. The behaviour related to the orientation dependency of the velocities is direct consequence of the elastic constants of the material. All the values of SOEC and TOEC can be utilized for the determination of the ultrasonic properties. Thus the work is very useful for the material characterization after production and during the processing well.

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