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# Lattice Dynamical Properties of Magnesium Germanide (Mg2Ge)

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**Abstract**: Solid-state physics, the largest branch of condensed matter physics, is the study of rigid matter, or solids, through methods such as quantum mechanics, crystallography, electromagnetism and metallurgy. Solid-state physics considers how the large-scale properties of solid materials result from their atomic-scale properties. Solid-state physics thus forms the theoretical basis of materials science, as well as having direct applications, for example in the technology of transistors and semiconductors. Semiconducting magnesium silicide (Mg2Si) and magnesium germanide (Mg2Ge) have an antifluorite structure (space group Fm3m) and have been proposed to be good candidates for high-performance thermoelectric materials, because of their superior features such as its large Seebeck coefficient, low electrical resistivity, and low thermal conductivity To study the properties of such materials of interest various theoretical; methods can be used. To study lattice dynamical properties de Launey angular force constant method can be considered as one of the best fitted method so in this study lattice dynamical properties of Mg2Ge has been studied using de Launey angular force constant model.

## I. INTRODUCTION

Semiconducting magnesium silicide ($Mg_2Si$) and magnesium germanide ($Mg_2Ge$) have an antifluorite structure (space group Fm3m) and have been proposed to be good candidates for high-performance thermoelectric materials, because of their superior features such as its large Seebeck coefficient, low electrical resistivity, and low thermal conductivity [1-6]. A wide variety of physical properties of $Mg_2Si$ and $Mg_2Ge$ at finite temperatures depend on its lattice-dynamical behavior. Therefore, it is important to understand the vibrational properties of $Mg_2Si$ and $Mg_2Ge$. In 1965, Whitten et al. [7] and Chung et al. [8] determined the elastic constants of $Mg_2Si$ and $Mg_2Ge$ from 80 to 300 K by a resonance technique and calculated the lattice vibration frequencies using the experimental elastic constants as well as optical data. However, theoretical work on the phonon of $Mg_2Si$ and Mg2Ge is very limited. In 1997 and 1999, Baranek et al. [9, 10] determined the phonon frequencies of $Mg_2Si$ at the center of the Brillouin zone by first-principles calculation within the frozen phonon approximation. In 2001, Arnaud and Alouani [11] calculated the excited properties of $Mg_2Si$ and $Mg_2Ge$ using all-electron GW approximation. To our best knowledge, no detailed for first-principles lattice dynamic calculation data such as phonon dispersion relations, phonon density of states, and thermodynamic properties such as vibrational entropy, specific heat, and Debye temperature, have been reported on $Mg_2Si$ and $Mg_2Ge$ exist. In this study, we present calculations of the structure, elastic constants, lattice dynamics, and some thermodynamic properties of $Mg_2Ge$. The computed thermodynamic properties will be compared to previous experimental data.

## II. METHODOLOGY

The intermetallic compounds $Mg_2Ge$ belongs to class of Zintl phases. Zentil phases are compound, which consist of two or more (main group) metals or semimetals with a relative large electronegtivity difference, which obey the concept of Zintl, Kelmm and Busmann (ZKB). The ZKB concept states that the valence electrons of the less electronegative element (often an alkali or alkaline earth metal) are completely transferred to more electronegative one. The latter, with a new number of valance electrons, now build up partial structures which are also built by main group elements with the corresponding number of valance electron, or, more generally speaking structures, which obey the (8-n) rule.-[21]

In case $Mg_2Ge$ four valence electrons are formally transferred from magnesium to germanium. This lead to 4+4=8 valance electrons at the germanium atom and corresponds to valance electron configuration of noble

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gas (krypton or xenon). In accordance with the (8-n) rule, solids built up by noble gases are characterized by isolated noble gas atoms. This phenomenon can also be found for $Mg_2Ge$ compound in the cubic anti $CaF_2$ structure. Eight magnesium atoms, forming a regular cube, surround the germanium atom. Magnesium in turn is tetrahedrally coordinated by germanium. DAF model involves two types of interatomic forces the harmonic force act only along the line joining two neighbors, and is called 'central force' also called radial force. A second type of force is one, which depends on the angle, which the lines joining the moving atoms make with the equilibrium position of the line. This type of force is known as 'angular force'. In this analysis the phonons of $Mg_2Si$ have been calculated by using de Launey angular force constant model. As this model is used for short range forces and magnitude of the forces generally diminishes after second neighbor, so interatomic interaction upto second nearest neighbor is considered. The separate force constants are used for the central and angular forces. In this study $\alpha_1$ and $\alpha_2$ are the force constants used for central force and $\alpha'_1$ and $\alpha'_2$ are force constants used for angular force for first neighbor and second neighbor respectively.

Now by using DAF model a dynamical matrix of (9x9) has been established and it is solved to obtained relations between force constants, frequency and elastic constants at zone centre. The obtained relations are as given below.

$$2aC_{11} = 4/3(\alpha_1 + 2\acute{\alpha}_1) + 4\alpha_2 + 12\alpha_3 \quad \text{------.1)}$$

$$2aC_{44} = 4/3(\alpha_1 + 2\acute{\alpha}_1) + 4\,\acute{\alpha}_2 + 6\alpha_3 - \frac{[4/3(\alpha_1 - \acute{\alpha}_1)]^2}{[4/3(\alpha_1 + 2\acute{\alpha}_1)]} \quad \text{-------- 2)}$$

$$2aC_{12} = 4/3(\alpha_1 - 4\acute{\alpha}_1) - 4\,\acute{\alpha}_2 + 6\alpha_3 \quad \text{--------3)}$$

$$4/3(\alpha_1 + 2\acute{\alpha}_1) = [mM/(2m+M)]\,\omega_{TO}^2 \quad \text{------4)}$$

$$4/3(\alpha_1 + 2\acute{\alpha}_1) + 4(\alpha_2 + 2\acute{\alpha}_2) = m\omega_R^2 \quad \text{-----5)}$$

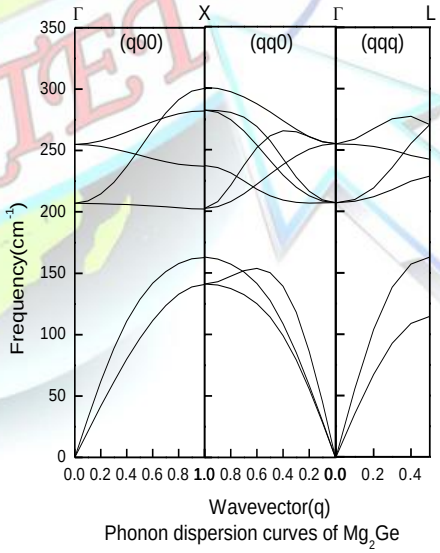
Table1. Input data

| Compound | Zone centre phonon frequencies [25] (cm-1) | | Elastic constant [25] (1011 dynes. cm-2) | | | Lattice constant (Å) |
|---|---|---|---|---|---|---|
| | $\omega_{TO}$ | $\omega_R$ | $C_{11}$ | $C_{12}$ | $C_{44}$ | a |
| $Mg_2Ge$ | 207 | 255 | 11.79 | 2.30 | 4.65 | 6.318 |

Table 2.Calculated force constants and zone centre (ZC) frequencies

## III. Results And Discussions

The calculated force constants listed in table 2. The present model appears to be realistic, since the force constants from this model are all-positive and diminish with increasing neighbor distance. It is also clear from table 2 that the interatomic interaction ($\alpha_1$) between Ge and Mg1 or Mg2 is strongest among all. It is also obvious from table 2 that the calculated zone center phonons of $Mg_2Ge$ are well in agreement with other's calculated results [25] the calculated phonon dispersion curves along three symmetric directions for $Mg_2Ge$ are shown in figure 2. It is obvious from these figures that there are three acoustic and six optic modes for all wave vectors along [KK0] directions. However, there are two acoustic and four optic modes along the high symmetry directions [K00] (Γ-X) and [KKK] (Γ-L), due to the degeneracy of the transverse modes in both acoustic and optic branches.



Phonon dispersion curves of $Mg_2Ge$

It is also visible from figure 1 that all the optical modes of $Mg_2Ge$ are found to be quite dispersive along the main symmetric directions of [K00], [KK0] and [KKK]. Due to mass difference between Mg and Ge atoms, there is very sufficient

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large gap between the acoustic and optic branches for $Mg_2Ge$. In particular, the frequencies of the lowest TO (transverse optical) and LA (longitudinal acoustical) modes are found to be 202 and 162 $cm^{-1}$ respectively at the X point. It is different from other calculation [25], which found overlapping of these modes. This difference may arise because of consideration of interatomic interaction only up to third nearest neighbor in the present simple model. It is found from eigen vector displacement calculation that all optic phonon modes are due to Mg atoms while acoustic phonon modes are mainly characterized by the motion of Ge atoms. Along the least symmetry direction [KK0] (Γ-X), the phonon branches show an appreciable amount of dispersion along this direction for both compounds. The present calculations are in good agreement with available theoretical results.

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