Accepted Manuscript

The first principle calculations of structural, vibrational, elastic, thermodynamic and electronic properties of MgX (X = La, Nd, Sm) intermetallics

S. Rameshkumar, G. Jaiganesh, V. Jayalakshmi

PII: S2352-2143(18)30148-5

DOI: 10.1016/j.cocom.2018.e00324

Article Number: e00324

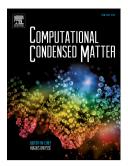
Reference: COCOM 324

To appear in: Computational Condensed Matter

Received Date: 14 May 2018
Revised Date: 18 July 2018
Accepted Date: 21 July 2018

Please cite this article as: S. Rameshkumar, G. Jaiganesh, V. Jayalakshmi, The first principle calculations of structural, vibrational, elastic, thermodynamic and electronic properties of MgX (X = La, Nd, Sm) intermetallics, *Computational Condensed Matter* (2018), doi: 10.1016/j.cocom.2018.e00324.

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.



ACCEPTED MANUSCRIPT

The first principle calculations of structural, vibrational, elastic, thermodynamic

and electronic properties of MgX (X = La, Nd, Sm) intermetallics

S. Rameshkumar¹, G. Jaiganesh² and V. Jayalakshmi^{1,*}

¹Department of Physics, SRM Institute of Science and Technology, Ramapuram Campus,

Chennai – 600089, India

²Materials Science Group, Indira Gandhi Centre for Atomic Research, Kalpakkam – 603102, India

Abstract

In the present work, we have investigated the structural, electronic, vibrational,

elastic, mechanical and thermodynamic properties of MgX (X = La, Nd, Sm) intermetallics in

B2, Ba, B1, B3, B20 and B32 cubic phases. Our obtained results show that B2 and Ba phases

are stable than the other B1, B3, B20 and B32 phases at ambient conditions. The estimated

ground-state properties are in good agreement with the available experimental and other

theoretical results. The metallic nature of these intermetallics is confirmed from the band

structure and density of state calculations. The phonon dispersion curve explains the

dynamical stability of these intermetallics. The elastic constants and mechanical properties of

these intermetallics as a function of pressure are also discussed. In addition to the above, the

thermodynamic property of these intermetallics as a function of pressures and temperatures

are reported.

Keywords: An ab-initio study; MgX intermetallics; ground-state properties; elastic constants;

Phonon dispersion

*corresponding author e-mail: jayam6480@gmail.com

1

Download English Version:

https://daneshyari.com/en/article/7956349

Download Persian Version:

https://daneshyari.com/article/7956349

Daneshyari.com