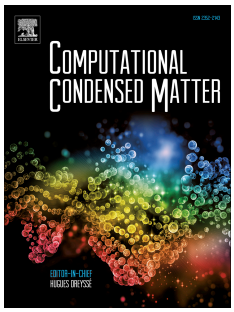
Accepted Manuscript



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.

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

S. Rameshkumar[1], *G. Jaiganesh*[2] *and V. Jayalakshmi*[1,*]

[1]*Department of Physics, SRM Institute of Science and Technology, Ramapuram Campus, Chennai – 600089, India*

[2]*Materials 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