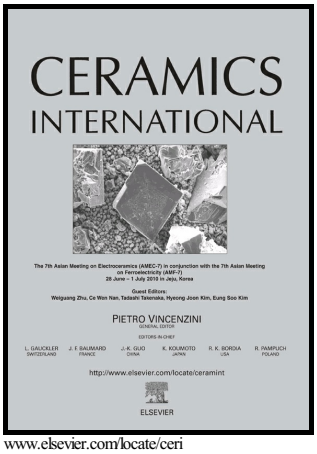

www.elsevier.com/locate/ceri

Phase stability, elastic, anisotropic properties, lattice dynamical and thermodynamic properties of $B_{12}M$ (M=Th, U, Np, Pu) dodecaborides

You Lv, Xudong Zhang, Wei Jiang

PII: S0272-8842(17)32076-X
DOI: http://dx.doi.org/10.1016/j.ceramint.2017.09.147
Reference: CERI16318

To appear in: *Ceramics International*

Received date: 28 August 2017
Revised date: 18 September 2017
Accepted date: 18 September 2017

Cite this article as: You Lv, Xudong Zhang and Wei Jiang, Phase stability, elastic, anisotropic properties, lattice dynamical and thermodynamic properties of $B_{12}M$ (M=Th, U, Np, Pu) dodecaborides, *Ceramics International,* http://dx.doi.org/10.1016/j.ceramint.2017.09.147

Phase stability, elastic, anisotropic properties, lattice dynamical and thermodynamic properties of $B_{12}M$ (M=Th, U, Np, Pu) dodecaborides

You Lv[a], Xudong Zhang[a]*, Wei Jiang[a,b]

[a] School of Science,Shenyang University of Technology, Shenyang 110870, China;

[a,b]School of Materials Science and Engineering, Shenyang University of Technology, Shenyang 110870, China

*Corresponding author. E-mail address: zxdwfc@163.com

Abstract: Dodecaborides are promising high strength ceramic and refractory materials, due to the excellent physical properties. However, the scarce systematic investigations of physical properties of $B_{12}M$ (M=Th, U, Np, Pu) dodecaborides hinder the better applications of these dodecaborides. By means of the first-principles approach, we systemically investigated the phase stability, elastic, anisotropic properties, dynamical stability and thermodynamic properties of $B_{12}M$ (M=Th, U, Np, Pu) dodecaborides. The optimized structure constants are consistent with available experimental data. The values of formation enthalpies and V/V_0 under pressure indicate $B_{12}M$ have good phase stability. The elastic parameters and modulus indicate that $B_{12}M$ dodecaborides are all brittle and superhard materials. The results of anisotropic factors, 3D surface contours and 2D projections of $B_{12}M$ indicate that they are all anisotropic, but the extent of anisotropy is relatively small. Anisotropy of acoustic velocities and the 2D planar projections of the minimum thermal conductivity are also calculated and discussed. The lattice dynamic properties indicate that four dodecaborides are all satisfied with the dynamic stability conditions. The