Accepted Manuscript

Novel 122-type Ir-based superconductors $BaIr_2Mi_2$ (Mi = P and As): A density functional study

Md. Zahidur Rahaman, Md. Atikur Rahman

PII: S0925-8388(17)31182-9

DOI: 10.1016/j.jallcom.2017.04.006

Reference: JALCOM 41407

To appear in: *Journal of Alloys and Compounds*

Received Date: 13 December 2016

Revised Date: 18 March 2017

Accepted Date: 1 April 2017

Please cite this article as: M.Z. Rahaman, M.A. Rahman, Novel 122-type Ir-based superconductors $BaIr_2Mi_2$ (Mi = P and As): A density functional study, *Journal of Alloys and Compounds* (2017), doi: 10.1016/j.jallcom.2017.04.006.

Novel 122-type Ir-based superconductors $BaIr_2Mi_2$ (Mi = P and As): A density functional study

Md. Zahidur Rahaman[1]

Department of Physics, Pabna University of Science and Technology, Pabna-6600, Bangladesh
zahidur.physics@gmail.com

Md. Atikur Rahman[2*]

Department of Physics, Pabna University of Science and Technology, Pabna-6600, Bangladesh
atik0707phy@gmail.com
[*]Corresponding author.

Abstract

We explore the structural, electronic, bonding, mechanical, thermodynamic and superconducting properties of two newly discovered isostructural bulk superconductors barium iridium phosphide $BaIr_2P_2$ (T_c ~ 2.1 K) and barium iridium arsenide $BaIr_2As_2$ (T_c ~ 2.45 K). The optimized structural parameters of both the compounds show good agreement with the experimentally evaluated values. The replacement of P by As mostly affects the *c* value, whereas *a* remains approximately the same. Metallic conductivity is observed for both the superconductors. The analysis of DOS, Mulliken atomic populations and total charge density revel a complex bonding in $BaIr_2P_2$ and $BaIr_2As_2$ with ionic, covalent and metallic characteristics. Mechanical and dynamical stability of both the phases is confirmed by analyzing the elastic constant data. According to the calculated Pugh's ratio both the intermetallics are ductile in nature. Both the superconductors demonstrate anisotropic nature whereas the elastic anisotropy of $BaIr_2P_2$ is higher than that of $BaIr_2As_2$. The hardness of $BaIr_2P_2$ and $BaIr_2As_2$ is evaluated to be 6.92 GPa and 5.02 GPa respectively indicating the relative hardness of $BaIr_2P_2$ than that of $BaIr_2As_2$ superconductor. The Debye temperature of $BaIr_2P_2$ and $BaIr_2As_2$ has been calculated by using the elastic constant data to be 293.06 K and 258.47 K respectively. Finally the electronic specific heat coefficient, electron-phonon coupling constant, coulomb pseudo potential and superconducting critical temperature have been evaluated for both the compounds. We found weakly and moderately coupled bulk superconductivity in $BaIr_2P_2$ and $BaIr_2As_2$ with transition temperature 0.0057 K and 6 K respectively.

Keywords: $BaIr_2P_2$, $BaIr_2As_2$, Superconductivity, Physical properties.

I. Introduction

The discovery of superconductivity in Fe-based compounds gives a clear spur to the search for new superconductors with high superconducting critical temperature [1]. The material combination of iron pnictide is very promising for practical discovery of superconductors with high transition temperature. The combination of ternary 122-type materials is alike as that of so called iron pnictide and hence in this structure type the substitution of iron by any other transition metals provides a fresh route for the exploration of high T_c superconducting materials.

On the other hand the rare-earth compounds with AM_2X_2 type structure (where, A = lanthanide element or any alkaline earth element; M = transition metal; X = P, As, Ge or Si) have attracted a large scientific community with their many attractive properties including heavy fermion behavior, superconductivity, exotic magnetic order, mixed valency and valence fluctuation [2]. Since one possible route to explore high T_c superconductors is the substitution of Fe by other transition elements in the AM_2X_2 type structure, $ThCr_2Si_2$ structured compounds can be the great choice with more than seven hundred representatives. $ThCr_2Si_2$ structure type was first reported in 1965 by Ban and Sikirica