Jan Dlugosz
University
in Czestochowa

www.ujd.edu.pl

Jan Dlugosz University in Czestochowa

CRYSTAL, ELECTRONIC STRUCTURE AND HYDROGENATION PROPERTIS OF $Zr_{5-x}Mg_xNiSn_3$

Agnieszka Balińska[1], Volodymyr Pavlyuk[1,2]

[1]Institute of Chemistry, Jan Dlugosz University in Czestochowa,
al. Armii Krajowej 13/15, 42-200 Czestochowa, Poland,
e-mail: a.balinska@ujd.edu.pl
[2]Department of Inorganic Chemistry, Ivan Franko National University of Lviv,
Kyryla and Mefodiya str. 6, 79005 Lviv, Ukraine

INTRODUCTION

New ternary compound of $Zr_{5-x}Mg_xNiSn_3$ was prepared from elemental zirconium (foil, 0.25mm thick 99.8 at.%, Aldrich), magnesium (powder, 98 at.%, Aldrich), nickel (powder, 99.7 at.%, Aldrich) and tin (granules, 99.85 at.%, POCH). The pieces of the pure metals were pressed into pellet. The sample was melted in arc furnace under continuous argon flow. X-ray powder diffraction of the samples were carried out using STOE powder diffractometer (Mo – radiation). Rietveld refinements of X – ray powder diffraction data were performed by using the FULLPROF program [1]. The phase content of synthesized alloy was carried out using the TESCAN electron microscope equipped with EDS detectors. Hydrogen absorption-desorption properties of the alloy was studied using a Sieverts type apparatus.

The crystal structure of $Zr_{5-x}Mg_xNiSn_3$ and $Zr_{5-x}Mg_xNiSn_3H_6$ phases were investigated by powder methods. The $Zr_{5-x}Mg_xNiSn_3$ and $Zr_{5-x}Mg_xNiSn_3H_6$ crystallises in the Hf_5CuSn_3-type with $P6_3/mcm$ space group, respectively a = 8.5051 Å, c = 5.8135 Å and a = 8.6904 Å, c = 5.9081 Å. The electronic structures of the compounds were calculated using the tight-binding linear muffin-tin orbital (TB-LMTO) method in the atomic spheres approximation (TB-LMTO-ASA) [2–4], using the experimental crystallographic data. The maximum electron localization around the Sn atoms are obtained.

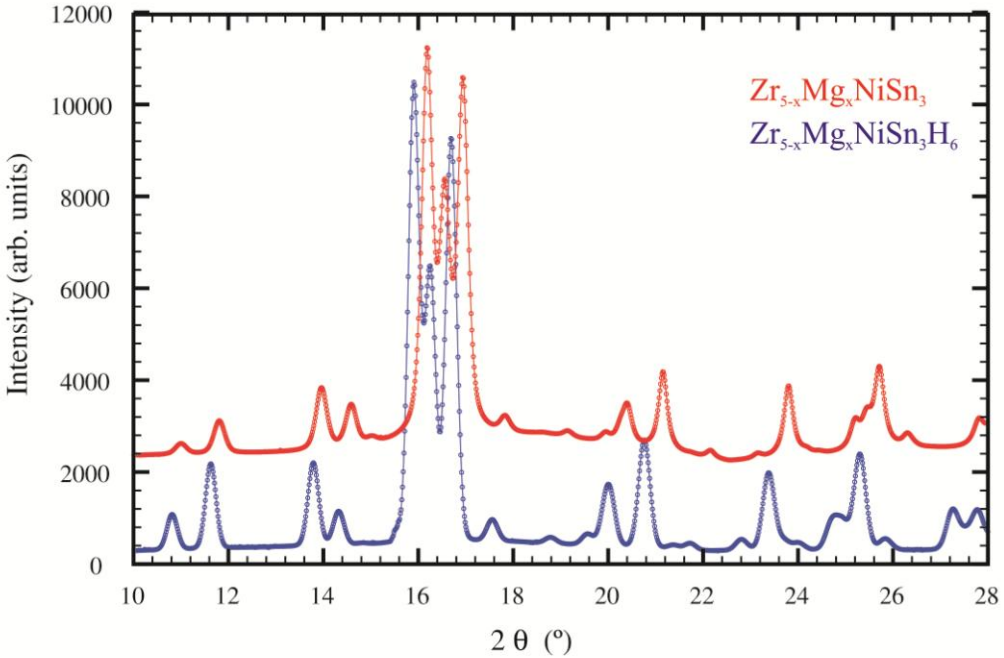

Figure 1. X-ray powder diffraction patterns for $Zr_{5-x}Mg_xNiSn_3$ and $Zr_{5-x}Mg_xNiSn_3H_6$

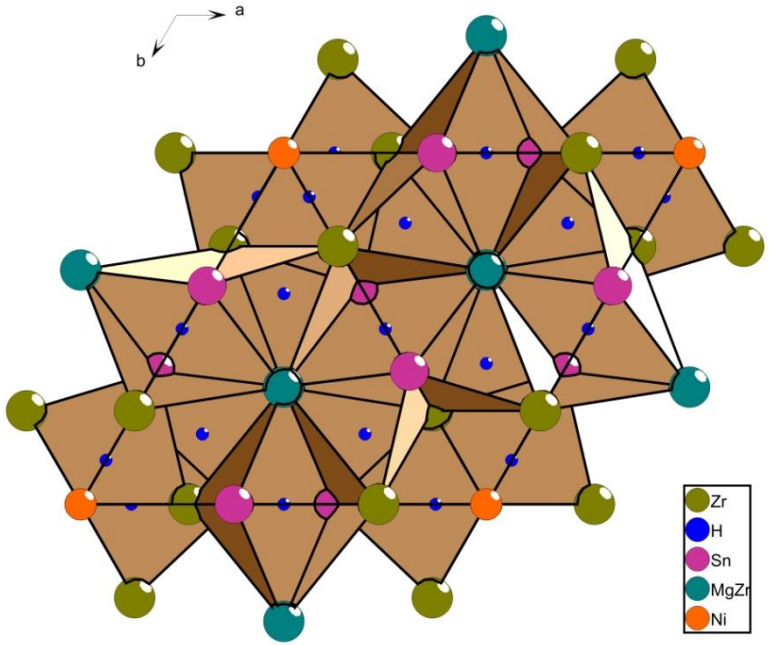

Figure 2. The unit cell and coordination polyhedra of atoms for $Zr_{5-x}Mg_xNiSn_3H_6$

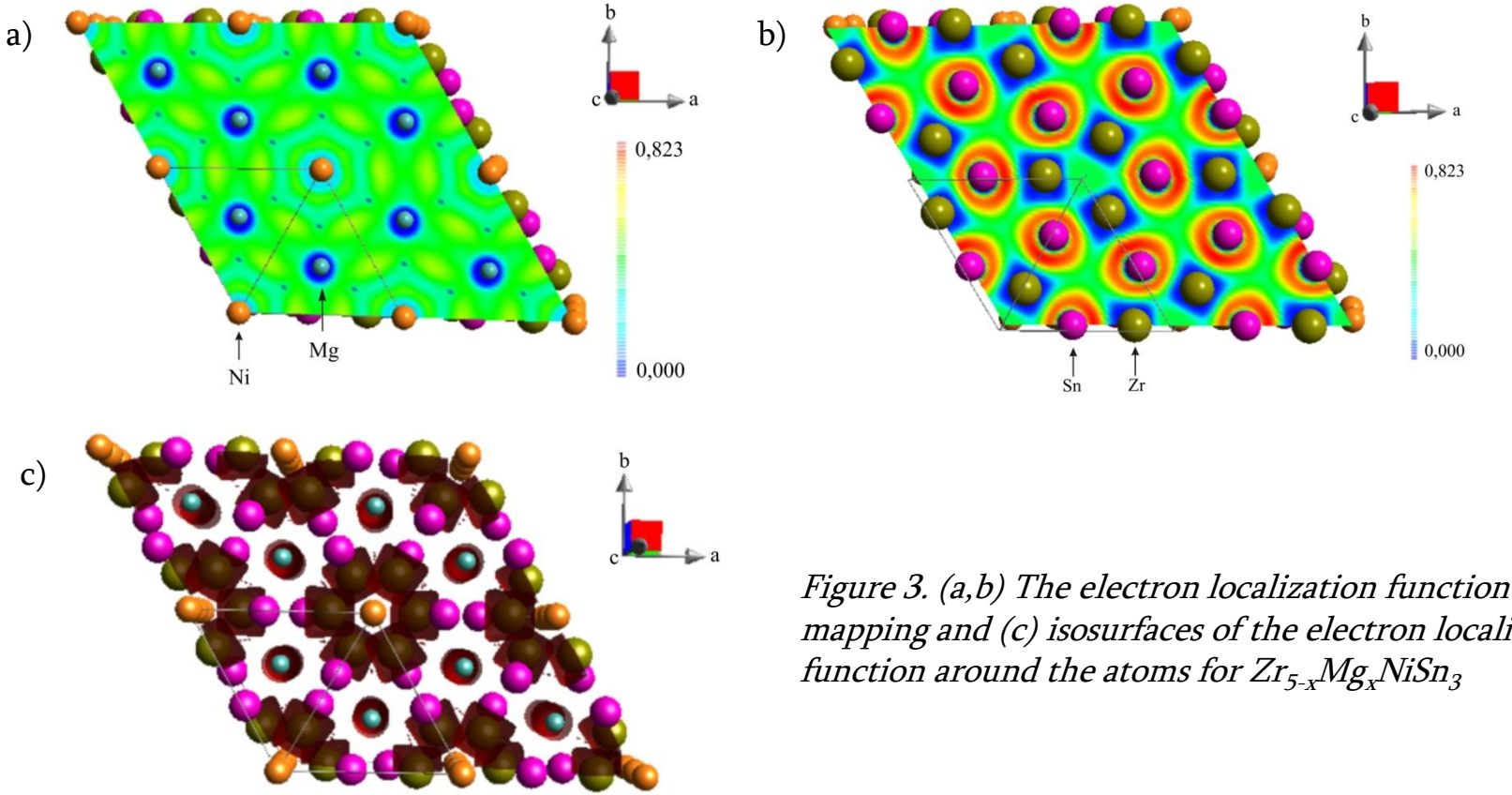

Figure 3. (a,b) The electron localization function (ELF) mapping and (c) isosurfaces of the electron localization function around the atoms for $Zr_{5-x}Mg_xNiSn_3$

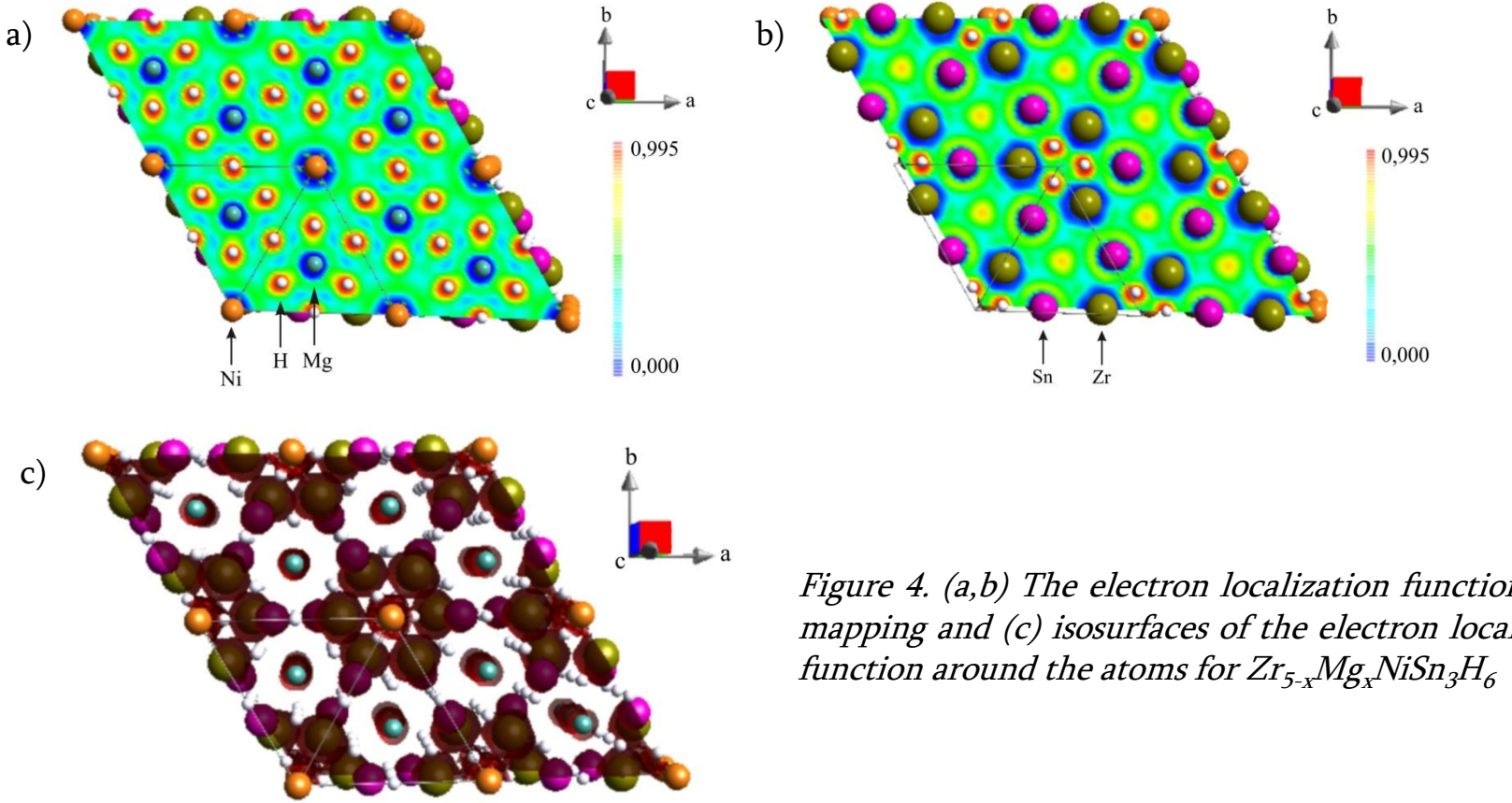

Figure 4. (a,b) The electron localization function (ELF) mapping and (c) isosurfaces of the electron localization function around the atoms for $Zr_{5-x}Mg_xNiSn_3H_6$

Jan Długosz University in Częstochowa

References

[1] J. Rodriguez-Carvajal, Recent advances inmagnetic structure determination by neutron powder diffraction, *Physica B*, 1993, 192, 55–69

[2] OK. Andersen, Linear methods in band theory, *Phys Rev B*, 1975, 12, 3060–3117

[3] OK. Andersen, O. Jepsen, Explicit, First-Principles Tight-Binding Theory, *Phys Rev Lett*, 1984, 53, 2571–2574

[4] OK. Andersen, Z. Pawlowska, O. Jepsen, Illustration of the linear-muffin-tin-orbital tight-binding representation: Compact orbitals and charge density in Si, *Phys Rev B*, 1986, 34, 5253–5269

Financial support from the National Science Centre, Poland NCN (No 2017/25/B/ST8/02179)