

International Centre for Diffraction Data and American Society for Metals database survey of thermoelectric half-Heusler material systems

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Phase diagrams and X-ray powder diffraction patterns provide critical information for thermoelectric (TE) research. We have conducted a survey of phase diagrams and powder diffraction patterns of TE systems in the ASM (American Society for Metals) Metal/Alloy database and ICDD (International Centre for Diffraction Data) PDF (Powder Diffraction File), respectively, for their availability and crystal systems. In this report, we focus on TE materials that have the half-Heusler XYZ structure, and related compounds, based on a set of materials selection rules. We found that among 306 potential XYZ compounds that we have surveyed, 234 have powder diffraction patterns in the PDF, but only 28 have phase diagram information, and 67 do not have any crystallographic information. Among the 234 phases with powder patterns, 84 were reported to have cubic $F43m$ half-Heusler type structure, and the remainder have hexagonal, orthorhombic or other structure types. Some XYZ compounds have both cubic and hexagonal phases. This information will provide the basis for future activities for the improvement of the databases. These activities include filling the missing gaps in both phase equilibria database and the PDF, as well as adding TE and pertinent physical properties to the PDF. © 2013 International Centre for Diffraction Data. [doi:10.1017/S0885715612000942]

Key words: thermoelectric half-Heusler compounds, ICDD PDF, ASM phase diagram database, survey

I. INTRODUCTION

A. Thermoelectric (TE) materials

In recent years, partly due to rising fuel prices and concern over the role of CO₂ emissions in the greenhouse atmospheric warming effect, TE material research has become increasingly important worldwide. The TE effect refers to phenomena by which either a temperature difference creates an electric potential or an electric potential creates a temperature difference (Martin *et al.*, 2010). These phenomena are known as the Seebeck effect (converting temperature to current), Peltier effect (converting current to temperature), and Thomson effect (conductor heating/cooling). Although all materials have a nonzero TE effect, in most materials it is too small to be useful for practical applications. Low-cost materials that have a large TE effect have potential to be used in applications including power generation and refrigeration.

TE materials can either allow heat to be pumped from one place to another using electricity or allow electricity to be generated from heat. The efficiency and performance of TE power generation or cooling are related to the dimensionless figure of merit (ZT) of the TE materials, given by $ZT = S^2\sigma T/k$, where T is the absolute temperature, S is the Seebeck coefficient or thermopower, σ is the electrical conductivity ($\sigma = 1/\rho$, ρ is electrical resistivity), and k is the thermal conductivity (Tritt and Subramanian, 2006). In order to develop efficient TE materials, efforts have been expended on synthesizing completely new materials as well as on

developing chemically doped materials with improved properties.

B. Phase diagrams and X-ray diffraction patterns

Phase diagrams contain important information for the development of new materials, control of structure and composition of critical phases, and the improvement of properties of technologically important materials. These diagrams very often can be thought of as “road maps” or “blue prints” for processing and for understanding materials’ properties, as they provide the theoretical basis for synthesis of materials. Applications of phase diagrams range from preparation of high-quality single crystals and single-phase materials to controlled precipitation of second phases and formation of melts. More specifically, the phase relationships described in a phase diagram can be used to correlate the phases present in X-ray diffraction patterns of material systems, and to understand whether a single phase or a mixture has been obtained.

For over 60 years, the American Ceramic Society (ACerS), in collaboration with National Institute of Standards and Technology (NIST), has evaluated and published the Phase Diagrams for Ceramists series of compilations. A parallel program in alloy phase diagrams is currently managed by the American Society for Metals (ASM). The ASM Alloy Phase Diagrams Center is copyrighted by ASM International, and the data in this product are copyrighted by Material Phases Data System, Vitznau, Switzerland. A portion of the binary diagrams is jointly copyrighted by Material Phases Data System and Japan Science and Technology Corporation, Tokyo, Japan. The availability of phase diagrams in these databases is critical for any branch

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of materials research, whether it concerns energy-related materials (TEs, superconductors, fuel cells, batteries or supercapacitors), or materials for a diverse array of other applications, such as optoelectronic devices, magnetic materials, ferroelectric materials, etc.

Since X-ray diffraction provides a non-destructive “fingerprint” technique for phase identification, X-ray diffraction reference patterns are especially important for phase characterization. Therefore, it is essential to have complete coverage of experimental/calculated patterns in the Powder Diffraction File (PDF), produced by the International Centre for Diffraction Data (ICDD), to serve as references.

C. ICDD TE task group

ICDD serves a dual role in the scientific community. It is a non-profit publishing house as well as a scientific organization that sponsors diffraction-related conferences and scientific committees for ensuring the high quality of the PDF. In the past two decades, the Ceramics Subcommittee of the Technical Committee of ICDD has created a number of material task groups to ensure extensive coverage of reference diffraction patterns of ceramics phases in the PDF. One of the task groups focuses on TE materials (code “TE” in the PDF). The working definition of TE is that “Thermoelectric materials are materials that have reasonably high Figure of Merit (ZT , $ZT = S^2\sigma/\kappa$; materials with high Seebeck coefficient (S), high electrical conductivity (σ), and low thermal conductivity (κ) for practical applications.” Some or all of the associated properties (Seebeck coefficient, electrical conductivity (or resistivity ($1/\sigma$)), thermal conductivity and ZT) should be added to the PDF and made available to the users.

An important activity of the TE task group is to fill in the gap of the PDF with those phases that have missing patterns and also provide added physical property information to the TE phases. A survey of the TE materials in the PDF is therefore important for the TE community (including the ICDD Grants-in-Aid recipients).

II. SURVEYING PLAN

We designed a survey with the aim of compiling the phase diagrams and X-ray diffraction patterns of TE compounds based on known TE systems. To efficiently accomplish this goal, we organized the TE materials in the PDF into five categories, namely half-Heusler compounds, skutterudites, clathrates, oxides, and other chalcogenides, silicides, and pnictides. This classification will cover a significant number of the state-of-the-art TE materials. The chosen compounds/systems are checked against the phase diagrams databases produced by ASM or by ACerS/NIST, and also against the PDF.

In this report, we will discuss our effort at tabulating information pertaining to the half-Heusler compounds. As these half-Heusler compounds are all semiconductors/metal-alloys, the ASM database was used exclusively.

III. SURVEY OF HALF-HEUSLER COMPOUNDS

A. Background information on half-Heusler compounds

The half-Heusler structure, XYZ, was first discovered by Heusler (Heusler, 1903). The half-Heusler compounds possess MgAgAs type structure (Jeitschko, 1970) that is closely

related to that of the full-Heusler alloys. The full-Heusler structure, X_2YZ , is built up from four interpenetrating *fcc* sublattices mutually shifted along the body diagonal by a $1/4$ distance. In other words, the unit cell of the full-Heusler structure, with space group $Fm\bar{3}m$, consists of four interpenetrating *fcc* lattices at offsets of $A = (0, 0, 0)$, $B = (1/4, 1/4, 1/4)$, $C = (1/2, 1/2, 1/2)$, and $D = (3/4, 3/4, 3/4)$, with site occupancies $A = Y$, $B = X$, and $C = Z$. If one of the two equivalent sites, $(1/4, 1/4, 1/4)$ or $(3/4, 3/4, 3/4)$, is empty, this will give rise to the half-Heusler XYZ structure that adopts the space group $F\bar{4}3m$. The half-Heusler structure is shown in Figure 1. These alloys, in general, have three components that often originate from different element groups. Most frequently, two of the groups are composed of transition metals and the third group consists of metals and metalloids. The structures of the full-Heusler and half-Heusler compounds exhibit different properties. For example, while the full-Heusler compounds MNi_2Sn ($M = Zr, Hf, Ti$) are metallic, removal of one of the two Ni sublattices and replacing them by an ordered lattice of vacancies leads to the formation of the half-Heuslers with semi-conducting character (Uher *et al.*, 1999).

Semiconductors with a small band gap in the density of states are favourable for TE applications. In recent years, half-Heusler compounds that obey the isoelectron rules (the sum of valence electron count (VEC)) of 18 per formula unit (Tobola *et al.*, 1998) have attracted increasing attention as new TE compounds because of their high thermoelectric power ($TEP = S^2\sigma$) (Ogut and Rabe, 1995; Kaczarska, *et al.*, 1998; Tobola *et al.*, 1998; Jung *et al.*, 2000; Tobola and Pierre, 2000; Asahi *et al.*, 2008) due to their narrow band gaps. Complex compounds such as TiNiSn phases are promising n-type thermoelectrical materials as illustrated by an exceptionally large figure of merit, $ZT \sim 1.5$ at high temperatures (Asahi *et al.*, 2008). Doped TiCoSb, a p-type material, exhibits a large thermopower of $S = -400 \mu V/K$ at 300 K. Larson *et al.* (1999) studied the electronic structure of a class of half-Heusler compounds $MNiPn$ where M is Y, La, Lu, and Yb, and Pn is a pnictogen Sb and Bi and found that all these systems except Yb are narrow gap semiconductors and are potential candidates for high-performance TE materials. Yang *et al.* (2008) conducted theoretical calculations on 36 representative half-Heusler compounds to

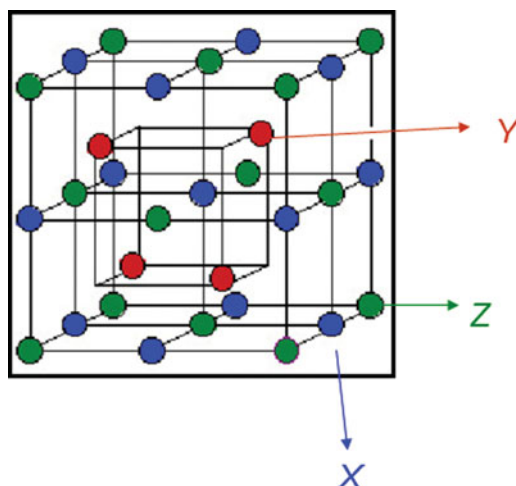


Figure 1. Structure of a half-Heusler compound XYZ that adopts the space group $F\bar{4}3m$.

TABLE I. Survey results of 306 intermetallic compounds, XYZ, where Z is Si, Ge, Sn, Sb, Bi using the ASM phase diagram data base and the PDF.

Compounds XYZ	Phase Diagram X-Y-Z ASM Database	Literature References	Cubic system, space group	Hexagonal system, space group	Orthorhombic system, space group	Other or unknown system, space group	ICDD Database, PDF#
HfNiSn	Y	Stadnyk Y.V., and Romaka L.P., J. Alloys Compd., Vol. 316, 2001, p 169–171	$F\bar{4}3m$				04-012-9150
HfPdSn	N		$F\bar{4}3m$				04-003-9106
HfPtSn	N		$F\bar{4}3m$				04-001-4047
NbCoSn	Y	Skolozdra R.V., and Okhrimovich K.O., THE Nb-Co-Sn AND Nb-Ni-Sn SYSTEMS, Russ. Metall., Vol. (6), 1971, p 135–138	$F\bar{4}3m$				00-052-0908
NbRhSn	N	–	$F\bar{4}3m$				04-012-9743
LaCuSn	N	–		$P6_3mc, P6_3/mmc$			01-074-8436 04-014-1200
CeCuSn	N	–		$P6_3/mmc, P6_3/mmc$			00-054-0363
PrCuSn	Y	Komarovskaya L.P., Mkhailiv L.A., and Skolozdra R.V., THE TERNARY Pr(Lu)-Cu-Sn SYSTEM, Russ. Metall., Vol. (4), 1989, p 204–208					01-079-3644
NdCuSn	Y	Riani P., Fornasini M.L., Marazza R., Mazzone D., Zanicchi G., and Ferro R., The isothermal section at 400 °C of the Nd-Cu-Sn ternary system, Intermetallics, Vol. 7, 1999, p 835–846		$P6_3mc, P6_3/mmc$			04-009-2179 01-078-9595
SmCuSn	Y	Senkovska I.V., Mudryk Y.S., Romaka L.P., and Bodak O.I., The (Sm,Er)-Cu-Sn ternary systems, J. Alloys Compd., Vol. 312, 2000, p 124–129		$P6_3mc, P6_3/mmc$			04-009-2180 01-078-9589
EuCuSn	N	–			<i>Imam</i>		00-051-1263
GdCuSn	N	–		$P6_3mc, P6_3/mmc$			0-009-2181 01-078-9586
DyCuSn	Y	Bodak O.I., Romaka V.V., Tkachuk A.V., Romaka L.P., and Stadnyk Y.V., Phase equilibria in the Dy-Cu-Sn ternary system, J. Alloys Compd., Vol. 395, 2005, p 113–116		$P6_3mc, P6_3/mmc$			01-073-4651 00-051-0895
HoCuSn	N	–		$P6_3mc, P6_3/mmc$			04-007-7234 01-078-9592
YCuSn	Y	Zhuang Y., Qin C., and Li J., The isothermal section (500 °C) of the phase diagram of the ternary system Cu-Sn-Y, J. Less-Common Met., Vol. 175, 1991, p 97–101		$P6_3mc, P6_3/mmc$			01-076-4964 01-078-9587
ErCuSn	Y	Senkovska I.V., Mudryk Y.S., Romaka L.P., and Bodak O.I., The (Sm,Er)-Cu-Sn ternary systems, J. Alloys Compd., Vol. 312, 2000, p 124–129		$P6_3mc, P6_3/mmc$			04-007-7238 00-054-0546
TmCuSn	N	–		$P6_3/mmc$			01-078-9594
YbCuSn	Y	Zanicchi G., Mazzone D., Fornasini M.L., Riani P., Marazza R., and Ferro R., Yb-Cu-Sn system: the isothermal section at 400 °C, Intermetallics, Vol. 7, 1999, p 957–966			<i>Pnam</i>		04-008-5177
LuCuSn	Y	Komarovskaya L.P., Mkhailiv L.A., and Skolozdra R.V., THE TERNARY Pr(Lu)-Cu-Sn SYSTEM, Russ. Metall., Vol. (4), 1989, p 204–208		$P6_3mc, P6_3/mmc$			04-014-1201 01-79-3628
LaAgSn	N	–		$P6_3/mmc, P6_3mc, P6_3/mmc$			04-004-9707
CeAgSn	Y	Boulet P., Mazzone D., Noel H., Riani P., Rogl P., and Ferro R., The system Ce-Ag-Sn: phase equilibria and magnetic properties, Intermetallics, Vol. 7, 1999, p 931–935					01-073-8216 04-004-9699

PrAgSn	Y	Mazzone D., Riani P., Zanicchi G., Marazza R., and Ferro R., The isothermal section at 400 °C of the Pr-Ag-Sn ternary system, <i>Intermetallics</i> , Vol. 10, 2002, p 801–809		$P6_3mc$		01-073-8217
NdAgSn	N	–		$P6_3mc, P6_3/mmc$		00-050-1330 01-073-8218
SmAgSn	N	–		$P6_3/mmc$		04-004-9706
EuAgSn	N	–			<i>Imam</i>	00-049-1733
GdAgSn	N	–		$P6_3/mmc$		04-004-9700
DyAgSn	N	–		$P6_3mc, P6_3/mmc$		01-077-5801 04-004-9701
HoAgSn	N	–		$P6_3mc, P6_3/mmc$		01-073-8221 04-003-9396
YAgSn	N	–		$P6_3mc$		04-013-4038
ErAgSn	N	–		$P6_3mc, P6_3/mmc, P\bar{6}2m$		01-073-8222 00-054-0378 04-014-9311
TmAgSn	N	–		$P6_3mc, P\bar{6}2m$		04-014-9312 04-013-4039
YbAgSn	N	–		$P6_3/mmc, P\bar{6}2m, P3m1$		04-004-9703 04-011-1835 04-010-0938
LuAgSn	N	–		$P6_3mc, P\bar{6}m2$		01-077-5799 04-013-4040
CeAuSn	Y	Boulet P., Mazzone D., Noel H., Rogl P., and Ferro R., Phase equilibria and magnetic studies in the ternary system Ce-Au-Sn, <i>J. Alloys Compd.</i> , Vol. 317/318, 2001, p 350–356		$P6_3mc, P6_3/mmc$		04-011-4994 01-079-2782
PrAuSn	N	–		$P6_3mc, P6_3/mmc$		01-073-7495 01-079-2817
NdAuSn	N	–		$P6_3mc, P6_3/mmc$		01-073-7496 04-014-3437
SmAuSn	N	–	$F\bar{4}3m$	$P6_3mc, P6_3/mmc$		04-014-9324 04-013-9219 01-079-2823
EuAuSn	N	–		$P6_3mc, P6_3/mmc$	<i>I2mm</i>	00-051-1264
GdAuSn	N	–	$F\bar{4}3m$	$P6_3mc, P6_3/mmc$		04-014-9323 04-013-9220 01-072-5277
DyAuSn	N	–		$P6_3mc, P6_3/mmc$		01-073-7498 01-079-2786
HoAuSn	N	–	$F\bar{4}3m$	$P6_3mc, P6_3/mmc$		04-014-2513 01-073-7499 01-079-2799
YAuSn	N	–		$P6_3mc, P6_3/mmc$		04-014-1182 01-079-2825
ErAuSn	N	–	$F\bar{4}3m$	$P6_3mc$		04-014-9322 04-014-9316
TmAuSn	N	–	$F\bar{4}3m$	$P6_3mc$		04-014-9321 04-014-9315

Continued

Table I. Continued

Compounds XYZ	Phase Diagram X-Y-Z ASM Database	Literature References	Cubic system, space group	Hexagonal system, space group	Orthorhombic system, space group	Other or unknown system, space group	ICDD Database, PDF#
YbAuSn	N	–			<i>Pnam, I2mm</i>		04-008-5179 01-073-4965
LuAuSn	N	–	$F\bar{4}3m$	$P6_3mc$			04-014-9320 04-014-9314
ScCuSn	N	–		$P6_3mc, P6_3/mmc$			04-014-1198 01-079-3651
ScAgSn	N	–		$P\bar{6}m2$	<i>Ima2</i>		04-015-1067 04-15-1066
ScAuSn	N	–	$F\bar{4}3m$	$P6_3mc$			04-014-1180 04-014-9313
TiNiSn	N	–	$F\bar{4}3m$				04-002-1680
TiPtSn	N	–	$F\bar{4}3m$				04-003-9768
ZrNiSn	N	–	$F\bar{4}3m$				00-023-1281
ZrPdSn	N	–	$F\bar{4}3m$				04-012-9745
ZrPtSn	N	–	$F\bar{4}3m$				04-001-4046
HfNiGe	N	–			<i>Pnma</i>		04-001-4360
HfPdGe	N	–				Monoclinic $P2_1/m$	01-077-5512
HfPtGe	N	–			<i>Pnma</i>		04-008-5933
NbCoGe	N	–			<i>Pnma</i>		00-015-0411
NbRhGe	N	–			<i>Pnma</i>		04-005-0826
NbIrGe	N	–			<i>Pnma</i>		04-011-4998
LaCuGe	N	–		$P6/mmm$			04-005-0182
CeCuGe	N	–		$P6_3/mmc, P6/mmm$			01-074-4477 01-077-6497
PrCuGe	N	–		$P6/mmm$			01-086-1456
NdCuGe	N	–		$P6/mmm$			04-005-0185
SmCuGe	N	–		$P6/mmm$			01-077-6491
EuCuGe	N	–			<i>Pnma</i>		00-054-0521
GdCuGe	N	–		$P6_3mc, P6/mmm$			04-013-4030 01-077-3690
DyCuGe	N	–		$P6/mmm, P6_3mc$			04-012-9165 04-005-0189
HoCuGe	N	–		$P6_3/mmc, P6/mmm$			04-005-0190
YCuGe	N	–		$P6_3/mmc$			01-073-8619
ErCuGe	N	–		$P6_3mc, P6_3/mmc$			01-086-1461 01-073-8612
TmCuGe	N	–		$P6_3/mmc, P6/mmm$			01-078-9354 04-005-0192
YbCuGe	N	–		$P6_3/mmc, P6_3mc$			00-049-1608 04-012-0641
LuCuGe	N	–		$P6_3/mmc$			01-073-8614
LaAgGe	Y	Bardin O.I., Bodak O.I., Belan B.D., Kryvulya L.V., and Protsyk O. S., THE La-Ag-Ge SYSTEM, Visn. L'viv. Derzh. Univ., Ser. Khim., Vol. 38, 1999, p 58–63 (in Ukrainian) + F41		$P6_3mc$			00-042-1281

CeAgGe	Y	Cordruwisch E., Kaczorowski D., Saccone A., Rogl P., and Ferro R., Constitution, Structural Chemistry, and Magnetism of the Ternary System Ce-Ag-Ge, J. Phase Equilib., Vol. 20, 1999, p 407–422	$P6_3mc$		00-042-1282	
EuAgGe	Y	Belan B.D., Soroka I.N., Kryvulya L.V., Bodak O.I., and Protosyuk O.S., ISOTHERMAL SECTION OF THE PHASE DIAGRAM Eu-Ag-Ge SYSTEM AT 670 K, Visn. L'viv. Derzh. Univ., Ser. Khim., Vol. 38, 1999, p 54–57 (in Ukrainian)		<i>Imam</i>	04-011-4958	
GdAgGe	N	–	$\bar{P}6_2m$		01-086-0849	
DyAgGe	N	–	$\bar{P}6_2m$		01-086-0850	
HoAgGe	N	–	$\bar{P}6_2m$		04-007-5930	
YAg _{1.1} Ge _{0.9}	N	–	$\bar{P}6_2m$		00-053-0506	
Er-Ag-Ge	N	–	$\bar{P}6_2m$		01-008-5931	
Tm-Ag-Ge	N	–	$\bar{P}6_2m$		01-078-2936	
Yb-Ag-Ge	N	–	$\bar{P}6_2m$		04-009-2132	
Lu-Ag-Ge	N	–	$P6_3mc$		01-77-5399	
La-Au-Ge	N	–	$P6_3mc$		04-013-0768	
CeAuGe	N	–	$F\bar{4}3m$	$P6_3mc$	<i>Pnam</i>	04-014-9329 04-012-0314 04-012-0315
NdAuGe	Y	Zaplatynsky O.V., INTERACTION BEHAVIOR OF ND AND AU WITH ELEMENTS OF GROUP IVA AT 600 °C, Visn. L'viv. Derzh. Univ., Ser. Khim., Vol. 39, 2000, p 87-91		–	–	
EuAuGe	N	–		<i>Im2m</i>	00-051-1070	
GdAuGe	N	–	$P6_3mc$		04-010-1327	
DyAuGe	N	–	$P6_3mc$		01-072-8537	
HoAuGe	N	–	$F\bar{4}3m$	$P6_3mc$	04-014-9330 04-013-0928	
YAuGe	N	–	$P6_3mc$		04-013-0767	
ErAuGe	N	–	$P6_3mc$		01-074-5374	
YbAuGe	N	–		<i>Pbnm, Imam</i>	04-008-5562 04-008-5564	
LuAuGe	N	–	$P6_3mc$		04-011-9787	
ScCuGe	N	–	$\bar{P}6_2m$		01-078-9521	
ScAuGe	N	–	$P6_3mc$		04-011-9786	
TaCoGe	N	–		<i>Pnam</i>	04-001-4358	
TaRhGe	N	–		<i>Pnam</i>	01-078-9407	
TiNiGe	N	–		<i>Pnam</i>	04-005-7620	
TiPdGe	N	–	$\bar{P}6_2m$	<i>Pnam</i>	04-015-1713 04-015-1712	
VCoGe	N	–		<i>Pnam</i>	00-015-0412	
ZrNiGe	N	–		<i>Pnam</i>	00-015-0487	
ZrPdGe	N	–		<i>Pnam</i>	04-005-0828	
ZrPtGe	N	–		<i>Pnam</i>	01-078-8109	
HfNiSi	N	–		<i>Pnam</i>	04-001-4355	
HfPdSi	N	–		<i>Pnam</i>	01-070-3871	
HfPtSi	N	–		<i>Pnam</i>	04-008-6303	
NbCoSi	N	–		<i>Pnam</i>	00-015-0719	
NbRhSi	N	–		<i>Pnam</i>	00-059-0001	
NbIrSi	N	–		<i>Pnam</i>	04-011-4997	

Table I. Continued

Compounds XYZ	Phase Diagram X-Y-Z ASM Database	Literature References	Cubic system, space group	Hexagonal system, space group	Orthorhombic system, space group	Other or unknown system, space group	ICDD Database, PDF#
LaCuSi	N	–		$P6_3/mmc$, $P6/mmm$			04-004-9633 04-005-0197
CeCuSi	N	–		$P6_3/mmc$			01-078-3320
PrCuSi	N	–		$P6_3/mmc$, $P6/mmm$			04-004-9634 04-005-0199
NdCuSi	Y	Salamakha P.S., and Zaplatynsky O.V., X-ray investigation of the ternary Nd-Cu-Si and Nd-Cu-Pb systems at 870 K, J. Alloys Compd., Vol. 260, 1997, p 127–130		$P6_3/mmc$, $P6/mmm$			04-008-5162 00-054-0450
SmCuSi	N	–		$P6_3/mmc$, $P6/mmm$			04-004-9632 04-005-0201
GdCuSi	Y	Chornobryvets L., Bodak O.I., and Berezyuk D.A., THE Gd-Cu-Si SYSTEM, Visn. L'viv. Derzh. Univ., Ser. Khim., Vol. 40, 2001, p 44–47 (in Ukrainian)		$P6_3/mmc$, $P6/mmm$			01-074-5744 04-005-0202
DyCuSi	N	–		$P6_3/mmc$, $P6/mmm$			04-004-9643 01-071-7652
HoCuSi	N	–		$P6_3/mmc$, $P6/mmm$			04-004-9644 04-005-7688
YCuSi	N	–		$P6_3/mmc$, $P6/mmm$			04-004-9642 04-005-0196
ErCuSi	N	–		$P6_3/mmc$, $P6/mmm$			00-054-0545 04-005-0206
YbCuSi	N	–		$P6_3/mmc$			04-004-9640
LuCuSi	N	–		$P6_3/mmc$			04-004-9641
LaAgSi	Y	Bardyn O., Belan B.D., Bodak O.I., Protsyk O.S., and Shpyrka Z.M., THE SYSTEM La-Ag-Si, Visn. L'viv. Derzh. Univ., Ser. Khim., Vol. 40, 2001, p 57–60 (in Ukrainian)				–	–
CeAgSi	Y	Belan B.D., Bodak O.I., Gladyshevskii R.E., Soroka I., Kuzhel B.S., Protsyk O.S., and Stets' I.N., Interaction of the components in the systems Ce-Ag-Si at 500 °C and Eu-Ag-Si at 400 °C, J. Alloys Compd., Vol. 396, 2005, p 212-216		$P6/mmm$			04-011-7256
PrAgSi	Y	Dzioba M.M., Savysyuk I.A., Shcherban O.O., and Gladyshevskii E. I., Pseudobinary CeAg ₂ -CeSi ₂ , PrAg ₂ -PrSi ₂ and PrAg ₂ -PrGe ₂ systems, Visn. L'viv. Derzh. Univ., Ser. Khim., Vol. 36, 1996, p 59–65 (in Ukrainian)				–	–
NdAgSi	Y	Zaplatynsky O.V., Prots Y.M., Salamakha P.S., Muratova L.O., and Bodak O.I., The X-ray investigation of the ternary Nd-Ag-Si system, J. Alloys Compd., Vol. 232, 1996, p L1–L4		$P6/mmm$			04-005-0859
SmAgSi	N	–		$\bar{P}6_2m$			04-008-8624
EuAgSi	Y	Belan B.D., Bodak O.I., Gladyshevskii R.E., Soroka I., Kuzhel B.S., Protsyk O.S., and Stets' I.N., Interaction of the components in the systems Ce-Ag-Si at 500 °C and Eu-Ag-Si at 400 °C, J. Alloys Compd., Vol. 396, 2005, p 212–2				–	–
GdAgSi	N	–		$\bar{P}6_2m$			04-008-8625
DyAgSi	N	–		$\bar{P}6_2m$			04-008-8626
HoAgSi	N	–				–	–

YAgSi	N	–		$\bar{P}6_2m$		04-008-8630
ErAgSi	N	–		$\bar{P}6_2m$		00-052-0924
TmAgSi	N	–		$\bar{P}6_2m$		04-008-8628
YbAgSi	N	–		$\bar{P}6_2m$		04-008-8623
LuAgSi	N	–		$\bar{P}6_2m$		04-008-8629
NdAuSi	Y		Zaplatynsky O.V., INTERACTION BEHAVIOR OF ND AND AU WITH ELEMENTS OF GROUP IVA AT 600 °C, Visn. L'viv. Derzh. Univ., Ser. Khim., Vol. 39, 2000, p 87-91	$P6/mmm$		04-008-5584
YAuSi	N	–		$P6_3mc$		04-007-7388
YbAuSi	N	–			$Im2m$	04-012-1392
LuAuSi	N	–		$\bar{P}6_2m$		04-009-4558
ScCuSi	N	–		$\bar{P}6_2m$	$Pnma$	04-001-5686
ScAuSi	N	–		$\bar{P}6_2m$		04-009-4557
TaCoSi	N	–			$Pnma$	00-015-0720
TaRhSi	N	–			$Pnma$	04-010-5237
TaIrSi	N	–			$Pnma$	04-011-4999
TiNiSi	N	–			$Pnma$	01-078-3555
TiPdSi	N	–			$Pnma$	04-005-0830
TiPtSi	N	–			$Pnma$	01-078-8110
VCoSi	N	–			$Pnma$	01-078-3549
ZrNiSi	N	–			$Pnma$	04-001-5367
ZrPdSi	N	–			$Pnma$	04-001-4352
ZrPtSi	N	–			$Pnma$	01-078-8108
CaCuSb	N	–		$P6_3/mmc$		03-065-0448
CaAgSb	N	–			$Pnma$	04-003-7967
CaAuSb	N	–		$P6_3/mmc$		01-071-4046
HfCoSb	N	–		$F\bar{4}3m$		04-003-9107
HfRhSb	N	–		$F\bar{4}3m$		04-001-4052
MgCuSb	N	–		$F\bar{4}3m$		04-010-8291
LaNiSb	N	–			Tetragonal $I4_1md$	00-055-0423
CeNiSb	N	–		$P6_3/mmc, P6/mmm$		00-050-0980 01-077-3694
PrNiSb	Y		Chykhrij S.I., and Smetana V.B., Phase equilibria and crystal structures of the compounds in the Pr-Ni-Sb system at 870 K, J. Alloys Compd., Vol. 400, 2005, p 100–105	$P6_3/mmc, P6/mmm$		04-012-7806 04-007-6980
NdNiSb	N	–		$P6/mmm$		04-007-6978
SmNiSb	N	–		$P6/mmm$		04-007-6981
GdNiSb	N	–		$F\bar{4}3m$	$P6/mmm$	00-050-0967 04-007-6982
DyNiSb	N	–		$F\bar{4}3m$		00-026-1019
HoNiSb	N	–		$F\bar{4}3m$		00-047-1192
YNiSb	N	–		$F\bar{4}3m$		00-047-1194
ErNiSb	N	–		$F\bar{4}3m$		00-047-1193
TmNiSb	N	–		$F\bar{4}3m$		01-072-2612
YbNiSb	N	–		$F\bar{4}3m$		04-012-9279
LuNiSb	N	–		$F\bar{4}3m$		00-050-1186
LaPdSb	N	–		$P6_3mc, P6_3/mmc$		04-005-1122 04-003-9156

Continued

Table I. Continued

Compounds XYZ	Phase Diagram X-Y-Z ASM Database	Literature References	Cubic system, space group	Hexagonal system, space group	Orthorhombic system, space group	Other or unknown system, space group	ICDD Database, PDF#
CePdSb	N	–		$P6_3mc, P6_3/mmc$			04-005-1129 00-048-1757
PrPdSb	N	–		$P6_3mc, P6_3/mmc$			04-005-1124 00-048-1758
SmPdSb	N	–		$P6_3mc, P6_3/mmc$			04-005-1126 00-048-1760
EuPdSb	N	–			$Pnma$		04-005-1121
GdPdSb	N	–		$P6_3mc, P6_3/mmc$			04-005-1128 04-004-9162
DyPdSb	N	–	$F\bar{4}3m$	$P6_3mc, P6_3/mmc$			00-050-1304 01-079-3731 04-005-1123
HoPdSb	N	–	$F\bar{4}3m$				00-048-1763
YPdSb	N	–	$F\bar{4}3m$				04-003-9152
ErPdSb	N	–	$F\bar{4}3m$				00-048-1764
TmPdSb	N	–	$F\bar{4}3m$				04-005-1117
YbPdSb	N	–	$F\bar{4}3m$				04-003-9152
LaPtSb	N	–		$P6_3/mmc$			04-001-3885
CePtSb	N	–		$P6_3/mmc$			04-001-3884
PrPtSb	N	–		$P6_3mc$			01-079-4749
NdPtSb	N	–		$P6_3mc, P6_3/mmc$			04-009-4725 04-001-3883
SmPtSb	N	–	$F\bar{4}3m$				04-001-3893
EuPtSb	N	–			$Pnma$		04-005-3879
GdPtSb	N	–	$F\bar{4}3m$				01-073-8683
DyPtSb	N	–	$F\bar{4}3m$				04-012-9300
HoPtSb	N	–	$F\bar{4}3m$				04-012-9288
YPtSb	N	–	$F\bar{4}3m$				04-007-7613
ErPtSb	N	–	$F\bar{4}3m$				04-012-9287
TmPtSb	N	–	$F\bar{4}3m$				04-012-9286
YbPtSb	N	–	$F\bar{4}3m$				04-012-9285
LuPtSb	N	–	$F\bar{4}3m$				04-012-9284
ScNiSb	N	–	$F\bar{4}3m$				01-072-5849
ScPdSb	N	–	$F\bar{4}3m$				04-013-8399
ScPtSb	N	–	$F\bar{4}3m$				01-071-6562
TiCoSb	N	–	$F\bar{4}3m$				04-006-6287
TiRhSb	N	–	$F\bar{4}3m$				04-001-4050
ZrCoSb	N	–	$F\bar{4}3m$				00-054-0448
ZrRhSb	N	–	$F\bar{4}3m$				04-001-4051
CaCuBi	N	–		$P6_3/mmc$			03-065-0449
MgCuBi	N	–	$F\bar{4}3m$				04-001-5873
PrNiBi	N	–	$F\bar{4}3m$				04-010-4647
NdNiBi	N	–	$F\bar{4}3m$				04-010-4648
SmNiBi	N	–	$F\bar{4}3m$				04-010-4649
GdNiBi	N	–	$F\bar{4}3m$				01-072-5583

DyNiBi	N	–	$F\bar{4}3m$	00-054-0538
HoNiBi	Y	Mozharivskiy Y.A., Kuz'ma Y.B., and Sichevich O.M., Y-Ni-Bi and Ho-Ni-Bi Systems, Neorg. Mater., Vol. 34, 1998, p 851–854 (in Russian)	$F\bar{4}3m$	04-010-4651
YNiBi	Y	Mozharivskiy Y.A., Kuz'ma Y.B., and Sichevich O.M., Y-Ni-Bi and Ho-Ni-Bi Systems, Neorg. Mater., Vol. 34, 1998, p 851–854 (in Russian)	$F\bar{4}3m$	04-012-9294
ErNiBi	N	–	$F\bar{4}3m$	04-010-4652
TmNiBi	N	–	$F\bar{4}3m$	01-072-5623
LuNiBi	N	–	$F\bar{4}3m$	01-072-5600
LaPdBi	N	–	$F\bar{4}3m$	04-010-4661
CePdBi	N	–	$F\bar{4}3m$	01-076-8856
PrPdBi	N	–	$F\bar{4}3m$	04-010-4662
SmPdBi	N	–	$F\bar{4}3m$	04-010-4663
GdPdBi	N	–	$F\bar{4}3m$	04-015-0507
ErPdBi	N	–	$F\bar{4}3m$	04-010-4665
TmPdBi	N	–	$F\bar{4}3m$	04-010-4666
YbPdBi	N	–	$F\bar{4}3m$	00-049-1736
LuPdBi	N	–	$F\bar{4}3m$	04-010-4667
LaPtBi	N	–	$F\bar{4}3m$	00-055-0471
CePtBi	N	–	$F\bar{4}3m$	04-010-4655
GdPtBi	N	–	$F\bar{4}3m$	01-072-5584
DyPtBi	N	–	$F\bar{4}3m$	01-072-5578
HoPtBi	N	–	$F\bar{4}3m$	01-072-5586
YPtBi	N	–	$F\bar{4}3m$	04-010-4653
ErPtBi	N	–	$F\bar{4}3m$	01-072-5580
TmPtBi	N	–	$F\bar{4}3m$	04-010-4657
YbPtBi	N	–	$F\bar{4}3m$	04-010-4657
LuPtBi	N	–	$F\bar{4}3m$	04-010-4659
ScNiBi	N	–	$F\bar{4}3m$	01-072-5622
ScPdBi	N	–	$F\bar{4}3m$	04-010-4660
ZrCoBi	N	–	$F\bar{4}3m$	04-008-1437

determine the band structure and predicted TE properties. The dependence of Seebeck coefficient, electrical conductivity, and power factor on the Fermi level was also reported. The electronic structure results predicted the band gaps, and provided an invaluable guide for further experimental work.

B. Material selection rules

In this survey, we focus our attention on the half-Heusler compounds using the following selection rules: (1) for alkali-earth elements, only Mg and Ca are selected (so far half-Heusler compounds containing alkali-earth elements Sr and Ba have no band gap); (2) for group IVB elements Sn, Ge, and Si are used (as Pb is considered toxic and therefore has been avoided), and for VB elements, Sb and Bi were used; and (3) lanthanide elements were chosen except for Pm and Tb.

C. Results of the survey

Table I provides the results of the phase diagram and powder diffraction pattern survey. This table is divided into columns of the chemical formula XYZ; whether the ASM database provides the specific phase diagram (“Y” indicates “Yes” and “N” indicates “No”); a reference to the phase diagram cited in the ASM database if available; the structure type of the XYZ phases, whether they are “cubic,” “hexagonal,” “orthorhombic,” or other; the set number of the reference powder patterns in the PDF (xx-xxx-xxxx). If either the phase diagram or crystallographic information is missing in the PDF, the symbol “-” is used.

Based on our selection rules, we found a total of 306 compounds with the chemical formula XYZ. The structures of these XYZ compounds have been found to be of several different types. Apparently, not all XYZ phases form the half-Heusler type structure (fcc, cF12, $F\bar{4}3m$), some form hexagonal structures ($P6_3/mmc$, $P6/mmm$, $P6_3mc$, and $P\bar{6}2m$), and some form the orthorhombic $Pnam$ structure. The size factor of each element is of great importance in determining the structure of intermetallics. As a specific example, the structure of the members of the RNiSb family that contain lighter elements (with larger covalent radius; $R = \text{La, Ce, Pr, Nd, Sm, Gd, and Tb}$) is of the hexagonal ($p6/mmm$ or $P6_3/mmc$) type, whereas the heavier Dy, Ho, Er, and Y alloys are of the cubic ($F\bar{4}3m$) type (Marazza *et al.*, 1980). In some cases, for example, RAuSn, both the cubic and hexagonal structures of the same XYZ formula can be prepared under different conditions. In other cases, while the lighter hexagonal members in the RAuSn ($R = \text{lanthanides}$) compounds crystallize in the space group of $P6_3/mmc$, the heavier ones adopt the $P6_3mc$ space group. In silicides, coexistence of two structure types was also reported: the Fe₂P type structure with space group $P\bar{6}2m$ (Dwight *et al.*, 1973) and the orthorhombic $Pnam$ phase (Kotur and Gladyshevskij, 1981). Most orthorhombic phases identified in Table I are metallic.

Among the 306 compounds, a total of 67 compounds have no information regarding phase diagrams or crystallographic data. These compounds are listed below as Sn-, Ge-, Si-, Sb, and Bi-containing compounds:

- (1). NbIrSn, LaAuSn, TaCoSn, TaRhSn, TaIrSn, TiPdSn, VCoSn, VRhSn, VIrSn

- (2). PrAgGe, Nd-Ag-Ge, Sm-Ag-Ge, PrAuGe, SmAuGe, TmAuGe, ScAgGe, TaIrGe, TiPtGe, VRhGe, VIrGe
- (3). EuCuSi, HoAgSi, LaAuSi, CeAuSi, PrAuSi, SmAuSi, EuAuSi, GdAuSi, DyAuSi, HoAuSi, ErAuSi, TmAuSi, ScAgSi, VRhSi, VIrSi
- (4). HfIrSb, MgAgSb, MgAuSb, EuNiSb, LuPdSb, TiIrSb, ZrIrSb
- (5). CaAgBi, CaAuBi, HfCoBi, HfRhBi, HfIrBi, MgAgBi, MgAuBi, LaNiBi, CeNiBi, EuNiBi, YbNiBi, EuPdBi, DyPdBi, HoPdBi, YPdBi, PrPtBi, NdPtBi, SmPtBi, EuPtBi, ScPtBi, TiCoBi, TiRhBi, TiIrBi, ZrRhBi, ZrIrBi

III. CONCLUSION

We found that among 306 potential XYZ systems that we have surveyed, 234 have powder diffraction patterns in the PDF, 28 have phase diagram information, and 67 do not have any phase diagram or crystallographic information. Among the XYZ systems with powder patterns, 84 are reported with cubic $F\bar{4}3m$ half-Heusler structures, and the others are hexagonal, orthorhombic or unknown. Some XYZ compounds have both the cubic half-Heusler and hexagonal structures, and others have hexagonal structure with different space groups, or both hexagonal and orthorhombic structures.

Although not all XYZ phases that we have discussed belong to the half-Heusler cubic type phase, from the point of view of filling the gap in both the phase diagram and powder diffraction databases, it is also important to fill the missing hexagonal and orthorhombic phases as well. In addition, a majority of the half-Heusler phases still need to have property data. It is hoped that this survey activity will provide a useful starting point for the TE and materials research community, phase diagram community, ICDD task group members and grants-in-aid recipients to provide missing phase diagrams, reference X-ray powder diffraction patterns, and property data to improve the coverage of the phase diagram databases and the PDF. Success of these database activities will lead to efficient and productive materials research and development.

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