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CRYSTAL STRUCTURE OF R. E. NiSn AND R. E. PdSn EQUIATOMIC COMPOUNDS*

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MASTER

Crystal Structure of R.E. NiSn and R.E. PdSn Equiatomic Compounds

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During an investigation of the Dy-Ni-Sn system a ternary compound DyNiSn was found and identified as the TiNiSi-type. Isotypic compounds were found in other R.E. NiSn and R.E. PdSn alloys.

The alloys were made by arc melting as described in Ref. 1 and annealed to 800° C. Debye-Scherrer X-ray films were taken with filtered Co radiation. Unit cell constants were calculated from three high angle reflections, and indexing was verified with the aid of calculated intensities. The cell constants and volume per formula weight (V/M) are given in Table I.

Table I. Unit Cell Constants.

Compound	a(Å)	b(Å)	c(Å)	V/M(Å)^3
LaNiSn	7.636	4.661	7.552	67.2
PrNiSn	7.440	4.56	7.706	65.4
NdNiSn	7.395	4.541	7.69	64.6
SmNiSn	7.304	4.509	7.68	63.2
GdNiSn	7.199	4.464	7.677	61.68
TbNiSn	7.146	4.448	7.661	60.87
DyNiSn	7.112	4.439	7.656	60.42
HoNiSn	7.063	4.438	7.64	59.84
ErNiSn	7.016	4.425	7.629	59.22
TmNiSn	7.000	4.414	7.621	58.87
YbNiSn	6.983	4.426	7.616	58.851
LuNiSn	6.93	4.401	7.601	57.96
YNiSn	7.115	4.449	7.665	60.66
NdPdSn	7.424	4.665	7.951	68.85
SmPdSn	7.323	4.639	7.929	67.33
GdPdSn	7.254	4.618	7.912	66.2
TbPdSn	7.182	4.598	7.916	65.3
DyPdSn	7.157	4.589	7.897	64.8
HoPdSn	7.117	4.581	7.884	64.5

HoPdSn also occurs[2] with the Fe_2P-type structure, as do (Er, Tm, Lu, Sc) PdSn compounds.

The unit cell constants are plotted against ionic radii of the rare earths, in Fig. 1. Several trends are noted:

1. The a_o constant rises with increasing ionic radius[3] more steeply than do the b_o and c_o constants. This derives from the fact that in the a_o direction the rare earth atoms form zig zag chains, with relatively short interatomic distances. Substitution of a larger rare earth (e.g., Nd for Gd) causes enlargement of the unit cell, but mostly along the rare earth chain.

2. Substitution of Pd for Ni causes a large increase in the b_o and c_o constants, and only a slight increase in the a_o. The shortest Ni-Sn and Pd-Sn interatomic distances are parallel to the b_o and c_o directions, and are dominated by the size of the Ni or Pd atom.

3. The c_o of the R.E. NiSn series reaches a maximum value for PrNiSn, then declines in LaNiSn. This is accompanied by an abnormal increase in b_o for LaNiSn, which is the distance between layers. This indicates that the pentagon which surrounds each R.E. atom has become stretched to its limit, and further increase in volume of the unit cell can only be accommodated by an increased separation of layers.

A portion of this work was performed at Argonne National Laboratory under auspices of the U.S. Department of Energy.

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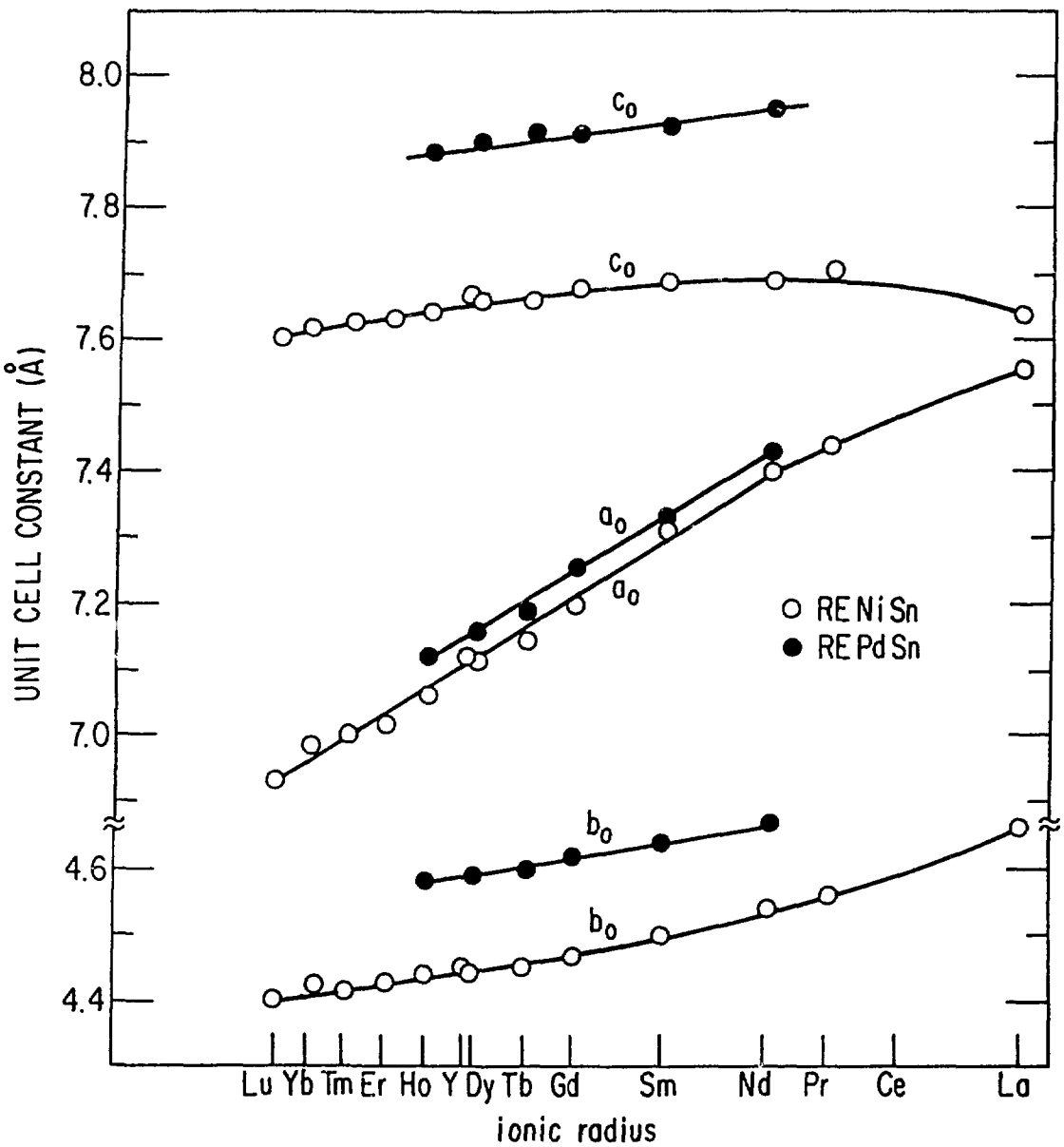

Fig. 1. Unit cell constants vs ionic radii for R.E. Ni(Pd)Sn compounds.