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Crystal structures of MgRh and ScRh. By VERA B. COMPTON, *Bell Telephone Laboratories, Incorporated, Murray Hill, New Jersey, U.S.A.*

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The compounds MgRh and ScRh were prepared and investigated for possible superconductivity by Matthias & Corenzwit (1957). Neither of the alloys is superconducting.

The alloys were prepared by heating the elements in stoichiometric proportion; for MgRh the reaction was carried out in a fused quartz tube at 1000 °C. and for ScRh in a helium arc furnace. X-ray diffraction powder photographs were taken of the resulting product, using a Norelco camera of 114.6 mm. diameter and Cu *K* radiation. The patterns were indexed on the basis of a primitive cubic cell with lattice constants given in Table 1.

Table 1. *Structural data*

Compound	a_0 (Å)	Interatomic distance $A-B$ (Å)	
		Exp.	Calc.
MgRh	3.099 ± 0.002	2.68	2.88
ScRh	3.206 ± 0.001	2.78	2.88

Relative intensities were computed for each of these compounds on the basis of a CsCl-type structure, suggested by the comparatively stronger intensities for planes with $h+k+l = 2n$. The formula used in this calculation is

$$I \propto p |F_{hkl}|^2 \frac{1 + \cos^2 2\theta}{\sin^2 \theta \cos \theta} \times 10^{-5},$$

where p is the multiplicity factor, $F(hkl)$ is the structure amplitude, and the remaining term is twice the combined Lorentz and polarization factors. The scattering factors

Table 2. *Comparison of calculated with observed intensities**

hkl	MgRh		ScRh	
	I_o	I_c	I_o	I_c
100	<i>vs</i>	144	<i>m</i>	82
110	<i>vs</i> †	292	<i>vs</i>	410
111	<i>m</i>	38	<i>w</i>	25
200	<i>m-s</i>	47	<i>m</i>	68
210	<i>m-s</i>	50	<i>w-m</i>	33
211	<i>vs</i>	93	<i>s</i>	135
220	<i>m</i>	30	<i>m</i>	44
300, 221	<i>m</i>	29	<i>w-m</i>	18
310	<i>m-s</i>	51	<i>m-s</i>	71
311	<i>w-m</i>	23	<i>w</i>	13
222	<i>w</i>	18	<i>w-m</i>	23
320	<i>w-m</i>	27	<i>w</i>	14
321	<i>vs</i>	136	<i>vs</i>	161
400	<i>w</i>	58	<i>w-m</i>	31
410, 322	$\theta > 90^\circ$		<i>m</i>	98

† Rh line coincident.

* Observed intensities for the two alloys are not comparable with each other because of differences in exposure.

for Mg and Sc were obtained from compilations in the *International Tables* (1935) and for Rh from the compilation by Thomas & Umeda (1957). Dispersion corrections from Dauben & Templeton (1955) were applied. The results are summarized in Table 2, together with the visually estimated intensities.

The good agreement between calculated and observed intensities confirmed a CsCl-type structure for both compounds. The observed intensity for the {400} reflection in the MgRh compound is considerably lower than the calculated value. This is probably the result of inaccurate estimation due to the considerable width of the line.

The MgRh compound contained excess rhodium and the ScRh contained Sc_2O_3 . The lines for each of these impurities were weak.

The CsCl structure, Type B2 (*Strukturbericht*, 1931), contains one formula weight in the unit cell and belongs to space group $O_h^1-Pm\bar{3}m$ with one atom in the position (a) 0, 0, 0; and the other atom in (b) $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$. Each atom is at the center of a cube of atoms of a different sort and therefore has a coordination number of eight.

The nearest-neighbor observed and calculated interatomic distances are given in Table 1. The observed values are determined from the relationship $d_{A-B} = \frac{1}{2}a_0/\sqrt{3}$ and the calculated values are the sum of the C.N. 8 radii of the elements. There is a 6.9% contraction for Mg-Rh and a 3.5% contraction for Sc-Rh. A similar contraction of 4.4% is calculated from experimental data for Al-Rh, which was found by Schubert (1957) to have a CsCl-type structure with $a_0 = 2.99$ Å. However, it is not possible to determine from these data which of the components in the alloys has changed its size. Laves (1956) discussed the variability of atomic size in CsCl-type compounds.

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