ESRF	**Experiment title:** A Study of the Ferromagnetic Superconductor $Ru_{1-x}Sn_xSr_2GdCu_2O_8$ using X-ray diffraction. (x=0, 0.05, 0.075)	**Experiment number**: HE-692
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Report:

Diffraction experiments were carried out on three samples of nominal composition $Ru_{1-x}Sn_xSr_2GdCu_2O_8$ (x = 0, 0.05, 0.075) at ambient temperature and ambient pressure. Samples were contained in 0.5 mm borosilicate capillaries and a wavelength of 0.32514 Å was used. An excellent Rietveld refinement fit was obtained with a tetragonal *P4/mmm* symmetry structural model for all samples as in the previous X-ray Synchrotron study of the ferromagnetic superconductor $RuSr_2GdCu_2O_8$ [1] (T_c (R=0) = 30 K, T_M = 132 K). Disorder of the oxygen atoms within the RuO_2 planes and of the apical oxygen atoms linking the CuO_5 units and RuO_6 octahedra was evidenced by large U values. This was modelled by using a single isotropic U- factor for all the oxygen atoms and splitting the sites (Table. 1)

Table 1.Refined atomic parameters for $Ru_{1-x}Sn_xSr_2GdCu_2O_8$.

Atom	**Site**	**Occu-pancy**		***x* = 0.0**	***x* = 0.05**	***x* = 0.075**
Ru/Sn	1(b)	1.00	U_{iso} (Å^2)	0.0037(2)	0.0039(2)	0.0046(2)

[1] A. C. Mclaughlin, W. Zhou, J. P. Attfield, A. N. Fitch and J. L. Tallon, *Phys Rev B*, **60**, 7512 (1999)

Sr	2(h)	1.00	*z*	0.30926(6)	0.30873(7)	0.30877(8)
			U_{iso} (Å^2)	0.0084(1)	0.0079(2)	0.0086(2)
Gd	1(c)	1.00	U_{iso} (Å^2)	0.0046(1)	0.0045(1)	0.0046(2)
Cu	2(g)	1.00	*z*	0.14611(9)	0.14607(9)	0.1458(1)
			U_{iso} (Å^2)	0.0052(2)	0.0051(2)	0.0053(2)
O(1)	8(s)	0.25	*x*	0.049(3)	0.054(3)	0.042(5)
			z	0.3332(4)	0.3340(4)	0.3331(5)
			U_{iso} (Å^2)	0.0127(7)	0.0120(7)	0.0155(9)
O(2)	4(i)	1.00	*z*	0.1304(3)	0.1308(3)	0.1304(3)
			U_{iso} (Å^2)	0.0127(7)	0.0120(7)	0.0155(9)
O(3)	4(o)	0.50	*x*	0.113(2)	0.116(2)	0.120(2)
			U_{iso} (Å^2)	0.0127(7)	0.0120(7)	0.0155(9)

The T_c (onset) increases with Sn doping from T = 39 K in the undoped sample to T = 51 K in the 7.5% Sn sample, whereas the Curie temperature T_M decreases from 132 K in the undoped sample to 105 K in the 7.5 % sample. The mismatch between lengths of the in-plane Ru-O and Cu-O bonds results in the rotations of the RuO_6 octahedra around c by 12.7º. A slight tilting of the polyhedra which reduces the Cu-O-Ru angle to 173º is also observed. The substitution of the larger Sn^{4+} atom for Ru^{5+} results in the increase of the bond mismatch between the in-plane Ru-O and Cu-O bonds. This is observed by an increase in the average Ru-O(3) bond and an increase in the rotations around c from 12.7º in the undoped sample to 13.6º in the 7.5 % Sn sample. (Table 2).

Table 2. Refined cell parameters, agreement factors, interatomic distances and angles in $Ru_{1-x}Sn_xSr_2GdCu_2O_8$.

	***x*=0**	***x*=0.05**	***x*=0.075**
***a* (Å)**	3.83955(1)	3.84157(1)	3.84162(1)
***c* (Å)**	11.57239(7)	11.58011(8)	11.58258(7)
V (Å^3)	170.602(1)	170.895(1)	170.936(1)
Ru-O(3) (Å)	1.968(1)	1.972(2)	1.976(2)
Sr-O(3) (Å)	3.226(5)	3.242(5)	3.254(6)
Sr-O(3) (Å)	2.661(4)	2.660(4)	2.652(4)
Ru-O(3)-Ru (º)	154.6(4)	153.8(4)	152.9(5)
R_{wp} (%)	8.9	9.01	10.53
R_p (%)	6.43	6.53	7.73
χ^2	1.98	1.88	1.41