The International Conference on Solid Compounds of Transition Elements

SCTE 2021

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Wrocław, Poland

organized by

Institute of Low Temperature
and Structure Research,
Polish Academy of Sciences,
Wrocław, Poland

Programme and abstracts

Scope

The SCTE Conference, organized biannually, is traditionally aimed to provide a platform to discuss recent discoveries and progress in research on **solid compounds containing d- and f-electron elements - in the field of solid state chemistry, physics and materials science**. It is also a unique opportunity to exchange ideas with other scientists in informal atmosphere and to start new collaboration.

The conference will address the latest progress in these fields in plenary talks to be given by experts for all the participants as well as invited lectures and oral contributions during parallel sessions for specialists in particular fields, and in poster presentations.

Due to the COVID-19 outbreak all the events of SCTE 2021 have exclusively a form of **on-line meetings**.

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- Magdalena Majewicz
- Orest Pavlosiuk
- Lan Maria Tran

LIST OF POSTER PRESENTATIONS

Poster session 1

1. E. Anikina
   "Study of hydrogen interaction with Ho_2Fe_{17} via Calvet-calorimetry method"

2. A. Broda
   "A Ternary Phase with the $Zr_2Nb_3Ge_4$ Structure Type in the Hf–V–Ge System"

3. M. Gamża
   "Antiferromagnetism in trigonal $CaMn_2P_2$"

4. V. Hreb
   "Phase separation in $Bi_{1-x}Ho_xVO_4$ system"

5. L. Kalandadze
   "Validity of effective medium theory in ferrofluids and nano iron films"

6. D. Kowalska
   "Band engineering of the narrow band gap LaN"

7. S. Królak
   "Physical property measurement and synthesis of ferromagnetic compound Pr_7Ru_3"

8. K. Łątka
   "Heat capacity studies of $EuAg_{5-x}Ga_x$ (x = 0.5 and 1)"

9. R. Martyniak
   "Element Substitution Effects on the Structure and Magnetic Properties of $(Cr,Ni)_{4-x}T_xSi$ Phases"

10. P. Mohanty
    "Effect of Site Mixing in $CoCr_2O_4$ Nanoparticles and Epitaxial Thin Films"

11. E. Murashova
    "Novel $RE_{10}RuAl_3$ Intermetallic Compounds with Heavy Rare Earth Metals"

12. U. Nwankwo
"Observing the Effects of P-Type-Metal-Doping of the Compact-TiO_2 Electron Transporting Layer on the Performance of Perovskite Solar Cells"

13. A. Pavlenko
"Phase equilibria in the Ag–Pd–Sn ternary at 500°C"

14. N. Pavlyuk
"Crystal structure of the novel MgT_6Ga_6 (T=Ni, Pd) ternary compounds"

15. M. Roman
"Crossover from charge density wave stabilized antiferromagnetism to superconductivity in $Nd_{1-x}La_xNiC_2$ series"

16. M. Samsel-Czekała
"The dual nature of the U 5f electrons in caged UTE_2Al_{10} systems with TE = Fe, Ru, and Os, exhibiting anomalous rattling"

17. D. Sedelnikov
"Intermetallic Compounds $RE_{26}(Ru_xIn_{1-x})_{17}$ (RE - Pr, Nd, Sm, Gd-Tm, Lu)

18. I. Stetskiv
"Electrochemical hydrogenation of $Tb_2Co_{16.5}Sb_{0.2}Li_{0.3}$"

19. M. Tihtih
"Study of the $BaTiO_3$ Electronic Structure Using Density Functional Theory Calculations"

20. A. Tursina
"Ternary Aluminides $Ce_{0.67}Pd_2Al_5$, $Ce_{1.33}Pd_3Al_8$, and $Ce_{1.74}Pd_{5.29}Al_{11.71}$"

21. M. Winiarski
"Electronic structure of $Tl_xLa_{1-x}N$ materials"

22. N. Zaremba
"New quaternary germanide $Ca_{0.265}Yb_{0.735}Ni_3Ge_2$"

23. A. Zarzecka
"Tuning the CePdIn magnetism by p-electrons and hydrogen"

Poster session 2

1. E. Aoun
   "The effect of calcination temperature on the photocatalytic performance of $SrNiO_{3-\delta}$ nanoparticuls for the degradation of Rose Bengal under UV irradiation"

2. N. Dominyuk
   "Crystal structure of $LaRh_{0.65}Ge_{0.35}In$, $CeRh_{0.71}Ge_{0.29}In$ and $SmRh_{0.67}Ge_{0.33}In$ compounds"

3. K. Górnicka
   "Characterization of the Laves-phase superconductors ROs_2 (R = Sc, Y, Lu)"

4. J. Rahman
   "Synthesis and crystal structure of Sb-based high entropy alloys"

5. R. Kara
   "On Electrochemical synthesis and characterization of p-type cuprous oxide thin films: Effects of Na aluminate solutions"

6. H. Krarcha
   "Theoretical study of structural, elastic, mechanical, thermic and vibrational properties of new transition metal iodide perovskites: Cs_2MI_6 (M=Zr, Ti, Hf &Pt)"

7. A. Kuchin
   "Cr or V - doped GdFeSi compound"

8. L. Litzbarski
   "Magnetic behavior of disordered ternary AlB_2-type intermetallics RE_2TGe_3"

9. D. Moço
   "Development of new thermoelectric materials – Tetrahedrite co-doped with Nickel and Selenium"

10. Y. Morozova
    "The phase equilibria of the Ce-Pt-Al system"

11. S. Nesterenko
    "Two polymorphs of Ce_2Rh_2Ga"

12. I. Oshchapovskyy
"Complementing diffraction data by first-principle calculations: hydrogen sublattice in Mg_2NiH_x (x=0.3) hydride"

13. V. Pavlova
"New intermetallic $SmRu_{0.26(1)}Sn_2$"

14. S. Pukas
"New Representatives of the Structure Type $Y_3NiAl_3Ge_2$"

15. P. Ruszała
"Tilted Dirac cone gapped due to spin-orbit coupling and transport properties of a 3D metallic system $CaIr_2Ge_2$"

16. M. Sahakyan
"Density Functional Theory study of electronic structure and magnetic properties of $CePd_2P_2$"

17. V. Shilov
"Electronic structure and magnetic properties of Heusler alloy $Mn_{1.5}Fe_{1.5}Al$"

18. H. Świątek
"Crystal structure and physical properties of $Mg_{2-x}In_xNi$ solid solution"

19. L. M. Tran
"Synthesis of single crystal $GdFe_{1-x}Co_xAs$"

20. J. Veretennikova
"Influence of irregularities on internal fields in multilayer granular systems"

21. N. Zapp
"YHO and HoHO – a Structural Exception in Rare Earth Chemistry"

22. O. Zaremba
"Four-Component Perovskite Phases in Ca–R–Fe–O Systems, where R = Rare-Earth Metal"

23. L. Zinko
"Crystal Structure of the $Hf_5Re_{1.36}Al_{2.64}$ Compound"

Wednesday Poster 2-13

New intermetallic $SmRu_{0.26(1)}Sn_2$

Vera Pavlova[1], Alexander Gribanov[1], Elena Murashova[1]

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In the process of studying the ternary system Sm-Ru-Sn, the sample of composition 30:10:60 was synthesized by high-temperature liquid-phase synthesis followed by annealing at 620 °C. Crystals suitable for carrying out X-ray diffraction analysis were found on the surface of the sample. Further studies of the alloy were carried out by the methods of local X-ray spectral and X-ray phase analysis. According to the results of X-ray diffraction analysis, the intermetallic $SmRu_{0.26(1)}Sn_2$ crystallizes in a orthorhombic structure (space group C*mcm*) with unit cell parameters a = 4.5398 (7) Å, b = 16.5651 (3) Å, c = 4.40448 (7) Å.

Local X-ray spectral analysis showed the composition of the main phase was $Sm_{30.8}Ru_{7.7}Sn_{61.5}$ and insignificant presence of the second phase of composition $Sm_{17.0}Ru_{66.0}Sn_{17.0}$.

The reliability of the obtained crystal model of $SmRu_{0.26(1)}Sn_2$ was confirmed by experiments on powder diffraction of synchrotron radiation.

The sample was used to obtain a diffraction pattern at the ID22 international synchrotron radiation station (ESFR, Grenoble, France).

The resulting intensities were processed using the MRIA program. Using the Rietveld method, it was confirmed that the crystalline model of the $SmRu_{0.26(1)}Sn_2$ compound belongs to the family derived from the structural type $CeNi_{1-x}Si_2$ [1] and has the same structure with $CePd_{0.427}Sn_2$ intermetallic, the obtained values of R_p = 0.038, R_{wp} = 0.050, χ^2 = 2.07 indicate the correctness of the structural model.

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[1] I. Bodak and E. I. Gladyshevskii, *Soy. Phys. Crystallogr.,* **14** 859 (1970).
[2] A. Tursina, S. Nesterenko, D. Gnida, A. Pikul, D. Kaczorowski, *J.Alloy Compd.,* **667** 282-286 (2016).