

MS26-O5**Electronic properties of incommensurately modulated novel and complex materials**

Edoardo Martino¹, Alla Arakcheeva¹, Gabriel Autès², Sergiy Katrych¹, Oleg V. Yazyev², Philip J. W. Moll³, Ana Akrap⁴, László Forró¹

1. Laboratory of Physics of Complex Matter, École Polytechnique Fédérale de Lausanne EPFL, Lausanne, Switzerland
2. National Centre for Computational Design and Discovery of Novel Materials MARVEL, École Polytechnique Fédérale de Lausanne (EPFL), Lausanne, Switzerland
3. Max-Planck-Institute for Chemical Physics of Solids, Dresden, Germany
4. Light Fermion Spectroscopy group, University of Fribourg, Fribourg, Switzerland

email: edoardo.martino@epfl.ch

Potential periodicity in crystalline materials define their band structure and ultimately their electronic properties. An open question is how electronic properties are altered when two incommensurate potentials coexists. In our research we aim at understanding the structure-properties relation for metals with incommensurately modulated structure.

In our recent work we investigated the new compound $\text{Sr}_2\text{Pt}_{8-x}\text{As}$, synthesised at high pressure and high temperature. The Pt vacancies ($x=0.215$) located only on one specific site, are long range ordered and incommensurately modulated. We attribute to the structural modulation the saturation of electrical resistivity, with a peculiar temperature variation of less than 5% from room temperature to 4.2 K. The mechanism of resistivity saturation was described by Belitz and Schirmacher, [1] as quantum interference of conduction electrons by a high density of scattering centers, and identified as universal behaviour in “disordered” metals by Mooij [2].

Our goal is to bridge the structural studies and properties investigation, to clarify the commonly undefined term of “disorder” and understand the role of incommensurated structural modulation.

I will also outline our following research on layered transition metal dichalcogenides, a group of well studied materials, where local lattice distortion due to formation of charge density wave results in modulated structures.

References:

-
- [1] Belitz, D. & Schirmacher, W. (1983). *J. of Phys. C: Sol. State Phys.* 16, 913-926.
 [2] Mooij, J.H. (1973). *Phys. Status Solidi (A)*, 17, 521-530.
-

Keywords: structure-properties, incommensurately modulated structure, Mooij correlation

MS27 Quasicrystals: theory and experiment

Chairs: Prof. Marc de Boissieu, Prof. Janusz Wolny

MS27-O1**Clusters in the $\text{Al}_{13}\text{TM}_4$ quasicrystalline approximants : role on the surface structures and properties**

Émilie Gaudry¹

1. Univ. Lorraine CNRS IJL, Nancy, France)

email: Emilie.Gaudry@univ-lorraine.fr

A wide range of intermetallic crystal structures are based on polyhedral entities, often called “clusters”, as first introduced by F.A. Cotton in the early 1960’s to describe compounds containing metal-metal bonds. This approach is also largely used to describe more complex intermetallic phases, like quasicrystals and their approximants. Termed four-layer decagonal approximants, the structures of the $\text{Al}_{13}\text{TM}_4$ compounds (TM = transition metal, like Co, Fe, Ru for the experimentally grown compounds) have been initially understood as a periodic stacking of pseudo-10-fold symmetric atomic layers, but are also described a three-dimensional stacking of 26-atom clusters.

While the bulk atomic arrangements of the $\text{Al}_{13}\text{TM}_4$ compounds are very similar, the structures of their pseudo-10fold surfaces differ. The cluster substructure is preserved up to the $\text{Al}_{13}\text{Fe}_4(010)$ surface, but $\text{Al}_{13}\text{Co}_4(100)$ presents an Al-rich dense termination. The situation is even more complex for $\text{Al}_{13}\text{Ru}_4(010)$, since a surface reconstruction is observed experimentally [1]. Such structural differences lead to contrasted surface properties, for example in catalysis [2].

A systematic determination of the bulk electronic structure and chemical bonding network in the $\text{Al}_{13}\text{TM}_4$ series, including hypothetical compounds (TM= Mn, Fe, Co, Ni, Ru, Rh, Os, Ir) is an essential step in the scope of understanding the stabilities of the structures for TM = Fe, Co, Ru, as well as the surface structures and properties. This is achieved here with a theoretical approach based on the Density Functional Theory (plane-wave implementation). The projected Crystal Orbital Hamilton Population (pCOHP) has been used to analyze the chemical bonding network [3]. This method re-extract Hamilton-weighted populations from plane-wave electronic structure calculations to develop a tool analogous to the crystal orbital Hamilton population method. The bonding strengths result from the pCOHP integration to the Fermi level. While variations are noticeable within the $\text{Al}_{13}\text{TM}_4$ series, as will be discussed in the talk, the general picture leads to a decrease of the bonding strength with the bonding distance.

These insights into the chemical bonding network of the $\text{Al}_{13}\text{TM}_4$ compounds are very useful for the understanding of their diverse surface structures and properties. It also enable the discussion of chemical-composition / crystal-structure / (surface) properties relationships.