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PhD projet (2020-2023)

New lamellar phases Cu/In/Ga/S for photoinduced applications

Host laboratory : Institut des Matériaux Jean Rouxel, Nantes, France (IMN) https://www.cnrs-imn.fr

Keywords

2D inorganic materials, fundamental research, chemical crystallography electron crystallography, thin films, PV devices, photocatalysis.

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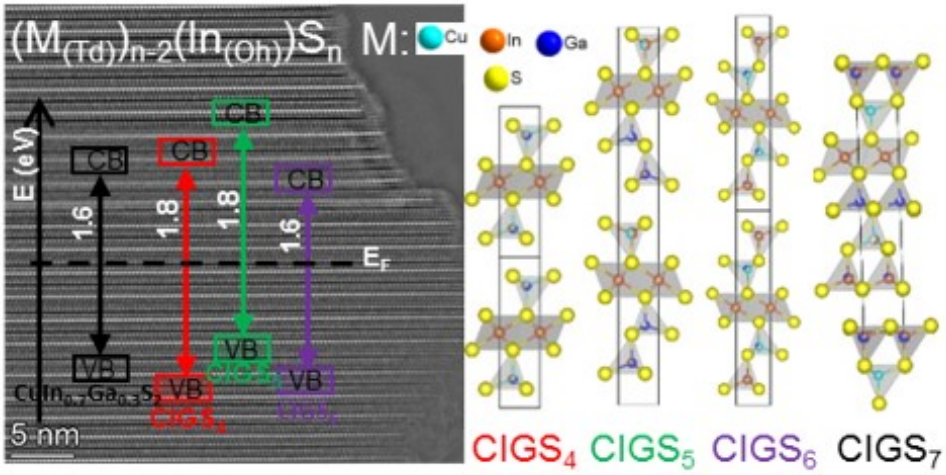
Description

Recently, we have identified new lamellar phases $(M\ (Td))_{n-2}\ (In\ (Oh))\ S_n$ (M = Cu, In, Ga) (named $CIGS_n$ [1]) in the pseudo-ternary system Cu_2S-In_2S_3-Ga_2S_3. These materials, with cations in sulfur tetrahedral (Td) and octahedral (Oh) environments (see figure below), have a strong 2D character with a van der Waals gap (~3.75 Å). The optical gap values of these new compounds of structural types $CIGS_4$, $CIGS_5$ and $CIGS_6$ are comparable to those of chalcopyrite $Cu(In_{0.7}Ga_{0.3})S_2$, currently studied as potential absorber in a tandem solar cell [2]. These materials can therefore have interesting physical characteristics, which can be modulated through their compositions for possible photovoltaic applications. In addition, their 2D character must allow layer deposition parallel or perpendicular to the substrates of the PV devices.

The aim of this PhD is to deepen the study of these new compounds as well as to identify their potential for photoinduced applications (e.g. photovoltaic, photocatalysis). First, we will continue to characterize the optoelectronic properties of the $CIGS_4$, $CIGS_5$ and $CIGS_6$ phases. At the same time, an exploratory research will be driven in order to identify new lamellar phases already detected by PEDT (precession electron diffraction tomography), a technique which has proven to be particularly suited to the complexity of this system. Secondly, several cationic and / or anionic substitutions could be envisioned in order to tune the optoelectronic properties of the compounds.

In a bottom-up approach (material to device), our objective will also concern the deposition of $CIGS_n$ compounds, for the first time as thin layers which will most likely exhibit great anisotropy in their physical properties. Indeed, the crystalline orientation of the layers relative to the plane of the substrate will have a noticeable influence on the properties of thin layers and on PV device performances [3].

The bulk samples will be prepared by ceramic route, but other synthesis methods (mechanosynthesis, microwaves, solvothermal) will also be used to adapt the microstructure of the powders to the targeted application. The thin films will be synthesized by coevaporation from elementary sources. The chemical crystallography study of these compounds will be carried out at the IMN, using conventional and advanced characterization tools: DRX, SEM, RAMAN, PEDT, HAADF-STEM imaging. The optoelectronic and photoinduced properties will be determined in our laboratory (diffuse reflectance, XPS, UV-V photoluminescence, transport measurements) as well as through national collaborations (flat band potentials, IR photoluminescence, photocatalytic activity). The devices will be characterized using I (V, T) measurements, quantum efficiency.



Requested skills

The candidate must have a well-trained in solid state science. He (she) must be motivated by the synthesis, materials shaping and their characterization. A spirit of initiative and rigor are needed, as well as a certain taste for teamwork. Facilities for oral and written expression as well as good interpersonal skills will would be an asset.

Financial Support

Grant of the « Ministère de l'Enseignement Supérieur et de la Recherche »
Net salary: around 1400 € / month

References

[1] M.T. Caldes, C. Guillot-Deudon, A. Thomere, M. Penicaud, Eric Gautron, P. Boullay, M. Bujoli-Doeuff Nicolas Barreau, S.Jobic, A.Lafond "New layered quaternary compounds in the Cu2S-In2S3-Ga2S3 system" (Inorg Chem 2020, accepted)

[2] Thèse Angelica Thomere, Univesité de Nantes, soutenue le 28 janvier 2020

[3] N Barreau and J C Bernède, MoS2 textured films grown on glass substrates through sodium sulfide based compounds, *J. Phys. D: Appl. Phys.* **35** 1197 (2002)