Chemical bonding networks and their role on the structure of complex metallic alloy surfaces

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Complex Metallic Alloys (CMAs), intermetallic compounds made of at least two elements, have a crystalline structure that differs from usual alloys by the number of atoms in their unit cell and the occurrence of highly symmetric clusters as alternative structural unit [1]. Recently, quantum chemical calculations performed on several types of Al-TM (TM=Cu, Co, Fe…) CMAs have highlighted the existence of specific covalent interactions within the bulk [2,3]. In the case of the $Al_{13}TM_4$ systems, this has led to a better understanding of their physical properties and to a description of their structure as 3-D cage compounds [3]. While well identified in the bulk materials, questions arise on how these chemical bonding networks will affect the atomic structure of CMA surfaces.

Here, we will present recent structural investigations of complex Al-TM surfaces using both experimental and *ab initio* computational methods [4,5]. It will be demonstrated that the surface terminations can be associated to planes present in the bulk crystal structure. For several phases, these planes remain incomplete when exposed at the surface. We will show how this reduced atomic density can be related to the presence of chemical bonding network in the materials.

Finally, among the systems studied, some of them have been recently considered as promising candidates for the heterogeneous hydrogenation catalysis [6]. We will discuss how their atypical surface structure and associated atomic ensembles could explain the catalytic properties reported in line with the site-isolation concept [7].

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Fields of Research

Surface, complex metallic alloys, thin films, quasicrystal

Publications

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