Chemical bonding networks and their role on the structure of $Al_{13}TM_4$ (TM= Fe, Ru) surfaces

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Recently, quantum chemical calculations performed on several types of Al-TM (TM=Cu, Co, Fe…) complex metallic alloys have highlighted the existence of specific covalent interactions within the bulk [1,2]. 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 [2]. While well identified in the bulk materials, question arises on how these chemical bonding networks will affect the atomic structure of CMA surfaces.

To this end, several $Al_{13}TM_4$ surfaces have been thoroughly characterised and will be presented here [3-5]. It will be shown that the $Al_{13}Fe_4$(010) surface consists of an incomplete puckered layer where only intact clusters have been preserved. For the $Al_{13}Co_4$(100) system, the terminating layer is also associated to a puckered plane but dissected clusters remain at the surface. The difference between both samples is explained by Al-TM bonding strength difference. Contrary to previous studies [3-5], a dislocation network is visible within the topmost $Al_{13}Ru_4$(010) surface layer. The dislocations run across terraces and appear as 'ditch'. They have been observed for annealing temperature ranging from 873 K to 1130 K. Within the 'ditch', bipentagonal motifs have been identified and resembles those observed on the $Al_{13}Fe_4$(010) surface, i.e. the topmost surface layer is once more related to a puckered plane present within the $Al_{13}Ru_4$ bulk structure.

Finally, among the systems studied, some of them have been recently considered as promising candidate for the heterogeneous hydrogenation catalysis [6]. We will discuss how their atypical surface structure could explain the catalytic properties reported in line with the site-isolation concept [7]. We will also show how surface defects can be used to influence the growth mode of fullerene molecules.

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