Crystallography vs. human masterpiece: $Li_{20}Mg_6Cu_{13}Al_{42}$, $Mg_9Ni_6Ga_{14}$ and Mg_3Ni_2Ga structures vs. ivory puzzle balls

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Beauty of our world we can see everywhere, but always two points of view are among scientists and artists, who is better: nature or human in the process of creativity. In our work we present three-shell clusters in intermetallic compounds and compare it with ivory puzzle balls. The crystal structures of all these intermetallic compounds were studied by single crystal method and confirmed by X-ray powder diffraction. $Li_{20}Mg_6Cu_{13}Al_{42}$ [1] (sp. gr. *Im*-3, a = 13.8451(2) Å) crystallizes as an ordered version of $Mg_{32}(Al,Zn)_{49}$, $Mg_9Ni_6Ga_{14}$ (sp. gr. *Fd*-3*m*, a = 19.8621(1) Å) and Mg_3Ni_2Ga (sp. gr. *Fd*-3*m*, a = 11.4886(17) Å) crystalizes in the own structure types. All these structures can be described as three-shell clusters: $[CuAl_{12}@Li_{20}Cu_{12}@Al_{60}]$ (fig. 1a) for the $Li_{20}Mg_6Cu_{13}Al_{42}$, $[Ni_6Ga_6@Mg_{20}@Ni_{18}Ga_{42}]$ (fig. 1b) for the $Mg_9Ni_6Ga_{14}$ and $[Mg_6@Ni_{12}Ga_6@Mg_{36}]$ (fig. 1c) for the Mg_3Ni_2Ga. Very easy to see, that the kind of packing of core shells for all these clusters is very similar to well-known human masterpiece ivory puzzle balls which are very popular in China (fig. 1d), but also known in Europe as "contrefait Kugeln" (fig 1e), which are created on the base of Johannes Kepler's Platonic Solids model of the Solar system from Mysterium Cosmographicum (fig 1f) [2]. The last one consists as second and third spheres octahedron and icosahedron like in first and second spheres of $[Mg_6@Ni_{12}Ga_6@Mg_{36}]$ cluster and as forth spheres dodecahedron with pentagons and hexagons which also form third sphere of $[CuAl_{12}@Li_{20}Cu_{12}@Al_{60}]$ and $[Ni_6Ga_6@Mg_{20}@Ni_{18}Ga_{42}]$ clusters.

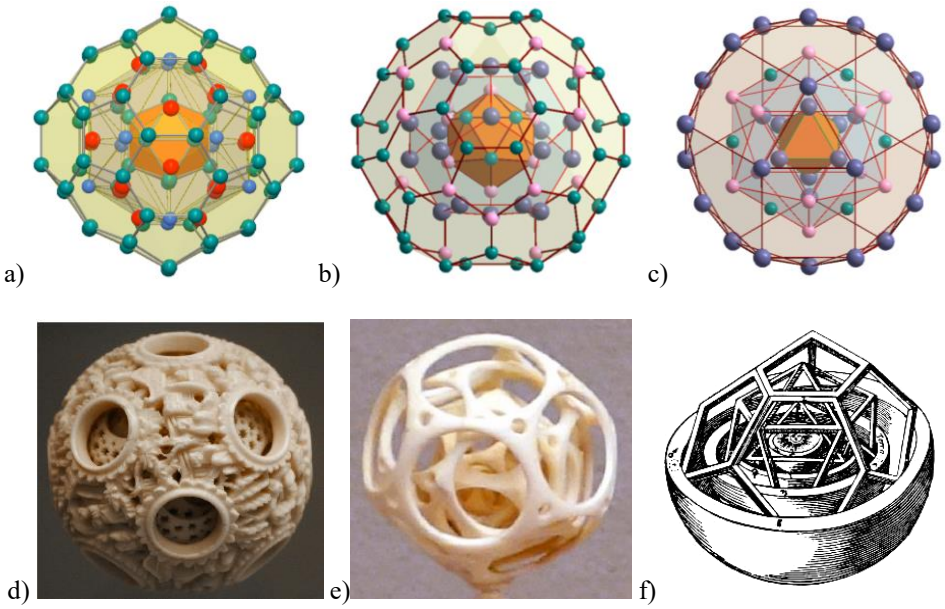

Figure 1. Atomic structure of a three-shell clusters $[CuAl_{12}@Li_{20}Cu_{12}@Al_{60}]$ (a), $[Ni_6Ga_6@Mg_{20}@Ni_{18}Ga_{42}]$ (b), $[Mg_6@Ni_{12}Ga_6@Mg_{36}]$ (c), Chinese ivory puzzle ball (d), Ivory puzzle ball from German workshop (e), Johannes Kepler's Platonic Solids model of the Solar system (f).

The results of electronic structure calculations for $Li_{20}Mg_6Cu_{13}Al_{42}$, $Mg_9Ni_6Ga_{14}$ and Mg_3Ni_2Ga confirm the three-shell clusters.

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