Atomic structure of Ca-based metallic glasses

Karel Saksl*, Juraj Ďurišin, Zuzana Molčanová, Pál Jovari, Ildiko Pethes, László Temleitner, Štefan Michalik, Michaela Šuliková, Katarína Šuľová, Miloš Fejerčák, Lukáš Kapuscinský

*ksaksl@saske.sk

The structure of biodegradable $Ca_{72}Mg_{28}$ at.% amorphous alloy was investigated by using neutron, X-ray diffraction and reverse Monte Carlo (RMC) modelling. The RMC configuration was decomposed into polyhedral holes whose faces are all triangles consisting of chemical bonds. Free volumes in the respective polyhedral holes were evaluated with reference to the packing efficiency of $CaMg_2$ tetragonal phase. The tetrahedral holes, which account for over 60% of the whole space, are regarded as densely packed units because the average packing efficiency of them is approximately equal to that of the corresponding crystal phase. On the other hand, various types of polyhedral holes, which have a certain free volume, are observed and some of them are connected with each other. The densely packed coordination polyhedra consisting only of tetrahedral holes tend to be clustered.

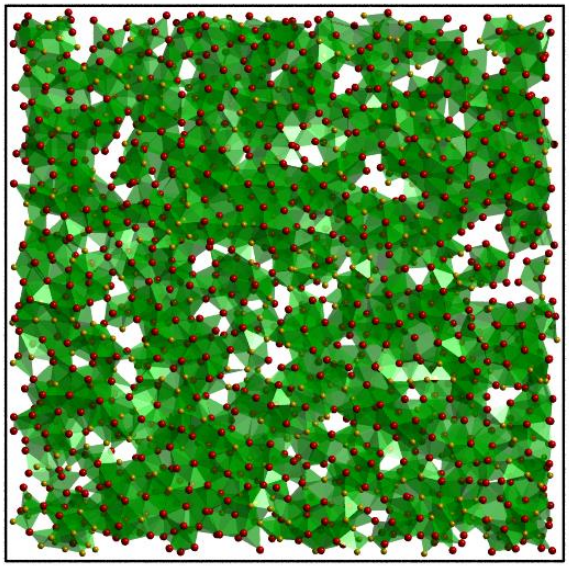

Fig. A 2Å thick slice of $Ca_{72}Mg_{28}$ at.%. RMC configuration with indicated tetrahedral holes