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Effect of excess electrons on hexagonal close-packed Mg and the model clusters for bulk metallic glasses MASAE TAKAHASHI, MIKIO FUKUHARA, AKIHISA INOUE, YOSHIYUKI KAWAZOE, Tohoku University — Though empirical rules for a large glass forming ability (GFA) were proposed, the formation mechanism of the bulk metallic glasses (BMGs) and the main factors for the GFA have not been clearly elucidated. The advantages of Mg-based BMGs are the lightness and abundance of resources, and a wide supercooled liquid region with the very high thermal stability and extremely large GFA. In 1991, Inoue *et al* developed glassy Mg–Cu–Y alloys with a maximum diameter of 4.0mm. We report here the effect of excess electrons on hexagonal close-packed Mg and the model clusters explained by an inflation process using density functional theory-based calculations, in order to understand the role of conduction electron concentration (CEC) in Mg-based BMGs [M. Takahashi et al, *J. Phys. D: Appl. Phys.*,**2008**, 41, 155424]. The CEC of Mg increase in Mg-based BMGs. In our model calculations, the increased CEC is artificially realized by the injection of electrons into Mg clusters and hcp Mg. We find the volume expansion and distortion to a higher c/aratio in the negative charge state. The increase in the values corresponding to the c/aratio is also observed in the model clusters. In the density of states at the equilibrium cell parameters expanded by charging, the pseudogap near the Fermi level by σ–π mixing becomes small and a spiky structure appears.

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