

Efficient atomic packing and amorphous phase separation in Al-rare earth metallic glasses

Jerzy Antonowicz

Faculty of Physics, Warsaw University of Technology, Koszykowa 75, 00-662 Warsaw, Poland

A relationship between dense atomic packing in a supercooled liquid and phase separation in binary aluminum – rare earth (Al-RE) metallic glasses [1,2] is discussed. Basing on an idea of Hume-Rothery of eutectic compositions and immiscible liquids [3] it is suggested that for binary Al-RE systems the efficient atomic packing related to formation of atomic clusters can produce an inflection in a free energy curve of the supercooled liquid phase. The inflection is located near the composition of optimal packing efficiency corresponding to highest glass-forming ability and results in a narrow metastable miscibility gap of the liquid. The results of free energy calculations performed using a complex formation approach [4] show that phase separation in a hypothetical binary A-B system with a tendency to form A-B clusters can be predicted if liquid phase is treated as a ternary mixture of atoms A, B and A-B atomic clusters. According to the calculations, a miscibility gap opens at low temperatures on a solute-poor side of the composition corresponding to maximal concentration of A-B clusters. The proposed model sheds light on the results of the small/wide-angle X-ray scattering (SAXS/WAXS) experiments which indicate amorphous phase separation prior to nanocrystallization in Al-RE metallic glasses [4]. The present approach can be considered as a thermodynamic foundation of the “lambda criterion” for crystallization behavior of aluminum-based amorphous alloys [5].

References:

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