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Correlation between the topological instability-electronegativity criterion and the glass forming ability in the Zr-Cu-Al system

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Abstract – The criterion of minimal topological instability combined with eletrectronegativity difference has been used for selection of glass forming compositions in many systems due to its simple formulation and usage. Although such criterion is not exact it makes the laborious process of selection easier and fast and is a promising tool among many others. This paper shows the correlation found between the prediction given by the method and the experimental results on glass forming ability of Zr-Cu-Al alloys.

The design of easy glass forming compositions in metallic systems still remains an interesting and unsolved problem. Many researchers have developed methods in order to forecast easy glass forming alloys based on thermodynamic, kinetic and structural models [1]. Although not so precise such methods save time since they reduce the number of trials thus shortening the experimental path to find easy glass forming alloys.

In the last two years we have proposed and used a simple method based on the topological instability parameter (λ) of crystalline phases and the mean electronegativity difference of an alloy to forecast new glassy compositions. The new criterion combines both factors assuming a synergetic effect that points to possible easy glass forming compositions in a given metallic system [2, 3, 4].

For a given alloy composition in any metallic system the λ parameter is calculated for all known phases and the minimum value is selected. This procedure generates a map of the minimum possible λ in the phase diagram. This means that the highest values in that minimum λ map refer to compositions where the topological instability reaches a maximum for all the surrounding phases simultaneously and thus rendering the crystallization more difficult during rapid quenching. To account the strength of the liquid against solute partitioning the average electronegativity difference is calculated assuming a random distribution of atoms. Both factors are thus multiplied considering a synergetic effect against crystallization. According to this criterion as high the calculated value as high the glass forming ability.

The figure 1 shows a selection map for the Zr-Cu-Al system generated by this new criterion. The agreement between the best glass formers found in the literature and the best region predicted by the method is remarkable [2].

In the present paper a correlation between this new criterion and the glass forming ability of alloys in the Zr-Cu-Al system is presented. The criterion is plotted against Tg/Tl values of many alloys since Tg/Tl is a well known parameter correlated to the glass forming ability (Tg – glass transition temperature, Tl – liquidus temperature).

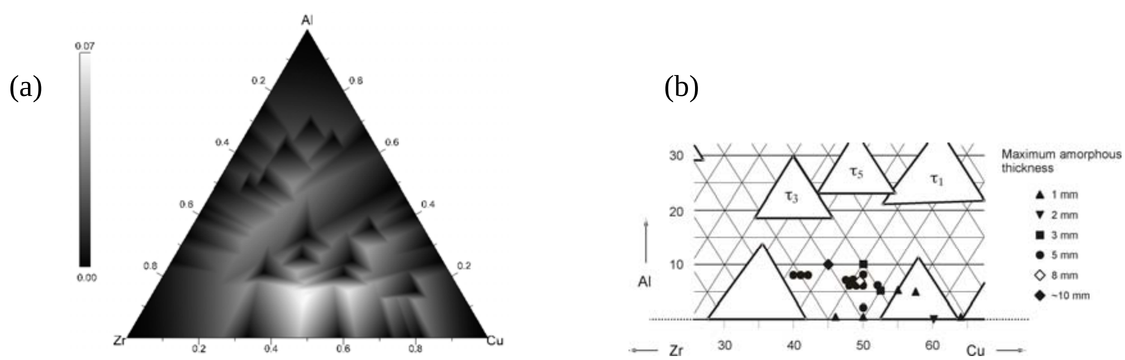

Figure 1: (a) Minimum topological instability and average electronegativity map for the Zr-Cu-Al system. Brighten areas refer to best glass forming compositions. (b) Maximum amorphous thickness in the best predicted region of (a), triangles refer to $\lambda < 0.1$.

References

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