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Choice and ambiguity of diffusion paths during formation and growth of intermediate phases and two-phase zones in ternary systems

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Predictive modeling of interdiffusion in alloys accompanied by the formation, competition and growth of intermediate phases is an important task of physical kinetics and materials science, including nanomaterials design. In case of binary alloys, the basic things now are more or less understood. On the other hand, for multicomponent alloys and, in particular, ternary systems, the problem remains a challenge. In particular, there is a problem of ambiguous choice of diffusion path in the concentration triangle, the problem of formation or non-formation of two-phase zones, the problem of instability of diffusion paths in two-phase zones, etc. Adding a third component to a binary system is a known way to optimize the bonding properties of materials. We concentrate on the known example of adding a few percent of zinc to a tin-based solder reacting with copper substrate. [1,2]. Such adding may reduce the porosity of joints as well as change the phase spectrum of the contact zone. We present two approaches to the modeling of diffusion path choice and phase competition in ternary systems – atomistic kinetic mean-field method and phenomenological analysis.

1. The recently developed modification of the mean-field kinetic method for describing the reaction diffusion and competition of intermediate phases [3-4] is generalized from the case of binary systems on ternary alloys (solid solutions, ordered intermediate phases and two-phase zones). At that, the interaction between atoms in the two coordination areas are taken into account (with opposite signs of mixing energies). To test the method, the temperature and interaction energies are chosen so that on the two sides (AB and BC) of the concentration triangle there is one or three intermediate ordered phases with a narrow interval of homogeneity, and on the third side (AC) there is complete solubility. The choice of the diffusion path and the kinetics of interdiffusion, ordering and growth of intermediate phases, depending on the composition of the original diffusion pair are studied.

2. Systematic kinetic study of various possible diffusion paths in the system Cu-(Sn+Zn) at various initial content of Zn in solder is made within phenomenological approach.

3. Results of both approaches are compared with the “candidates to general criteria” of evolution path choice like maximum Gibbs energy release rate etc.

References

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