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while forming the nuclei γ_{vs} effect will start to fade and γ_{cr} and γ_{sc} will increase thus

$$\Delta G = -l^2 h \Delta G_v + (4hl + l^2)\gamma_{cr} + l^2\gamma_{sc} - l^2\gamma_{vs}$$

$$\frac{\partial \Delta G}{\partial l} = 0 \longrightarrow \underbrace{-2lh\Delta G_v + (4h + 2l)\gamma_{cr} + 2l(\gamma_{sc} + \gamma_{vs})}_{\text{I}}$$

$$\frac{\partial \Delta G}{\partial h} = 0 \longrightarrow -l^2\Delta G_v + 4l\gamma_{cr} = 0 \longrightarrow$$

$$+l^2\Delta G_v = 4l\gamma_{cr} \longrightarrow l^* = \frac{4\gamma_{cr}}{\Delta G_v} \quad \text{II}$$

Plugging II in I $\rightarrow$

$$-2\times \frac{4\gamma_{cr}}{\Delta G_v} \times h \times \Delta G_v + 4h\gamma_{cr} + \frac{8\gamma_{cr}^2}{\Delta G_v} +$$

$$\frac{8\gamma_{cv}}{\rho\Delta G_v}(\gamma_{sc}-\gamma_{vs})=0 \xrightarrow{\times 1/\gamma_{cv}}$$

$$\frac{\cancel{8h-4h}}{h}=\frac{\overset{2}{\cancel{8}}(\gamma_{cv}+\gamma_{sc}-\gamma_{vs})}{\Delta G_v}$$

$\Downarrow$

$$h^{*}=\frac{2(\gamma_{cv}+\gamma_{sc}-\gamma_{vs})}{\Delta G_v}$$

$\downarrow$

$$\Delta G^{*}=-\frac{(\gamma_{sc}+\gamma_{vs}+\gamma_{cv})^2\cdot 16}{\Delta G_v}+\frac{16\gamma_{cv}^2}{\Delta G_v^2}(\gamma_{cv}+\gamma_{sc}-\gamma_{vs})$$

$$+\frac{16(\gamma_{sc}+\gamma_{cv}-\gamma_{vs})^2\cdot\gamma_{cv}}{\Delta G_v^2}$$

“Prediction of Interface Reaction Products between Cu and Various Solder Alloys by Thermodynamic Calculation”

Introduction:

Efforts are being made to develop Pb-free solder alloys to replace Sn-Pb solder. Sn-based multicomponent alloys with Ag, Zn, In, Bi, Sb, and/or Cu are promising. Intermetallic compounds that form at the substrate/solder interface during the soldering process affect the mechanical properties of the substrate/solder joint and solder wettability. The present work suggests a scheme to predict the first-forming intermetallic compound at the substrate/solder interface

Results:

A new scheme to predict the intermetallic compound which forms first at the substrate/solder interface during the soldering process has been suggested. A local equilibrium was assumed at the interface between the substrate and the liquid solder. By calculating metastable equilibria between the substrate and the liquid solder phases and by comparing the calculated driving forces of formation for individual phases, the compound which forms first at the substrate/solder interface could be successfully predicted. Thermodynamic calculations was done based on the CALPHAD. The composition of the liquid interface could be estimated using the point on the substrate and liquid/liquid metastable phase boundary where the ratios of liquid elements match those of the initial solder alloys. The prediction of interface reactions obtained by isothermal section calculation at 250 °C between Cu substrate and Sn-Pb, Sn-Bi and Sn-Zn binary eutectic solder was in agreement with already known experimental results.

Conclusion:

The article discusses how the thermodynamic state at the interface between substrate and liquid solder alloys can be determined by calculating metastable equilibria. The interface composition of the liquid can be estimated based on the substrate and liquid/liquid metastable phase boundary. By selecting the phase with the highest driving force under metastable equilibrium, it is possible to predict the intermetallic compound that forms first at the substrate/solder interface. The same method can be applied to any combination of solid/liquid metals or ceramics with diffusion-controlled reactions at the interface, provided that phase diagram information is available.

“Prediction of Ti/Al2O3 Interface Reaction Products by Diffusion Simulation”

Introduction:

It would be helpful to alloy design or process design if the reaction products could be predicted and controlled by some methods. Since the metastable tie-line cannot be determined by only thermodynamic calculations similar to in solid/liquid reactions, this paper presents a diffusion simulation study aimed at predicting the reaction products formed at the interface between titanium (Ti) and alumina (Al2O3).

Results:

A new model suggested based on thermodynamic calculation and diffusion simulation. Basically, a diffusion controlled reaction and a local equilibrium were assumed at the interface. The thermodynamic state at the interface before the formation of reaction product was regarded as to correspond to a metastable equilibrium between the two initial phases. A multicomponent diffusion simulation was performed for determination of the boundary compositions. By selecting the phase with the highest driving force of formation (calculated at metastable equilibrium state) as the first-forming interface reaction product, the order of formation as well as the interface layer sequence could be predicted. By using this methodology for prediction of interface reaction between pure titanium and alumina at 1100°C, It was expected that TiAl always forms first at the beginning of the interface reaction, but the stability of TiAl depends on the oxygen potential in the Ti matrix. The effect of the initial Ti layer thickness on the stability of TiAl was also clarified. If the initial layer of titanium is thin, the saturation of the Ti matrix with oxygen occurs quickly Thus the TiAl layer that was formed initially transforms into Ti3Al, resulting in a layer sequence of αTi-Ti3Al-Al203. By increasing thickness sequence changes to βTi-αTi-Ti3Al-TiAl-Al2O3.

Conclusion:

The diffusion simulation model presented in this paper provides a useful tool for predicting the reaction products formed at the interface between titanium and alumina. The model accurately predicts the formation of intermetallic compounds. This study demonstrates the importance of understanding the diffusion behavior of atoms at interfaces, and the potential of simulation methods in predicting material’s reaction product.