REPORT

POSTECH

POHANG UNIVERSITY OF SCIENCE AND TECHNOLOGY

제목 : **Homework #4**

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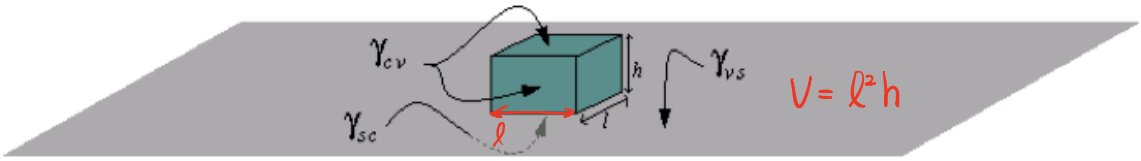
problem #1

1. The following figure illustrates a nucleation of a completely faceted cubic particle on a flat substrate. Write down an expression for the energy change due to the formation of nuclei in a functional form if its size. Then, find the critical size (h^*, l^*) and energy barrier of nucleation.



surface energy gradient $\Delta\gamma = (4hl + l^2)\gamma_{cv} + l^2\gamma_{sc} - l^2\gamma_{vs}$

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

$$0 = 2hl + l^2\frac{\partial h}{\partial l}, \quad \left(\frac{\partial h}{\partial l} = -\frac{2h}{l}\right)$$

① $$\frac{\partial \Delta G}{\partial l} = -2\Delta G_v lh - \Delta G_v l^2\frac{dh}{dl} + \left(4h + 4l\frac{dh}{dl} + 2l\right)\gamma_{cv} + 2l\gamma_{sc} - 2l\gamma_{vs}$$

At the critical size, equation ① is zero

$$-2\Delta G_v lh \overset{\circ}{\underset{\|}{-}} \Delta G_v l^2\left(\frac{2h}{l}\right) + (4h - 8h + 2l)\gamma_{cv} + 2l\gamma_{sc} - 2l\gamma_{vs} = 0$$

$$(-4h + 2l)\gamma_{cv} + 2l\gamma_{sc} - 2l\gamma_{vs} = 0, \quad l = \frac{2h\gamma_{cv}}{\gamma_{cv} + \gamma_{sc} - \gamma_{vs}}$$

$\gamma_{cv} + \gamma_{sc} - \gamma_{vs} = x$

$$\Delta G = -\Delta G_v \cdot \frac{x}{2\gamma_{cv}} \cdot l^3 + xl^2 + 4l\frac{x}{2\gamma_{cv}} l\gamma_{cv} = -\Delta G_v \frac{x}{2\gamma_{cv}} l^3 + 3xl^2$$

$$\frac{d\Delta G}{dl} = 0, \quad 6xl = \frac{3x\Delta G_v}{2\gamma_{cv}} \cdot l^2 \quad \begin{cases} l = \dfrac{4\gamma_{cv}}{\Delta G_v} \\ h = \dfrac{2(\gamma_{cv} + \gamma_{sc} - \gamma_{vs})}{\Delta G_v} \end{cases}$$

$$\therefore \Delta G = \frac{-32x}{\Delta G_v^2}\gamma_{cv}^2 + \frac{16x}{\Delta G_v^2}\gamma_{cv} + \frac{32x}{\Delta G_v^2}\gamma_{cv}^2 = \frac{16\gamma_{cv}^2}{\Delta G_v^2}(\gamma_{cv} + x - \gamma_{vs})$$

"Prediction of Interface Reaction Products between Cu and Various Solder Alloys by Thermodynamic Calculation," Byeong-Joo Lee, N.M. Hwang and H.M. Lee, Acta Materialia, 45, 1867-1874 (1997).

Abstract: The paper proposes a novel approach to anticipate the initial intermetallic compound formed at the interface of substrate and solder. The method considers a local equilibrium at the interface between the substrate and the liquid, and by calculating the metastable equilibria between the two phases, it predicts the first-forming compound. The approach involves comparing the driving forces of formation of individual phases to determine the one with the highest driving force, which is then predicted to form first.

Introduction provides an overview of the significance of Cu-solder interface reactions in electronic packaging, and the challenges associated with predicting the reaction products due to the complexity of the Cu-solder system. The methodology used in their study was described, which involves the use of thermodynamic calculations based on the CALPHAD (CALculation of PHAse Diagrams) approach. The results of the thermodynamic calculations are presented with a focus on the prediction of reaction products between Cu and various solder alloys, including eutectic Sn-Pb, Sn-Zn, Sn-Ag, Sn-Ag-Cu, and Sn-Bi alloys. The authors point out that thermodynamic calculations can provide valuable insights into the reaction products formed at the Cu-solder interface, and can aid in the selection of suitable solder materials for specific applications.

The thermodynamic state of the interface between the substrate and liquid solder alloys was determined by calculating the metastable equilibria between the initial phases. It was demonstrated that the composition of the liquid interface could be estimated using the point on the substrate + liquid/liquid metastable phase boundary where the ratios of liquid elements match those of the initial solder alloys. By selecting the phase with the highest driving force under the metastable equilibrium, the intermetallic compound that forms first at the substrate/solder interface could be predicted successfully, consistent with known experimental results in the case of Cu substrate and Sn-Pb, SnBi, Sn-Zn binary eutectic solder. If a diffusion-controlled reaction occurs at the interface and the phase diagram information of the related systems is available, this method can also be applied to the interface reaction of any combination of solid/liquid metals or ceramics.

"Prediction of Ti/Al2O3 Interface Reaction Products by Diffusion Simulation," ByeongJoo Lee, Acta Materialia 45, 3993-3999 (1997).

Abstract: A new method has been proposed for predicting the products of interface reactions at the interface between metals and ceramics. This method involves using both thermodynamic calculations and diffusion simulations. The initial state at the interface, before the reaction product is formed, is considered to be in a metastable equilibrium between the two starting phases. To determine the composition of the boundary, a simulation of multicomponent diffusion is carried out. By calculating the driving forces for the formation of all possible phases under the metastable equilibrium state, the phase with the highest driving force can be selected as the first-formed product of the interface reaction. This allows for the prediction of the order of formation and the layer sequence of the interface.

The paper then describes the methodology used in the study, which involves the use of diffusion simulation to predict the formation of interface reaction products. Furthermore, they explain the principles and assumptions underlying the diffusion simulation method, including the calculation of diffusion coefficients from experimental data. The author also discusses the factors that can influence diffusion, such as temperature, composition, and lattice structure. The results of the diffusion simulations are presented with a focus on the prediction of interface reaction products between Ti and Al2O3. It was discussed that the thermodynamic stability of the predicted reaction products, their composition, and the temperature range at which they are expected to form. The effects of the was predicted reaction products on the mechanical properties, thermal properties, and performance of Ti/Al2O3 interfaces, and provides insights into the factors that can influence the formation of specific reaction products.

When applying the current method to the reaction at the Ti/Al203 interface at a temperature of 1100°C, it was observed that TiAl is always the first to form at the interface. However, the stability of TiAl decreases as the Ti matrix becomes saturated with oxygen. If the initial layer of titanium is thin, the saturation of the Ti matrix with oxygen occurs quickly. In this case, the TiAl layer that was formed initially transforms into Ti3Al, resulting in a layer sequence of (αTi)/Ti3Al/Al203. On the other hand, if the initial layer of titanium is thick, the saturation of the Ti matrix with oxygen takes a longer time, and TiAl can be observed, resulting in a layer sequence of (βTi)/(αTi)/Ti3Al/TiAl/Al2O3.