Theoretical Study of Adhesive Interfaces between Epoxy Resin and Metal Surface in Semiconductor Packages

鶴見, 直明

（様式２）

氏　　名　：鶴見　直明

論 文 名　：Theoretical Study of Adhesive Interfaces between Epoxy Resin and Metal Surface in Semiconductor Packages (半導体パッケージにおけるエポキシ樹脂と金属表面の接着界面に関する理論的研究)

区　　分　：甲

論　文　内　容　の　要　旨

In this thesis, essential interactions of adhesion in electronics packages have been clarified by using quantum chemical calculations. In semiconductor packages, it is important to maintain the adhesion to ensure the long-term reliability of the device. However, the actual adhesion can easily delaminate depending on the operating environment, which is a major risk in ensuring the reliability of the products. To overcome this issue, it is necessary to understand the ideal adhesion structure and the bonding mechanism. The purpose of this study is to clarify the intrinsic interactions at the adhesive interfaces between epoxy resin and metal surface used in semiconductor packages. Chapter 1 provides a general introduction to the role of semiconductor packages, the basic theory of adhesion, and a method for calculating the theoretical adhesive force by using first-principles calculations.

In Chapter 2, a die bonding structure using a conductive adhesive is the subject of the research. Assuming the mounting structure of a light emitting diode (LED), the adhesive interface between the Au surface and the epoxy resin was theoretically investigated. We selected diglycidyl-ether of bisphenol-A (DGEBA) as the epoxy resin and dicyandiamide as the hardener, which are the same materials commonly used in actual assembly process. A fragment molecule formed by the curing reaction of DGEBA and dicyandiamide was proposed, and the ideal adhesive structure between the epoxy fragment and the Au (1 1 1) surface was calculated by using the density functional theory (DFT). The results show that the theoretically predicted maximum adhesion stress was as high as 1.15 GPa (see Fig.1). The cyano group involved in the hardener has been found to interact strongly with the ideal, smooth gold surface. This interaction is likely to come from σ-donation and π-back donation. It is revealed that a hardener would not only cure the epoxy resin but also make a bond to the surface atoms, at least on the ideal surface.

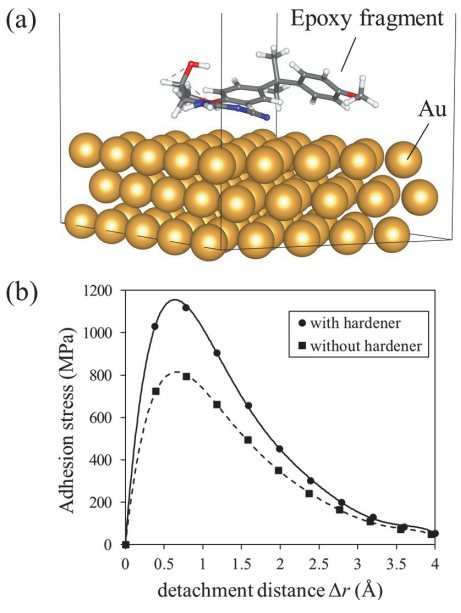

Fig.1. (a) Optimized adhesion structure (b) calculated adhesion stress

In Chapter 3, the actual bonding interface between the gold surface and the conductive adhesive was

investigated. A small lap-share specimen was designed and made with a package substrate including the die pad, and conductive adhesive. Then, the actual adhesive stress was measured by tensile tests. The obtained results were compared with the theoretical calculation results in Chapter 2, and the difference between the ideal and actual structures of the die bonding interface was discussed. The actual adhesive strength measured by using the lap-shear test was about 27 MPa at room temperature, decreasing with elevated temperature. Analytical methods indicated that there should be an altered layer with a thickness of several angstroms terminated with the compositions of Au(CN)x on the top of the plated gold surface. The observation of such a layer should cause a change of the interaction mechanism from that predicted from the DFT calculation to the one based on hydrogen bonding.

In Chapter 4, the adhesion interface between the epoxy molding compound (EMC) and the Cu-based leadframe was analyzed by using DFT calculations at the molecular level. In power devices, the delamination between the leadframe and the mold resin is a major reliability issue. Since the leadframe is mainly made of copper, a metallic Cu surface and an oxidized Cu_2O surface were selected as the adherends. A fragment molecule was prepared based on the molecular structure obtained from the curing reaction of *ortho*-cresol novolac epoxy resin (ECN) and phenol novolac resin (PN), which are standard mold encapsulation materials. The resin fragment was placed on the surface of Cu (1 1 1) and Cu_2O (1 1 1), and the ideal adhesive structures were calculated. It was found that the ECN-PN fragment adheres to the Cu (1 1 1) surface on the basis of the dispersion force. On the other hand, when the ECN-PN fragment adheres to the Cu_2O (1 1 1) surface, a OH group and a phenyl group in the fragment can form chemical bonds with the coordinatively unsaturated Cu atoms of the Cu_2O surface, resulting in a very strong adhesion (see Fig.2). The maximum adhesive stress was calculated to be 1.6 GPa for the Cu (1 1 1) and 2.2 GPa for the Cu_2O (1 1 1), respectively. The ECN-PN fragment bonded to the Cu_2O surface was stabilized by an energy of 0.5 eV compared to that bonded to the Cu surface due to the electron exchange interaction. Since these strong bonds inhibit the separation between the EMC and the leadframe surface, the adhesive failure does not occur at the molecular interface, but rather within the oxide layer of the leadframe or within the EMC, as the cohesive breakage.

Chapter 5 summarizes the findings of this study and discusses future research prospects. It is clear that the adhesion mechanism in semiconductor packages differs significantly depending on the combination of the atomic structures of the adherends and resin components. Through this study, we have been able to elucidate the ideal adhesive structures of semiconductor packages, which were previously unknown.

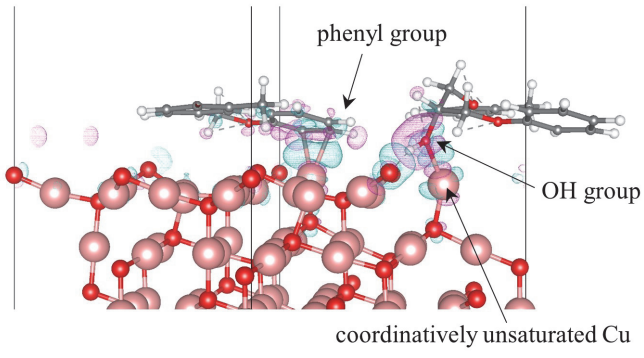

Fig.2. Electron density difference plot calculated for the adhesive interaction between the ECN-PN fragment and the Cu_2O (1 1 1) surface. The areas of charge accumulation and depletion are shown in light blue and purple, respectively.