First-Principles Study on Adhesive Strength between Metal Layer and Silane Coupling Agents

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Abstract

It is important for industry products to keep enough adhesive strength between inorganic materials and organic materials. Therefore, various silane coupling agents are employed to improve adhesive strength. Silane coupling agents consist of hydrolyzable group which reacts to an inorganic material and organic functional group which reacts to an organic material. Although the combination of hydrolyzable group and organic functional group should be designed, its variation is huge and difficult to examine by experiments. In this study, we investigated silane coupling agent on adhesive strength with metal layers through first-principle calculation. As an example calculation γ-mercapto propyl trimethoxy silane (MPS) and γ-amino propyl trimethoxy silane (APS) were selected and chromium layer was employ for inorganic materials. The computation indicated cohesion energy of the APS was 9.12% larger than MPS.

Keywords: First-principle calculation, Silane coupling agent, Adhesive strength, Cohesion energy, Chromium layer

Introduction

In recent years, it is important for industry products to keep enough adhesive strength between inorganic materials and organic materials. However, it is difficult to agglutinate inorganic materials and organic materials. Therefore, we use silane coupling agents to bond inorganic materials and organic materials[1][2]. In general the silane coupling agent possesses the hydrolyzable group (H group) to combine with an inorganic material and the organic functional group (O group) to combine with organic material. The variation of their combination is huge and difficult to examine by experiments. Therefore first-principles calculation are applied to adhesive strength test and fundamental mechanical characteristic of silane coupling agents have been revealed[3]. In this study, to support the design of silane coupling agents, we focus on two factors, molecular structure and crystal face of metal surface, and investigate the influence on adhesive strength.

Calculation Method

In this study, the density function theory was employed for first-principles calculation and Generalized Gradient Approximation (GGA) was utilized for exchange-correlation term. We consider a monomolecular of silane coupling agent and the surface of metal layer to adhesive strength (see Figure 1). As an example of typical silane coupling agents, γ- mercapto propyl trimethoxy silane (MPS: $(CH_3O)_3Si(CH_2)_3SH$) and γ-amino propyl trimethoxy silane (APS: $(CH_3O)_3Si(CH_2)_3NH_2$) were selected and chromium was set to metal layer. The length of long axis of stable MPS and APS monomolecular were 9.52 nm and 9.26 nm. The lattice constant of chromium was 0.285 nm and the dimension of metal layer were 0.782 nm, 0.838 nm and 2.791 nm, respectively in case of (110) surface. The monomolecular was located in the vacuum layer with 2.4 nm high. First, the stable structure of silane coupling agents and the chromium layer contacting with the vacuum layer were investigated. And then silane coupling

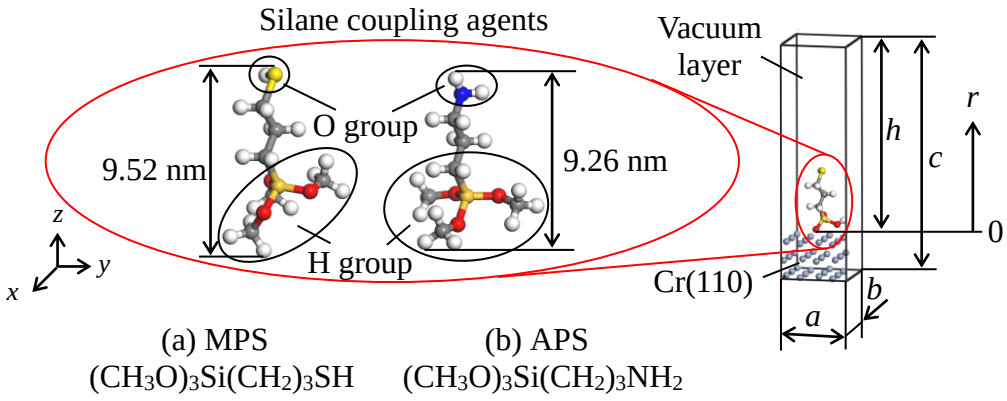

Figure 1. Silane coupling agents and metal layer

agent was arranged in the vacuum layer on the surface of chromium layer. The total energy of the above system was calculated as changing the distance between the silane coupling agent and the chromium layer.

Calculation Results

Figure 2 shows the relation between the total energy and the distance from metal surface in case of (110) crystal face. The total energy of both silane coupling agents increases linearly and then the maximum, which is corresponding to the cohesion energy, appears at approximately r=0.9 nm after gradual non-linear increase. The cohesion energy of APS was 9.12% larger than MPS.

Figure 3 compares the cohesion energy between MPS and metal layer among different crystal faces. The computation indicates that (001) surface has the highest cohesion energy and it is 23.7% larger than (110) surface.

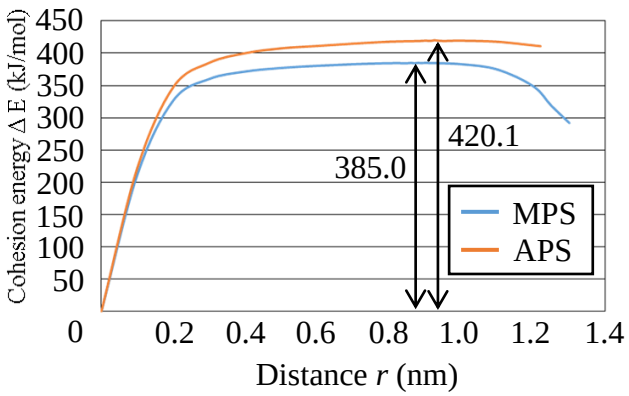

Figure 2. Relation between total energy and distance from metal surface

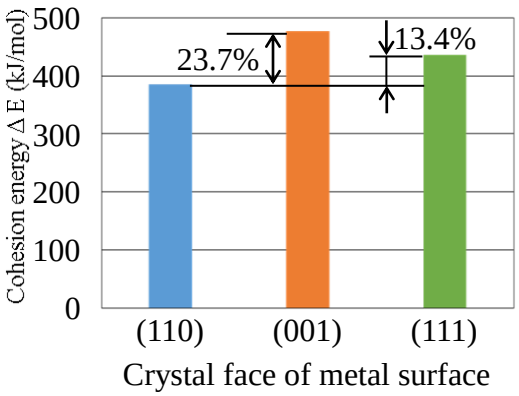

Figure 3. The comparison of cohesion energy of MPS among different crystal faces

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