Ab initio investigation of interfacial layer formation in the Mo/Si boundary for extreme ultraviolet lithography

In-Yong Kang*, *Yoon-Suk Kim, and Yong-Chae Chung
Department of Materials Science and Engineering, Hanyang University, Seoul, Korea

The extreme ultraviolet lithography (EUVL) is known to be the most promising technique for manufacturing ultra-large-scale integration devices for the 32-nm node. In EUVL system, the alternating Mo/Si multilayers optimized for Bragg reflection, are used as masks, as well as mirrors, during the pattern transfer process. The optical performance of Mo/Si multilayer is directly related to the interface characteristics of each Mo/Si boundaries. It was reported that the interfacial layer of Mo/Si multilayer can be asymmetrically formed between bcc Mo(110) and amorphous Si layers. Therefore, many works have been trying to figure out the formation mechanism of interfacial layer to minimize intermixing thickness in Mo/Si boundaries [1-2]. This work intends to show quantitative analysis of energy barrier and bonding nature in the initial deposition stage of Si adsorption on Mo(110) surface in an attempt to clarify the formation mechanism of silicide layers.

The Vienna *ab initio* simulation package (VASP) based on the density functional theory has been employed to perform the *ab initio* total energy calculations [3]. Our calculations are based on the density functional theory (DFT) and the generalized gradient approximation (GGA) for the exchange-correlation energy. The projector-augmented-wave (PAW) potentials are employed to describe the electron-ion interaction.

In order to find the adsorption sites, corresponding adsorption energies and the potential energy surface (PES) have been calculated. The PES obtained by using (2x2) cell (Fig. 1) shows that the Si adatom favors the hollow site of Mo(110) as the adsorption site with the adsorption energy of 6.27eV/Si. The barrier for hopping is located at the bridge site and the barrier height is calculated to be 0.64 eV. In order to analyze the bonding nature between Si adatom and Mo(110) surface, the total valence electron density and its change upon adsorption is plotted in Fig. 2. It can be clearly seen that most electrons are located around Mo atoms as shown in (a) and (c). In addition, the electron density difference revealed the formation of four Mo-Si covalent bonds per adsorbed Si atom as shown in (b) and (d). The density of state for each orbital and the electronic structure upon Si incorporation will be discussed.

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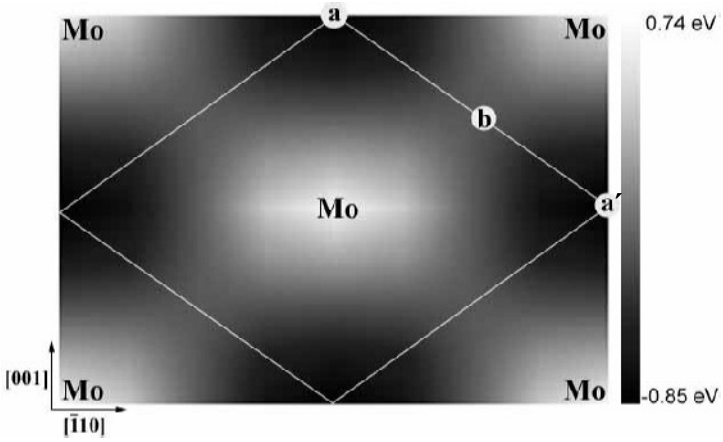

Fig. 1 The potential energy surface of a Si adatom on the Mo(110) surface. The symbol ⓐ represents a favored site, hollow site, for Si adatom and ⓑ represents a bridge site. The solid white line, ⓐ-ⓑ-ⓐ′, is the suggested path for surface diffusion for Si adatom. Here ⓐ′ is the adjacent hollow site.

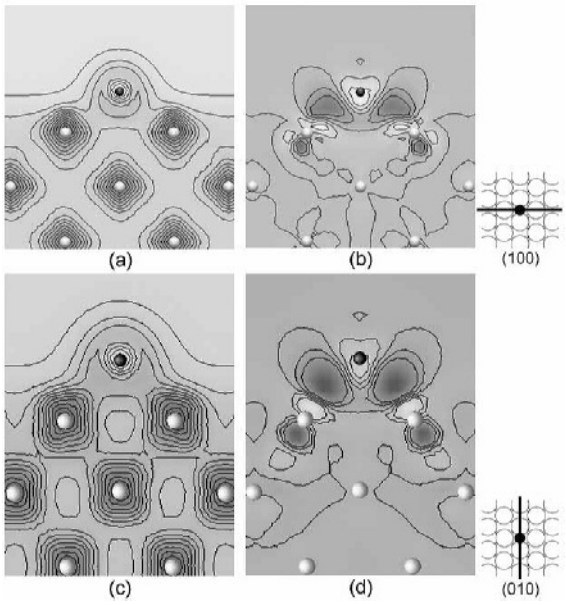

Fig. 2 Total electron density (a), (c) and its change upon Si adsorption (b), (d) plotted on the (100) and (010) plane. The contour lines are indicated every 0.138 e/Å^3 for total electron density difference and 0.017 e/Å^3 for its change. Black and white circles represent for Si and Mo atoms, respectively. The darker shaded contour indicates the higher electron density in (a) and (c). In (b) and (d), the dark and the bright shaded contours indicate electron accumulation and depletion, respectively.