



Interfacial chemical bonding between carbon nanotube and aluminum substrate modulated by alloying elements



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ABSTRACT

The effects of alloying elements (Mg, Zn, Cu, Sc and Ti) on the interfacial bonding between a carbon nanotube (CNT) and an Al(111) surface are studied systematically using first-principles total energy calculations. The redistribution of the charge density of the Al(111) surfaces induced by the five alloying elements, the projected densities of state, and the crystal orbital Hamilton population analysis of the atomic pairs in the vicinity of the interface are analyzed in detail. Thereby, it is revealed that the bonding characteristic between the CNT and the Al(111) surfaces are modified when alloying with the early transition metals Sc and Ti that occupy subsurface positions. Also for the other alloying elements a weak interaction between CNT and the substrates is found although these elements occupy surface positions in the Al(111) surface. Through a detailed study of the interaction potential energy and the restructuring energy, we demonstrate that different mechanisms are responsible for the substrate–CNT interactions.

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1. Introduction

In order to reduce fuel consumption and pollution, it is advantageous to reduce the weight of traditional vehicles like cars, trains, and aircrafts. Therefore, a large scientific interest in lightweight and high strength materials has developed. As a rust-free light metal, aluminum (Al) is assumed being an environmentally benign material. However, its use is still limited mainly due to its poor mechanical strength compared to, e.g., its steel counterpart [1]. As a complementary reinforcing phase in Al matrix composites, carbon nanotube (CNT) possesses exceptionally high Young's modulus of ~1 TPa and tensile strength in the region of 150 GPa [2,3]. As promising high strength-to-weight ratio materials, CNT-reinforced Al matrix composites, first fabricated by Kuzumaki et al. [4], have demonstrated a significant improvement of mechanical properties [5–8] and have accordingly potential to be widely used in the near future. To make the most efficient use of the reinforcing function of the CNTs, a homogeneous dispersion of CNTs in the Al matrix and a proper interfacial bonding between CNTs and Al substrate are of fundamental importance [9–12]. In situ synthesis of composite powders through chemical vapor deposition is one efficient method to

achieve integral and well-dispersed CNTs in an Al matrix [13,14]. The CNTs can pin dislocations and increase resistance against mechanical failure in a conventional way [15]. More importantly, the high tensile strength of the CNTs can be utilized efficiently only if the CNTs are connected to the Al matrix via strong chemical bonds [16]. It is believed that the limited formation of nano-sized Al₄C₃ layers at the nanotube surface is of advantage for the interfacial bonding [17–20]. In recent years, some theoretical studies on the interactions between non-defective CNTs and pure Al surfaces have found that these are weak [21,22]. When aiming at keeping the structural integrity of the CNT, varying the composition of the Al substrate provides an alternative way of modifying the interactions between the substrate and the CNTs.

On the other hand, Al alloys have higher initial mechanical properties compared with those of pure Al. Some recent studies [23–32] were dedicated to the CNT-reinforced Al alloy composites on account of the demand of structural engineering applications. Thus, it is necessary to clarify the role of alloying element in CNT reinforced Al matrix composites. No literature has reported whether the alloying elements could have the ability to influence the homogeneous dispersion of CNTs in the Al matrix, but some researches confirm that it is an effective method to improve the wettability between carbon materials and Al matrix through adding alloy elements [33,34]. However, a detailed understanding of the effects of alloying elements on the interfacial properties between CNTs and Al has not hitherto been reported in literature. This includes the question whether the alloying elements in the Al

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substrate modify the chemical bonding between an intact CNT and an Al substrate, which can offer guidelines to design the optimal substrate component for making the most efficient use of carbon nanotube.

Magnesium (Mg), zinc (Zn), copper (Cu) and titanium (Ti) are the main alloying elements in 2024 aluminum alloy which was widely used as matrix to be reinforced with CNTs by mechanical alloying [29, 31]. In addition, scandium (Sc) and Ti act as effective grain refiners in aluminum alloys [35,36]. Therefore, the effects of these five alloying elements on the interfacial bonding between (5,5) single-walled carbon nanotube (SCNT) and Al(111) surface are systematically studied through first-principles total-energy calculations in the present work. The changes in the charge density of the Al substrate with and without alloying elements, the partial densities of states (DOS), and the crystal orbital Hamilton populations (COHP) analysis are used to obtain information on the change of interfacial property due to the alloying elements.

2. Method and models

In our first-principles calculations, an idealized structural model for the interface between CNT and Al(111) surface was considered. The Al(111) surface was modeled through a repeated slab with 7 atomic layers in the form of ABC stacking. A supercell consisting of 70 atoms (69 Al atoms and 1 substituted alloying atom) was considered as substrate for the adsorption of CNT. Two substitution positions of the alloying atoms, i.e., at the top layer (TL) and at the subsurface (SS) of the Al(111) slab, were both studied, as shown in Fig. 1(a) and (b). An armchair (5,5) SCNT with a diameter of 6.78 Å was placed on the Al(111) surfaces. The axial direction of the (5,5) SCNT was placed along the [112] direction. A single Al(111) surface unit cell can then accommodate two unit cells of the CNT with a lattice mismatch of only about 0.6%. A vacuum region of 20 Å was used to separate the repeated slabs, and the CNTs belonging to different supercells were well separated in the lateral direction by 7.3 Å. We considered two different arrangements of the (5,5) SCNT on the Al(111) surface: in one (T0) the C–C bonds closest to the substrate form a zigzag line parallel to the tube axis, and in the other (T18) the C–C bonds closest to the substrate are oriented perpendicular to the tube axis, as shown in Fig. 1(c) and (d).

A local-density approximation (LDA) [37] within density-functional theory as implemented in the Vienna ab initio simulation package (VASP) [38] was used. The projector-augmented wave method [39,40] was used to model electron-ion interactions with a cutoff energy of 400 eV. In the geometrical optimization, the two bottom layers of the substrate were fixed, and all the other atoms in the system were allowed to move until the forces acting on each atom converged to 0.01 eV/Å or less. The atomic positions are relaxed using the Methfessel–Paxton [41] technique for the reciprocal-space integration, and a $3 \times 1 \times 1$ Γ point centered k -mesh was used in k -space sampling. For the converged structures, subsequent calculations with a larger $9 \times 3 \times 1$ k mesh were performed. The convergence criterion for the energy and electronic properties calculations was set to 10^{-5} eV, and the tetrahedron method together with Blöchl corrections [42] was used.

3. Results and discussion

At first, the relative energies of the TL and SS substitutions for each alloying element were calculated, in order to identify the most stable position of the alloying atoms in the Al(111) slabs. According to the relative energy ΔE_1 listed in Table 1, the TL position is more stable for Mg and Zn atoms, whereas for Cu, Sc and Ti atoms, the SS position is more stable. This difference can be associated with the experimental surface energy viz. E_{surf} [43,44] of these atoms. The E_{surf} of Mg and Zn is smaller than that of Al, so they are prone to segregate to the Al(111) surfaces, opposite to the cases for Cu, Sc, and Ti atoms. Besides the effect of E_{surf} , Mg and Zn with their closed electronic shells have a smaller tendency towards high coordination. On the other hand, differences in the

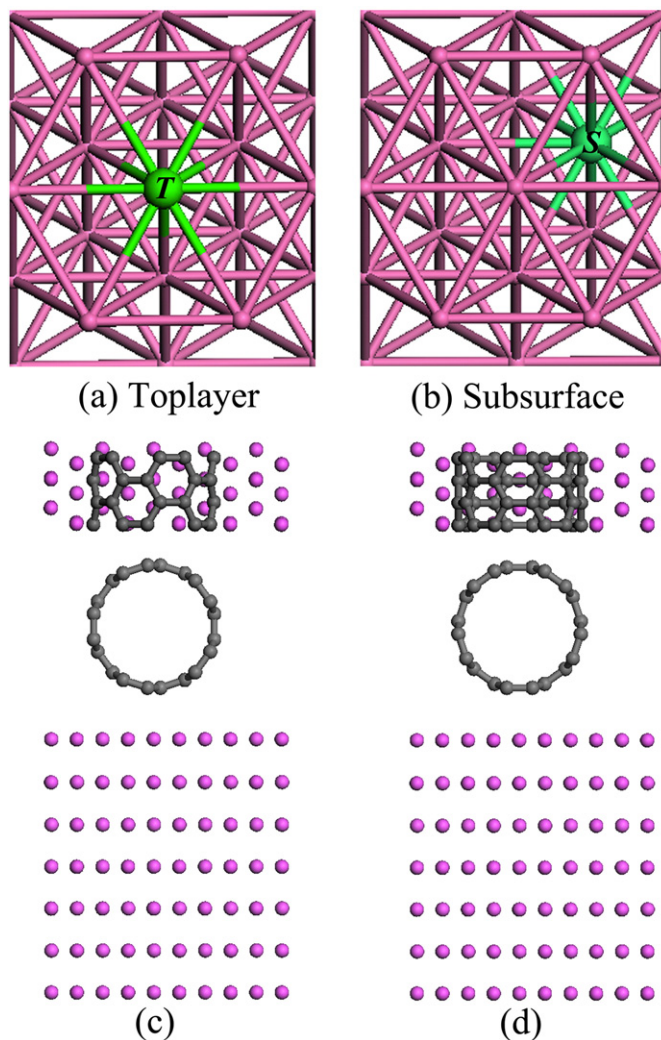


Fig. 1. Schematic representation of the Al(111) surfaces containing substitutional alloying elements in the top layer (a) or in the subsurface layer (b). (c) and (d) show the initial adsorption configurations for the CNT/Al(111) systems, with (c) the bottommost C–C bonds forming a zigzag line parallel to the tube axis (T0) and (d) the bottommost C–C bonds oriented perpendicular to the tube axis (T18). The upper panels and the lower panels in (c) and (d) give a top view and a front view, respectively.

atomic radii seem to be less relevant in explaining the differences in preferred sites.

After the optimized structure of Al(111) surfaces with alloying elements have been determined, the adsorption behavior of CNTs on Al(111) surfaces is investigated. The resulting structures are shown in

Table 1

The energy difference ΔE_1 (in eV) between the TL and SS configurations for the substitutionally doped surfaces, as well as the energy difference ΔE_2 (in eV) between T0 and T18 configurations for the combined CNT/Al(111) systems. Negative values of ΔE_1 and ΔE_2 indicate that TL and T0 are energetically more favorable, respectively. Al-X marks that the Al(111) surface is doped with an X atom. The d_{eq} (in Å) is the vertical distance between the bottommost carbon atom of the CNT and the top layer of the Al(111) slab. E_b , E_i and E_R (in eV) are interfacial binding energy, interaction energy without internal geometry relaxation, and restructuring energy between CNTs and Al(111) surfaces with and without alloying elements, respectively.

System	Pure Al	Al–Mg	Al–Zn	Al–Cu	Al–Sc	Al–Ti
ΔE_1	0.000	–0.262	–0.031	0.110	0.069	0.560
ΔE_2	0.011	–0.048	0.025	0.026	0.036	0.025
d_{eq}	2.80	2.90	2.70	2.85	2.20	2.15
E_b	0.431	0.565	0.426	0.444	0.616	0.540
E_i	0.411	0.538	0.390	0.428	–0.091	–0.391
E_R	0.020	0.027	0.036	0.016	0.707	0.931

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