



First-principles investigation on the interaction of Boron atom with Nickel part I: From surface adsorption to bulk diffusion



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ABSTRACT

In this work, Boron atom adsorption, absorption and diffusion on the surface of and in the bulk of the Nickel are studied with a first-principles density functional theory approach and the climbing image nudged elastic band method. The calculated results indicate that, on the Ni (111) surface, there are three stable sites for B atom adsorption, which are Top site, Hcp-hollow site and Fcc-hollow site, and Hcp-hollow site is the most preferred one. While below the surface, the Boron atom prefers to reside at the Oct site with the absorption energy of -1.38 eV, and the energy barrier for Boron atom diffusing from Hcp-hollow site to Oct site is 1.22 eV. In bulk Ni, the Tet and Oct sites are both stable ones for solution of the B atoms, the energy barrier for B atom diffusing from Tet site to its nearest neighboring Oct site is 0.29 eV, while that for B atom diffusing between two neighboring Oct sites are 1.65 eV, which indicate that the B atom diffuses between two neighboring Oct sites is harder than that from Tet site to neighboring Oct site.

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1. Introduction

In recent years, Ni and its alloys have been widely used in aerospace field because of the high ductility and the excellent corrosion-resistance [1–3]. In order to remedy the disadvantage on hardness and wear resistance, Ni and its alloys usually joint ceramic materials on surface before they were applied [4,5].

The Ni alloys/ceramic materials jointing methods are various, such as melting, self-propagating high temperature synthesis joining, solid state diffusion bonding, and so on [6–8]. In all the jointing methods, the transient liquid phase (TLP) bonding get the most recognized because of the high efficiency and the excellent reliability [9,10]. On the TLP bonding processing, the diffusion of the melting-point depression element (in most cases is B) is the most important, which is the essential reason for liquid zone broadening, oxide film breaking and isothermal solidification. Actually, the melting-point depression element B fully diffuses to Ni alloys and the induced reasonable change of the middle tier components are the lifeblood for a successful Ni alloys/ceramic materials TLP bonding [11–13].

Although the adsorption and diffusion of element B at the Ni alloys side is crucial, the corresponding mechanism is still not be understood, the main reason is that it is difficult to research this issue by traditional experimental methods. First-principles calculation based on density functional theory (DFT) and approximation conditions is a novel method considers the interactions between atom and atom, atom and electron, and electron and electron, which are usually used to investigate the atom adsorption and atom diffusion, the results are widely recognized.

Ivanovskaya [14] investigated the hydrogen adsorption on graphene by first principles calculations and indicated that the hydrogen chemisorption energy barrier is independent of the optimization technique and system size, being associated with the relaxation and rehybridization of the sole adsorbent carbon atom. Pašti [15] researched the adsorption of d-metals (Pd, Pt, Cu, Au) and p-metals (Sn, Pb, Bi) on the Pt (111) surface systematically by means of DFT calculations, and found that the adsorption trends were determined on the basis of strength of substrate-adsorbate and adsorbate-adsorbate interactions. Zhou [16] investigated the diffusion of hydrogen in a tungsten grain boundary using a first-principles method, and indicated that due to the much lower diffusion barrier of 0.13 – 0.16 eV from the bulk to the grain boundary in comparison with the segregation energy, it is quite difficult for the trapped hydrogen to escape out of the grain boundary.

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In the present work, the first-principles calculations have been performed to systematically investigate the B atom adsorption/absorption on Ni (111) surfaces (which is the close-packed surface and preferentially interact with B atoms) and B atom penetration/diffusion in bulk Ni, which can clear the mechanism for adsorption and diffusion of B atom at the Ni alloys side, and then provide theoretic foundation for optimizing technology of TLP bonding.

2. Computational details

DFT (density functional theory) [17,18] with ultrasoft pseudo-potentials was employed in the Vienna Ab initio Simulation Package [19] code utilizes plane-wave pseudopotential to perform first-principles quantum mechanics calculations. The Generalized Gradient Approximation-Perdew-Burke-Ernzerhof (GGA-PBE) [20] functional was employed to describe the electron exchange-correlation potentials.

The energy cutoff for the plane-wave basis set was set to 360 eV based on a convergence test. The conjugate gradient algorithm [21] was applied to optimize the geometry and the convergence criterion for the force was set to 0.03 eV/Å. The Monkhorst-Pack method [22] was used to sample the Brillouin zone. The smearing function proposed by Methfessel and Paxton [23] was used with $N = 2$ and $\sigma = 0.3$ eV to determine the partial occupancies of each wave function.

In order to research the adsorption/absorption behavior of the B atom on the Ni (111) surface and subsurface, a 2×2 super-slab model with five atomic layers was used, in which the upper two atomic layers were relaxed and the bottom three layers were fixed in their bulk like positions. A 12 Å vacuum layer was added to prohibit the interactions between two successive slabs and the k-point mesh was set to $6 \times 6 \times 1$. Then, a $2 \times 2 \times 2$ supercell was used to model the diffusion of the B atom in bulk Ni, where the k-point mesh of $4 \times 4 \times 4$ was employed.

To quantitatively estimate the amount of charge that was transferred between the B atom and the Ni surface/bulk, the Mulliken charge analysis was performed [24]. The diffusion behaviors of the B atom on the surface, into the subsurface and in the bulk of Ni were all studied with the climbing image nudged elastic band (CI-NEB) method, which determined the minimum energy paths (MEPs) and the corresponding energy barriers between the given initial and final configurations [25].

The adsorption energy of B atom on the Ni surface E_{ads} , the absorption energy of B atom into Ni subsurface E_{abs} and the solution energy of B atom in bulk Ni E_{sol} all can be defined as Eq. (1):

$$E_{ads/abs/sol} = E_{system}(B/Ni) - E_{surface/bulk}(Ni) - E_{atom}(B) \quad (1)$$

where $E_{system}(B/Ni)$ is the total energy of the B/Ni system, $E_{surface/bulk}(Ni)$ is the total energy of either the surface of the Ni slab or the bulk, $E_{atom}(B)$ is the energy for an isolated B atom.

3. Results and discussion

3.1. Structure of bulk Ni and Ni (111) surface

Fig. 1 shows the optimized structure for Bulk Ni. From it, the crystal structure of Ni is face-centered cubic with a space group FM-3M, and each Ni cell contains four atoms. Moreover, the optimized lattice parameters for Ni were determined to be $a = b = c = 3.524$ Å, together with a bond length between the adjacent Ni atoms of 2.492 Å. The results are all in agreement with the experimental data ($a = b = c = 3.525$ Å, bond length_{Ni-Ni} = 2.493 Å) [26] as well as other GGA results [27–29].

Fig. 2 indicates the band structure and density of states for Bulk

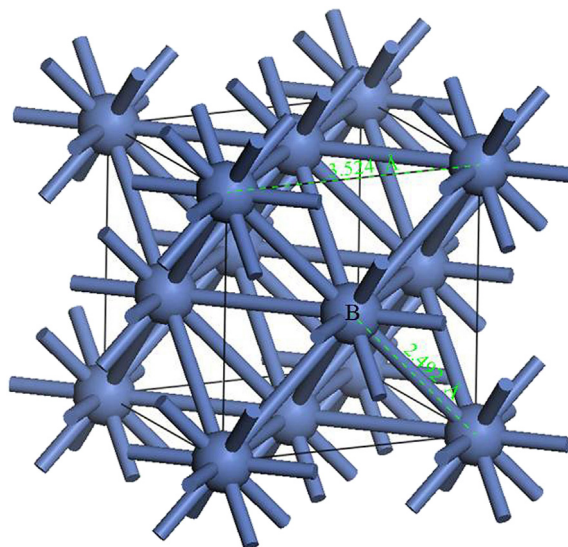


Fig. 1. Optimize structure for Bulk Ni.

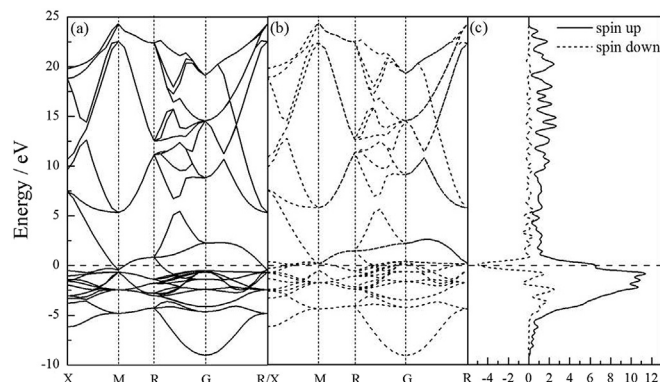


Fig. 2. (a) Spin up band structure, (b) spin down band structure and (c) density of states for Bulk Ni.

Ni. From Fig. 2(a), in the spin up band structure, the near Fermi-level states are occupied by the d orbitals of Ni atoms, as well as the slight influence by p orbitals, and the corresponding state density peak appears at -0.85 eV, in Fig. 2(c). Moreover, the band structure between -1.25 eV and -3.5 eV presents the symmetry at high symmetry point R. As shown in Fig. 2(b), the spin down band structure is very similar with the spin up one, except that the Fermi-level moves to conduction band, which leads to the state density peak appears at Fermi-level. From Fig. 2(c), the electron of Ni crystal presents strong spin polarization at Fermi-level, it is the reason that Ni possesses ferromagnetism.

Before investigate the adsorption/absorption behavior of the B atom on the Ni (111) surface and subsurface, the constructed Ni (111) surface was structural relaxed. After relaxed, there was no structural reconfiguration and only some surface atoms slightly moved in the direction of perpendicular to the surface, which leads to the small increment on the layer distance. In which, the layer distance between layer-1 and layer-2 of the relaxed structure has increased $+0.04\%$ compared with that of the un-relaxed structure, the layer distance between layer-2 and layer-3 has increased $+0.02\%$ while that between layer-3 and the fixed layer-4 has no change. The small change on layer distance indicates that the surface microstructure changes little in the structural

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