Vol 17 No 2, February 2008
1674-1056/2008/17(02)/0662-07

Chinese Physics B

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Atomistic simulation of kink structure on edge dislocation in bcc iron*

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(Received 9 October 2006; revised manuscript received 21 June 2007)

Based on the general theory of dislocation and kink, we have constructed the three kink models corresponding to the 1/2 ⟨111⟩{011} and 1/2 ⟨111⟩{112} edge dislocations (EDs) in bcc Fe using the molecular dynamics method. We found that the geometric structure of a kink depends on the type of ED and the structural energies of the atom sites in the dislocation core region, as well as the geometric symmetry of the dislocation core and the characteristic of the stacking sequence of atomic plane along the dislocation line. The formation energies and widths of the kinks on the 1/2 ⟨111⟩{011} and 1/2 ⟨111⟩{112} EDs are calculated, the formation energies are 0.05 eV and 0.04 eV, and widths are 6.02b and 6.51b, respectively (b is the magnitude of the Burgers vector). The small formation energies indicate that the formation of kink in the edge dislocation is very easy in bcc Fe.

Keywords: molecular dynamics, edge dislocation, kink structure, bcc iron
PACC: 6185, 6155F, 6170G

1. Introduction

The mechanical properties of metals are governed by many extremely complex mechanisms. One of the most important factors is the structure and mobility of dislocation.[1] At present it is commonly accepted that at finite temperature the dislocations in crystals glide in the Peierls relief due to nucleation of kinks and their propagation along the dislocation lines. This mechanism determines the dislocation mobility in covalent crystals but can also be essential in the bcc metals. It is found that the dislocation mobility depends exponentially on the formation and migration energies of kinks.[2] Kink excitations are responsible for some peaks of characteristic absorption spectra in metals.[3] Meanwhile, kinks are also of intrinsic interest. So the structure and energetics of kinks is of fundamental importance in metals.

In the classical papers, Duesbury[4,5] studied the structures, the Peierls stresses, and the formation energies of the isolated kinks and the kink pairs in the 1/2⟨111⟩ screw dislocation in potassium and bcc iron, and obtained a width of ∼6b with the energies between 0.01 and 0.5 eV for the isolated kinks in bcc iron. The formation energies of kinks in screw dislocations in Ta[6] and Mo[7] had been determined in a high accuracy by simulations with Green's function boundary conditions. A comprehensive study for the kink in the 1/2⟨111⟩ screw dislocation in bcc tantalum was performed by Wang *et al*,[8] who studied the multiplicity, the structural features and formation energies of the kinks. Nunes *et al*[9,10] studied the structures, the formation and migration energies of the kinks in the 90° partial dislocation in silicon. In their work, it was found that the asymmetric core reconstruction generates at least four distinct kink species as well as soliton defects, and that there exist certain low-energy kinks.

In contrast to extensive investigation on the structures and the formation energies of the kinks in screw dislocations, there exist few studies in the literature on the kinks in the EDs. Though it may be believed that kink mechanisms in the motion of ED are less important than in the screw dislocation due to low Peierls barrier in the ED, the formation of kinks in the ED are easier than that in the screw dislocation because the formation energy of a kink is directly proportional to the Peierls energy. Bacon *et al*[11,12] have conducted a comprehensive study for the core structure, static and dynamical behaviours of the ED in bcc Fe. Re-

*Project supported by the National Basic Research Program of China (Grant No 2006CB605102) and the Science Foundation of Central South University of Forestry & Technology, China (Grant No 06y016).
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cently, Tapasa *et al*[13] have studied the atomic-scale behaviour of a carbon interstitial atom in the core of a $1/2\,[111]\,(1\bar{1}0)$ ED in bcc Fe. Chang *et al*[14] have performed molecular dynamics simulations of the motion of edge and screw dislocations in bcc Mo. They found that at low temperatures the ED moves primarily through kink nucleation, whereas the mobility of the screw dislocation is strongly facilitated by the presence of a kink. So it is essential to understand the structure and energetics of kinks in the ED in metals. In this work, we will investigate the structures, widths and energies of kinks in the different types of EDs in bcc Fe using the molecular dynamics (MD) method.

2. The foundation of kink structure models

We use the MD simulation to study the structures and energies of the kinks in the EDs in bcc Fe by employing the Finnis–Sinclair (F-S) potential.[15,16] For bcc transition metals, the F-S potential is effective to simulate defects such as dislocation, grain boundaries and cracks.[17−19] The MD method is widely used in the static and dynamic simulations of material structure and property.[20−22]

2.1. Core structures of dislocations

In order to obtain the equilibrium atomic configurations of the EDs, we first adopt the MD method to simulate the $1/2\langle 111\rangle\{011\}$ and $1/2\langle 111\rangle\{112\}$ EDs. The initial configurations of the $1/2\langle 111\rangle\{011\}$ and $1/2\langle 111\rangle\{112\}$ EDs are constructed on the basis of the elastic stress field theory.[1] The blocks we use in our simulation contain 499392 and 452150 atoms for the $1/2\langle 111\rangle\{011\}$ and $1/2\langle 111\rangle\{112\}$ EDs respectively, consisting of 51 repeated cells along the Burgers vector direction (x axis), 32 repeated cells along the direction normal to the slip plane (y axis), and 51 repeated cells along the dislocation line direction (z axis).

We adopted the MD method to relax the initial configurations of the two types of EDs. We employ fixed boundary conditions for two directions normal to the dislocation line, while the periodic boundary condition is applied to the direction of dislocation line. After relaxation, we got the equilibrium atomic configuration with C_2 symmetry for the $1/2\langle 111\rangle\{011\}$ ED, while the $1/2\langle 111\rangle\{112\}$ ED appears the asymmetric core.[23] The structural model for the $1/2\langle 111\rangle\{011\}$ ED consists of six nonequivalent (112) planes (designated respectively as *A, B, C, D, E* and *F* planes) perpendicular to the dislocation line, and two nonequivalent (011) planes for the $1/2\langle 111\rangle\{112\}$ED (designated as *A* plane and *B* plane). The orders of stacking along the direction of dislocation line for the two types of EDs are *ABCDEF* and *AB*, respectively. The core structures of the $1/2\langle 111\rangle\{011\}$ and $1/2\langle 111\rangle\{112\}$ EDs are shown in Figs.1 and 2. Figure 1 gives the atomic configurations in the x-y plane, and Fig.2 in the x-z plane (Only two layers of atoms above and under the slip plane for each type of ED are drawn). It is obvious that the structure of the dislocation core is different from that of bulk bcc Fe.

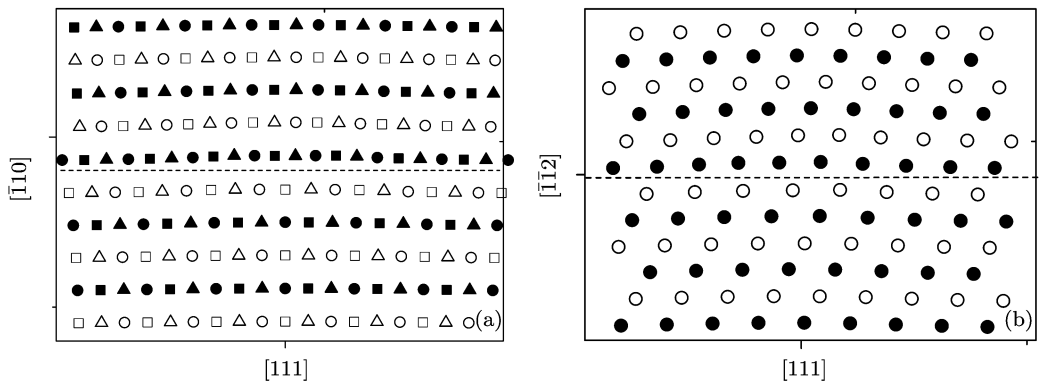


Fig.1. The atomic configuration of the dislocation system in the x-y plane after the relaxation. The symbols of solid circle, open circle, solid square, open square, solid triangle, and open triangle denote the atoms on the stacking planes *A, B, C, D, E* and *F*, respectively. The dashed line indicates the slip plane. (a) the $1/2\langle 111\rangle\{011\}$ ED; (b) the $1/2\langle 111\rangle\{112\}$ED.

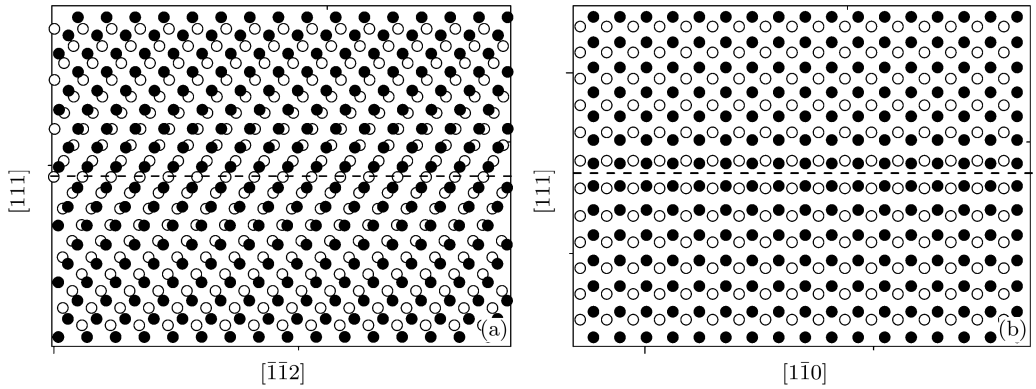


Fig.2. The atomic configurations of the dislocation system in the x-z plane after the relaxation (only two layers of atoms above and under the slip plane for each type of ED are drawn). The solid circles denote a layer of atoms located above the slip plane, and the open circles denote the layer of atoms located below the slip plane. (a) the 1/2⟨111⟩{011}ED; (b) the 1/2⟨111⟩{112} ED. Dislocation lies along dashed line.

2.2. Kink structures

2.2.1. Construction of initial structure of kink

In this section, we study the structure of a geometric kink. According to the definition of the kink, it is known that the dislocation line can only be kinked on the slip plane. On the basis of the relaxed structures of ED cores, we construct the initial configurations of the kinks corresponding to the two types of EDs, in which the kink is assumed to be located centrally in the crystal, and all atoms with the coordinate $z > 0$ are translated a height of kink along the Burgers vector direction. The kink height, which is the distance between two nearest Peierls valley, is $\frac{\sqrt{3}}{2}a_0$ (a_0 is the lattice constant). For the 1/2⟨111⟩{112}ED, two different initial configurations of kinks appear to be possible. In the same way, there are six possible different initial configurations of kinks for the 1/2⟨111⟩{011}ED. These possible initial configurations are schematically illustrated in Fig.3.

2.2.2. Relaxation effect and atomic configuration of kink

After constructing the initial kink configurations, we relax the various structures to their minimum energy states by the MD method, in which fixed boundary conditions are applied to the x, y and z directions. We obtain the atomic configurations of the three types of kinks and they are presented in Fig.4. For the 1/2⟨111⟩{112}ED, there is one type of kink, while for the 1/2⟨111⟩{011}ED there are two types of kinks. The kinks on the 1/2⟨111⟩{011} and 1/2⟨111⟩{112} EDs have the same symmetry as the corresponding EDs.

In order to see the reconstruction of atoms in the kinks clearly, we analyse the structure change of the kink before and after the relaxation, for example, the kink in the 1/2⟨111⟩{011} ED. In Fig.5(a), we have drawn the initial atomic configuration of the kink corresponding to Fig.3(e) in the x-y plane. The atomic configuration of the kink after the relaxation corresponding to Fig.3(l) is shown in Fig.5(b).

From Fig.5(a), it can be seen that the central atoms of the dislocation core—Fe2, Fe3, and Fe6 in the A atomic plane—form an inverted triangle, while the central atoms of the kink in Fig.5(b)—Fe2, Fe5 and Fe6 atoms in the A' atomic plane—form a normal triangle. That is because the atoms in the kink are rearranged after relaxation and the rearrangement results in the configuration of the A' atomic plane in the kink similar to that of B atomic plane in the 1/2⟨111⟩{011}ED. Another distinction between the relaxed kink and the unrelaxed kink is that the centre of the normal triangle on the A' atomic plane in Fig.5(b) (we regard it as the centre of the kink) is displaced by 0.1242 nm (approximately half height of the kink) parallel to the [$\bar{1}\bar{1}\bar{1}$] Burgers vector direction relative to the centre of the inverted triangle in the A atomic plane in Fig.5(a). Similarly, for the kink on 1/2⟨111⟩{112}ED, the core is reconstructed, and the centre of the kink is also displaced by 0.1242 nm. Therefore, the atomic configurations of the two types of kinks are different from those of the corresponding EDs. A kink has its unique structure.

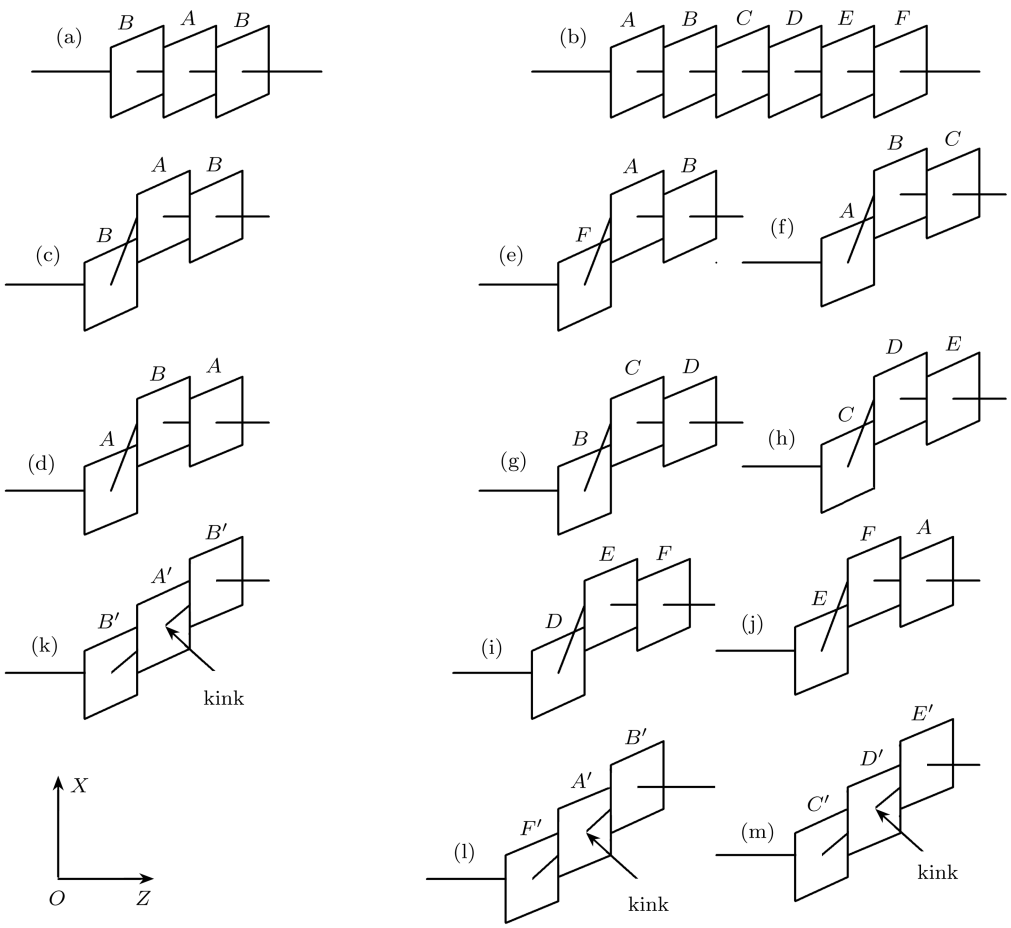


Fig.3. A schematic representation for the stacking sequence of atomic planes in the EDs, the types of the initial kinks, and the types of the kinks after the relaxation. (a) the $1/2\langle 111\rangle\{112\}$ ED; (b) the $1/2\langle 111\rangle\{011\}$ED; (c) and (d) the initial kinks for the $1/2\langle 111\rangle\{112\}$ED; (e)–(j) the initial kinks for the $1/2\langle 111\rangle\{011\}$ ED; (k) the kink in the $1/2\langle 111\rangle\{112\}$ED after the relaxation; (l) and (m) the kinks in the $1/2\langle 111\rangle\{011\}$ED after the relaxation.

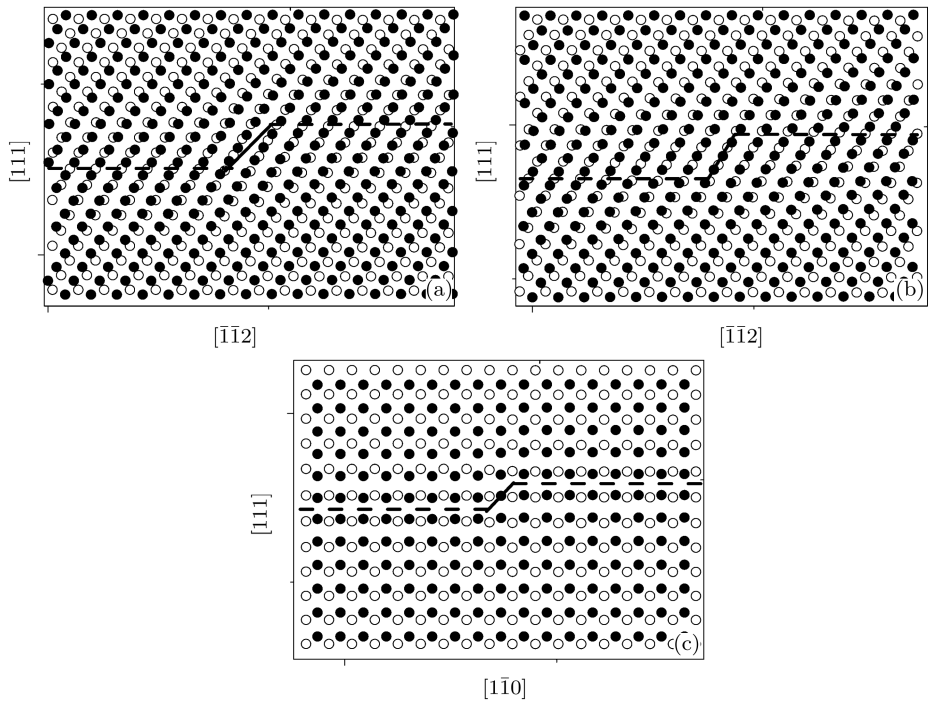


Fig.4. The atomic configurations of kinks in the x-z plane after the relaxation. The meaning of the symbols is the same as that in Fig.2. (a) the kink I in the $1/2\langle 111\rangle\{011\}$ ED; (b) the kink II in the $1/2\langle 111\rangle\{011\}$ ED; (c) the kink in the $1/2\langle 111\rangle\{112\}$ ED. Dislocation lies along the dashed line.

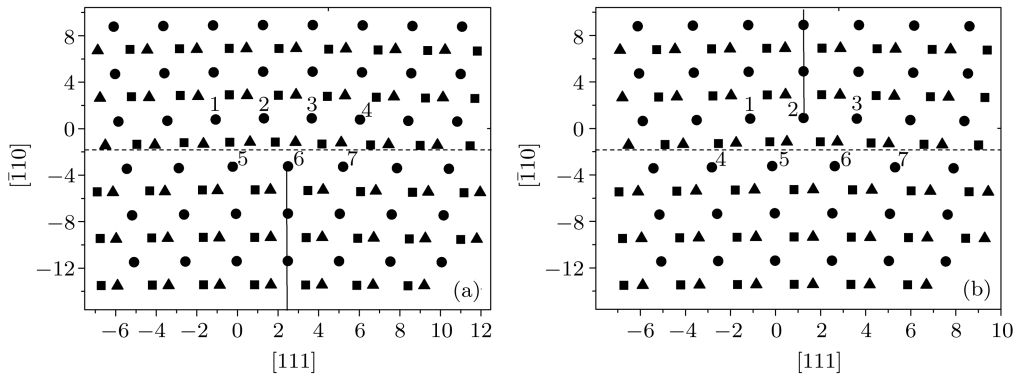


Fig.5. The atomic configurations of the kink on the 1/2⟨111⟩{011} ED before and after the relaxation. The symbols of square, circle and triangle denote the successive three layers of atoms in the kink, which correspond to the atoms in F, A and B atomic planes in Fig.3(e) and the atoms in F', A' and B' atomic planes in Fig.3(l), respectively. The dashed line denotes the slip plane. The vertical line is drawn to show symmetry in the region of dislocation core in $A(A')$ plane. (a)the unrelaxed kink; (b) the relaxed kink.

2.2.3. Structure analysis of kinks

The 1/2⟨111⟩{112}ED corresponds to one type of kink, and the dislocation line is kinked at the A atomic plane. While 1/2⟨111⟩{011}ED corresponds to two types of kinks, the dislocation line can be kinked at the A and D atomic plane, separately. From the characteristics of the kink structure as described above, one can say that the type of ED is not the only factor determining the structure of kink. In order to discuss this problem further in detail, we calculate the structural energies of the atomic sites in nonequivalent atomic planes of these EDs, and the results are shown in Fig.6.

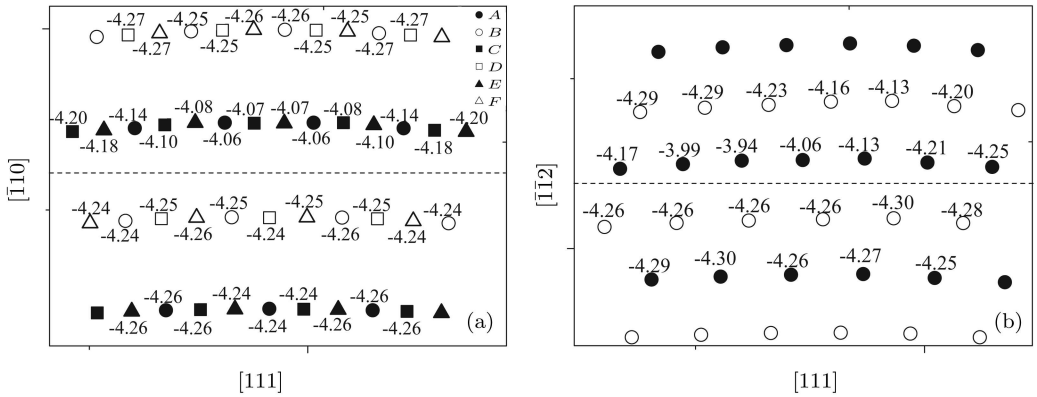


Fig.6. The structural energies (eV) of the atomic sites in the ED core. (a) the 1/2⟨111⟩{011}ED; (b) the 1/2⟨111⟩{112}ED. The dashed line denotes the slip plane.

From Fig.6, one can see that the structural energies of the atomic sites on the slip plane at the core region in the A atomic plane are higher (absolute value is small) than those in other atomic planes for the two types of kinks. This implies that the atoms at the core region in the A atomic plane are easier to move than those in other atomic planes; consequently, the formation energy of the kink along the A atomic plane is smaller than that along other atomic planes. Meanwhile, in order to decrease the energy of the kink system the configuration of the A' atomic plane at the kink should be similar to that of the B atomic plane at the corresponding ED. For the 1/2⟨111⟩{011}ED core, though the structural energies of the atomic sites at the core region in the D atomic plane are lower than those in the C and E atomic planes, the symmetry of the kink are higher when the kink occurs along D or A atomic plane. Based on the above analysis, we can find that the formation and structure of kinks depend not only on the type of ED and the structural energy of the atomic sites at the core region, but also on the geometric symmetry of the dislocation core and

the characteristic of the stacking sequence of atomic planes along the dislocation line.

3. Energy and width of kink

We define the kink formation energy as the energy difference between the kinked dislocation and the straight one. The formation energies of the kinks on the $1/2\langle 111\rangle\{011\}$ and $1/2\langle 111\rangle\{112\}$EDs are 0.05 eV and 0.04 eV, respectively. The small formation energies indicate that formation of kink in the ED is very easy in bcc Fe, which may be related to the low Peierls barrier in the ED. We have also calculated the electronic structure of the kink in the $1/2\langle 111\rangle\{011\}$ED.[24] The calculated formation energy of the kink is 0.06 eV, which is consistent with the present result.

The width of a kink is the measure of the spatial extent of the kink displacement field parallel to the dislocation line.[4] While the structural energy variation of the atomic sites in a kink may be used to determine the width of the kink. The difference between the structural energies of the atoms in the kinked dislocation line and the corresponding position on the straight dislocation line ($\Delta E_{\rm l}$) is plotted against coordinate z in Fig.7. When the energy variation $\Delta E_{\rm l}$ tends to zero, the kink displacement field will disappear. Form Fig.7, the widths of the kinks may be estimated, which are 6.02b and 6.51b for the kinks in $1/2\langle 111\rangle\{011\}$ and $1/2\langle 111\rangle\{112\}$ EDs, respectively.

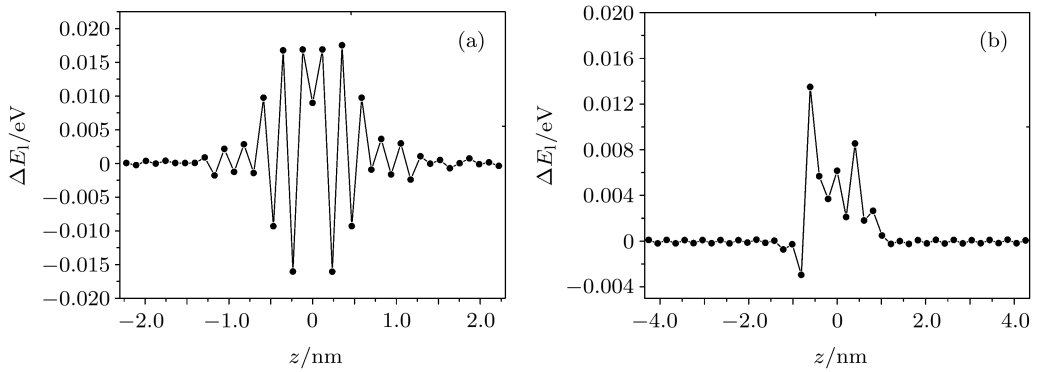


Fig.7. The energy difference between atoms in the kinked dislocation and the corresponding atoms in the straight dislocation vs z-coordinates. (a) the kink in $1/2\langle 111\rangle\{011\}$ ED; (b) the kink in $1/2\langle 111\rangle\{112\}$ED.

If the kink lies in the region of lattice distortion, the corresponding atoms would possess a larger activity. This makes the kink mobility increase evidently. The motion of the kink along the dislocation line causes the entire dislocation line to pass from one Peierls valley to the adjacent one. Therefore, the formation of the kink usually benefits the movement of the dislocation.

4. Conclusions

We have constructed the three kink models corresponding to the $1/2\langle 111\rangle\{011\}$ and $1/2\langle 111\rangle\{112\}$ EDs in bcc Fe using the MD method. In $1/2\langle 111\rangle\{011\}$ ED there exist two types of kinks, while in $1/2\langle 111\rangle\{112\}$ ED, there is only one type of kink. We find that the structure of a kink not only depends on the type of ED (Burgers vector is an important parameter) and the structural energy of the atomic sites in the dislocation core region, but also on the geometric symmetry of the dislocation core and the characteristic of the stacking sequence of atomic plane along the dislocation line. We have also calculated the formation energies and widths of the kinks in the different types of EDs, and found that the formation energies of the kinks are low. This indicates that the formation of kink in the ED is very easy in bcc Fe.

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