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Dissociation of super-dislocations and the SISF energy in γ-TiAl based alloy with Nb-doping, as studied by HRTEM

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Abstract The dissociation of super-dislocations in γ-TiAl in Nb-doped Ti-48 at.% Al-5 at.% Nb has been studied by high resolution transmission electron microscopy (HRTEM). The SISF energy in γ-TiAl in Ti-48 at.% Al-5 at.% Nb was calculated to be 35 mJ/m^2 according to the dissociation width. It is concluded that Nb addition may affect the electronic structure of TiAl and furthermore decrease SF energies in TiAl alloys, which is partly responsible for the strengthening effect of Nb-doping.

γ-TiAl based intermetallics as potential high temperature structural materials in aerospace and automotive industries have attracted extensive research interest owing to their unique combination of properties at elevated temperature [1–4]. However, their further application is still hindered by the limited ductility and poor fracture toughness at room temperature [5, 6]. Microstructural control and alloying are the main methods to improve the properties of these alloys [7, 8]. The most promising TiAl alloys are based on the composition of Ti-48 at.% Al with ternary or quarternary additions [9]. Besides, it has been recognized that Nb addition can enhance the high temperature strength, oxidation and creep resistance [10–12]. The strengthening mechanism related to Nb addition has been discussed extensively, involving solid solution strengthening, refinement of microstructure, and the increase of critical resolved shear stress (CRSS) for the cross slip of dislocations. However, studies concerning the influence of Nb addition on the stacking fault (SF) energies are still limited [13–15] and the results are not entirely consistent. The SF energy is expected to affect the glide, climb and multiplication processes of dislocations, as well as the twinning process and stability of the interfaces. Therefore, further studies concerning the influence of Nb addition on SF energy are needed.

In this letter, we report the superlattice intrinsic stacking fault (SISF) energy of γ-TiAl in Ti-48 at.% Al-5 at.% Nb alloy. The SISF energy γ_{SISF} was calculated from the width of the dissociated $[1/2<11\bar{2}]$ super dislocation as observed by the high resolution transmission electron microscopy (HRTEM) method. The result will be analyzed and discussed.

The Ti-48 at.% Al-5 at.% Nb alloy was prepared from high purity Ti (99.9 wt.%), Al (99.9 wt.%) and Nb (99.9 wt.%) elements by levitation melting under argon atmosphere. The hearth-button ingot of about 200 g was reversed and remelted three times in order to reduce segregation. The samples with size $4 \times 6 \times 7$ mm^3 were cut from the as-cast ingots. The 3 mm diameter disks with a 0.4 mm thickness were prepared from the sample by utilizing spark discharge cutting. The TEM disks were prepared by standard procedures. The microstructures of the specimens were studied in a Tecnai F20 field emission scanning and transmission electron microscope (STEM) equipped with an energy dispersive X-ray spectrometry (EDX) unit operated at 200 kV.

The as-cast Ti-48 at.% Al-5 at.% Nb consists of mainly γ-TiAl lamellae with $L1_0$-structure, γ-TiAl twin lamellae and some α_2-Ti_3Al lamellae with $D0_{19}$-structure, which are arranged alternately. The orientation relationship between γ and α_2 complies with the Blackburn relationship. In Fig. 1, the area indicated with an arrow shows a dislocation with dot-like contrast in a γ-TiAl lamella. The image was recorded under $[\bar{1}01]$ direction. This contrast character

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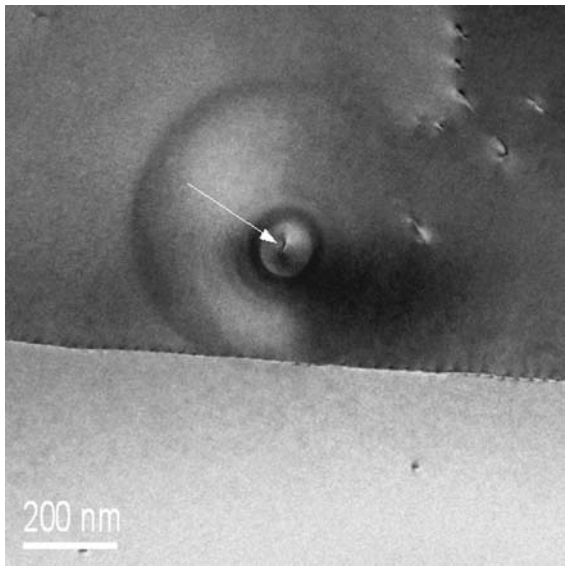

Fig. 1 The dislocation indicated with an arrow shows dot-like contrast, which implies that the dislocation line is nearly parallel to the beam direction. The image was taken along the [$\bar{1}$01] direction

implies that the line direction of the dislocation is nearly parallel to [$\bar{1}$01] direction. HRTEM is one of the most powerful techniques to disclose the microstructure of the dislocation core. Figure 2a shows the HRTEM image of the corresponding dislocation marked in Fig. 1. The dislocation core has an extended region. Inserted in Fig. 2a are the fast Fourier transform (FFT) patterns from different areas, the top left and the bottom right FFT patterns from left and right square, respectively, is not absolutely same, the former shows diffraction character of SF displaying extended line perpendicular to stacking fault plane (111) and the latter shows the diffraction pattern of [$\bar{1}$01] zone axis without the character of an SF. Figure 2b is the magnified inverse fast Fourier transform (IFFT) image. Two partial edge dislocations with the same sign can be observed in Fig. 2b, their slip plane is (111) according to the FFT pattern inserted in Fig. 2a. The Burgers vectors of the two partials have unequal projections in magnitude on the ($\bar{1}$01) plane along [$\bar{1}2\bar{1}$] direction and their projection signs are same. The projection lengths determined by the well-known Burgers circuit method are about 1/6[$\bar{1}2\bar{1}$] and 1/12[$\bar{1}2\bar{1}$], respectively. Referring to all the dislocation dissociations mechanism of γ-TiAl reported in the literature [16], with reasonable assumption the magnitudes of the projections are consistent with the projected length of the vectors of 1/3[$11\bar{2}$] and 1/6[$11\bar{2}$] on the ($\bar{1}$01) plane. So the Burgers vectors of the two dissociated partials are determined to be 1/3[$11\bar{2}$] and 1/6[$11\bar{2}$], respectively. The dislocation dissociation shown in Fig. 2 is consistent with the reaction on (111) plane as follows:

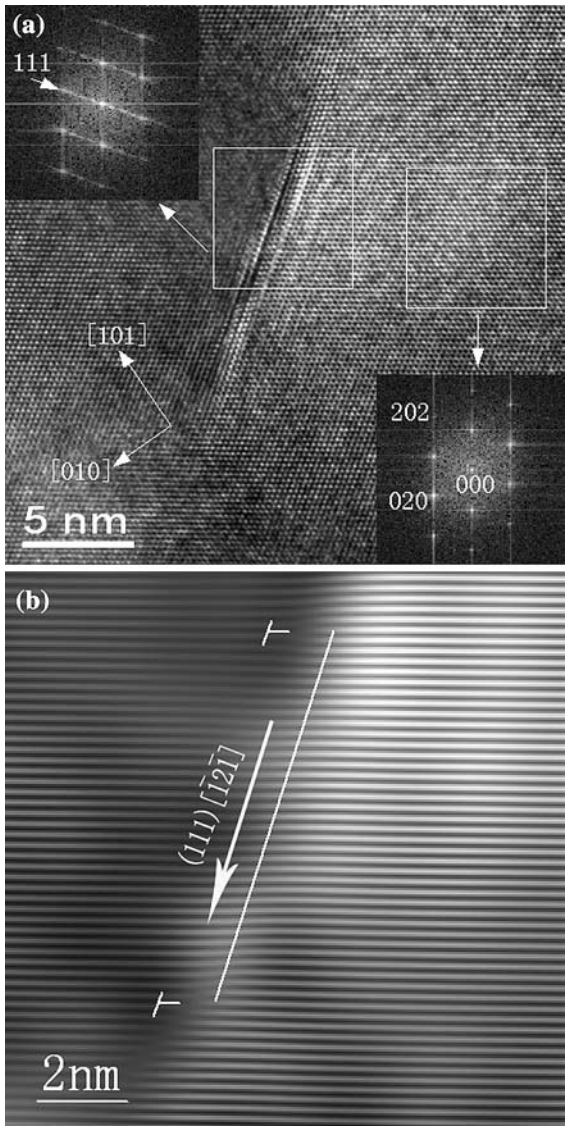

Fig. 2 (**a**) HRTEM micrograph shows dissociation of the dislocation, stacking fault marked with the left square can be observed clearly, the two inserted FFT patterns are not exactly the same, the top left one from the area with the left square shows diffraction character of SF displaying extended line perpendicular to stacking fault plane (111), while the bottom right one from the area with the right square shows diffraction pattern of [$\bar{1}$01] zone axis without character of SF (**b**) The magnified IFFT image of (a), two partial dislocations with the same sign can be observed, the slip plane is (111) according to FFT pattern inserted in (a)

$$1/2[11\bar{2}] \rightarrow 1/6[11\bar{2}] + \mathrm{SISF} + 1/3[11\bar{2}].$$

Figure 3 is the schematic drawing depicted the dislocation dissociation, only three successive atomic layers of ABC stacking are shown here and the atom plane is (111). The two vectors with dashed line along [$\bar{1}2\bar{1}$] in Fig. 3 are

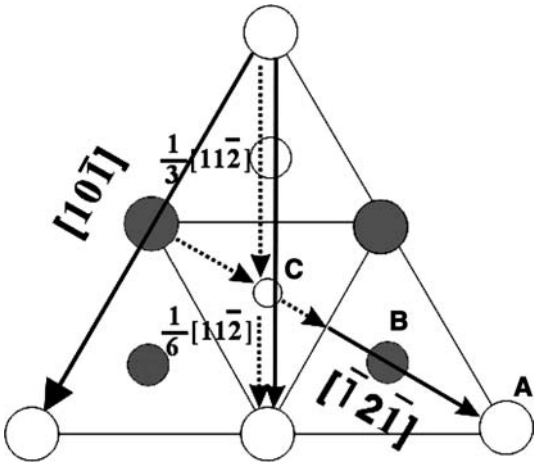

Fig. 3 Arrangement of atoms in the three successive (111) planes in γ-TiAl. Solid circles represent Ti and open circles Al. Three different sized circles represent three successive (111) layers in the ABC stacking sequence. The 1/2[11$\bar{2}$] super-dislocation dissociates into 1/6[11$\bar{2}$] and 1/3[11$\bar{2}$] partial dislocations with a SISF

1/6[$\bar{1}$2$\bar{1}$] and 1/12[$\bar{1}$2$\bar{1}$], which is the projection of 1/3 [11$\bar{2}$] and 1/6[11$\bar{2}$] along [10$\bar{1}$], respectively. The [10$\bar{1}$] dislocation was a mixed dislocation before its dissociation, the angle between the dislocation line and the Burgers vector is 30°.

In this case, there exists a repulsive elastic force between the two partials and an attractive force of SISF acts on the dissociated dislocations. Assuming that the two forces balance each other, the SISF energy can be calculated from the following equations [17]:

$$\gamma_{\mathrm{SISF}} = \mu b^2(2-v)/8\pi d_0(1-v) \quad (1)$$

and

$$d = d_0\{1 - [2v/(2-v)]\cos 2\Phi\} \quad (2)$$

where γ_{SISF} is the SISF energy, μ is the shear modulus (70 GPa [18]), v is Poisson's ratio (0.23 [18]), b is the Burgers vector of the partial dislocation, d is the separation width of the two partials and Φ is the angle between line direction of super-dislocation and the Burgers vector. Here, d is approximately 8.4 nm as measured from Fig. 2b and Φ is 30°. By substituting the corresponding values, the SISF energy is calculated to be 35 mJ/m^2.

In view of factors such as elastic anisotropy, interaction of dislocations and equilibrium separation, some error may be introduced, however, the SISF energy attained here can serve as an effective evaluation. Compared with the related report, the SISF energy decreases from 67 mJ/m^2 in Ti-48 at.% Al [13] to 35 mJ/m^2 in Ti-48 at.% Al-5 at.% Nb. The electronic structure of γ-TiAl with Nb addition is different from that without Nb addition. Nb atoms can decrease the degree of covalent bonding around themselves locally [19], this may result in the decrease of stacking fault energy. Therefore, it can be concluded that Nb addition decreases the SISF energy in TiAl alloys, which might account greatly for the strengthening in such alloys by doping Nb.

In summary, the dissociation of super-dislocations in Ti-48 at.% Al-5 at.% Nb was studied with the help of HRTEM. The SISF energy of γ-TiAl in Ti-48 at.% Al-5at.% Nb is about 35 mJ/m^2. Nb addition may affect the electronic structure of TiAl and furthermore decrease SF energies in TiAl alloys, which is partly responsible for the strengthening effect of Nb-doping.

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