DEBYE TEMPERATURE AND VALENCE ELECTRON STRUCTURE IN INTERMETALLIC TiAl①

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ABSTRACT

The Debye temperature θ_D of intermetallic compound TiAl at room temperature was determined by means of X-ray diffraction. The experiments show that the Debye temperature of TiAl is 515 K, which is obviously higher than that of Al (394 K) or Ti (380 K). The experimental results indicate that the bonding in the intermetallic compound TiAl is stronger than that in pure metal Ti or Al, which is in good agreement with the calculation of its valence electron structures. The relationship between the Debye temperature of TiAl and its brittle-ductile transition temperature is also dealt with in the paper.

Key words: Debye temperature intermetallic TiAl X-ray diffraction

1 INTRODUCTION

In recent years, much attention has been paid to intermetallic compound TiAl with the Ll_0 structure because of its numerous attractive characteristics which make it a potential candidate for high temperature structural applications. The Debye temperature in a solid may not only represent the interatomic force but also be related to many physical parameters, such as Young's modulus, vacancy formation energy and surface energy. The Debye temperature of intermetallic compound also provides important physical understanding of its bonding mechanism.

According to thermal vibration of atoms, the Debye temperature in a solid can be decided by measuring the relative change of Bragg intensities with powder samples. In the paper, the Debye temperature of intermetallic compound TiAl at room temperature was given by means of X-ray diffraction, and the relationship among the Debye temperature, valence electron structures and brittle-ductile transition temperature are discussed, too.

2 PRINCIPLES OF CALCULATION

For some crystals with known structure, the integrated intensity of Bragg diffraction in a powder sample is given by the kinematic approximation at temperature T

$$I_{(hkl)}(T) = KP(\theta)N|F^{T}_{(hkl)}|^2 \times \exp(-2\bar{B}\sin^2\theta / \lambda^2) \qquad (1)$$

where K is a constant; $P(\theta)$, the Lorentz polarization factor which is a function of Bragg diffraction angle, θ; $F^{T}_{(hkl)}$ is the theoretical

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structure factor; N, the multiplicity factor; $\overline{B}$, a mean Debye-Waller factor of measured materials ; λ and θ are the wave-length of the incident X-ray and Bragg diffraction angle respectively.

By taking logarithm of Eq. (1) and let

$$(F^{E}{}_{(hkl)})^{2}=I_{(hkl)}(T)/P(\theta)\cdot N,$$

the Eq (1) reduces to

$$\ln(F^{T}_{(hkl)}/F^{E}_{(hkl)})=\overline{B}\cdot\sin^{2}\theta/\lambda^{2}+C \qquad (2)$$

where $C=-\ln K$

If the integrated intensity of different Bragg diffraction at temperature T are made, the mean Debye-Waller factor B can be decided by the least squar method. The mean Debye temperature θ_D at room temperature can be expressed as

$$\theta_{D}=\sqrt{\frac{6h^{2}T}{M_{a}K_{B}\overline{B}}[\varphi(x)+\frac{1}{4}x]} \qquad (3)$$

where h—Planck's constant; K_B—Boltzman's constant; M_a— the mean mass of an atom; $\psi(x)$— Debye fuction; x— the ratio of Debye temperature to the experimental temperature.

3 EXPERIMENTAL PROCEEDURES

Alloy $Ti_{45}Al_{55}$ (at.−%) was melted in a vacuum high-frequency furnace and was drop-cast into dia 21 mm copper chill mold. The error of chemical composition was within 1 at.−%. The cast sample was annealed in a vacuum at a temperature of 1,350 ℃ for 50 h to ensure homogeneity and milled into powder less than 400 mesh (37 μ). The powder sample used by X-ray diffraction was annealed in vacuum at 700 ℃ for 10 h to minimize the residual stress.

The X-ray diffraction experiments were carriedd out on APD−10 X-ray diffraction equipment. The Cu K_α radiation with power of 35 kV−35 mA and graphite monochrometer were employed in the experiments. After the ranges of each Bragg peak were decided by fast scanning, the integrated intensities were measured by step scan with step length of 0.05 ° and holding time of 3 seconds. In this paper, the Gauss-Lorentz distribution was used to separate the over lapping peak in the diffraction profile of intermetallic compound TiAl with Ll_0 structure and the integrated intensities were calculated respectively.

4 EXPERIMENTAL RESULTS AND DISCUSSION

4. 1 *Mean Debye Temperature* θ_D *of* TiAl

Supposing a part of Ti was replaced by extra Al and the atomic scattering factors of Ti and Al were revised by anomalous scattering, the integrated intensity $I_{(hkl)}(T)$, theoretical structure factor $F^{T}_{(hkl)}$ and in $[F^{T}_{(hkl)}/F^{E}_{(hkl)}]$ of different Bragg diffraction with a range from (001) to (400) for TiAl were calculated (Table 1). B were calculated only by fundamental Bragg diffraction which can minimize the influence of order on the experimental results. The in $[F^{T}_{(hkl)}/F^{E}_{(hkl)}]$ of the fundamental as a function of $\sin^2\theta/\lambda$ was given in Fig. 1.

Based on the gradient calculated by the linear least square method, the mean

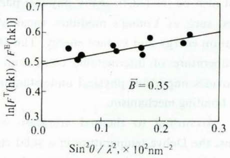

Fig. 1 The $\ln[F^{T}_{(hkl)}/F^{E}_{(hkl)}]$ as a function of $\sin^2\theta/\lambda^2$ for TiAl

Debye-Waller factor can be deduced as $\bar{B} = 0.35 \times 10^{-2}$ nm^2. The Debye temperature of TiAl could be obtained from Eq. (3), $\theta_D = 515$ K.

4.2 *Debye Temperature θ_D and Valence Electron Structures of* TiAl

The Debye Temperature in a solid represents interatomic force. The Debye temperature of TiAl at room temperature measured by X–ray diffraction in this paper is obviously greater than that of pure Ti or Al, which are 380 K and 394 K, respectively. This result indicates that intermetallic compound TiAl has a stronger bond than pure Ti or Al[1~3].

Table 1 The integrated intensity $I_{(hkl)}(T)$, theoretical structure factor F^T(hkl)and ln $[F^T_{(hkl)} / F^E_{(hkl)}]$ for TiAl at room Temperature

hkl	$\sin^2\theta \cdot \lambda^2 / \times 10^2$nm	$F^E_{(hkl)}$	$F^T_{(hkl)}$	$\ln[F^T_{(hkl)} / F^E_{(hkl)}]$
001	0.015	7 270	14.17	0.527
110	0.031	4 346	12.94	0.646
111*	0.046	100 437	48.94	0.550
002*	0.060	17 647	46.48	0.506
200*	0.062	31 830	46.08	0.526
201	0.077	2 730	10.14	0.458
112	0.091	1 535	9.51	0.582
202*	0.122	18 798	38.85	0.559
220*	0.125	9 368	38.63	0.542
003			7.99	
221	0.140	418	7.86	0.786
130	0.156	665	7.48	0.444
113*	0.166	11 228	35.24	0.549
131*	0.171	22 319	34.89	0.528
222*	0.185	8 745	33.95	0.594
132	0.216	552	6.55	0.623
004*	0.240	1 656	30.82	0.569
400*	0.250	3 037	30.33	0.598

* fundamental Bragg diffraction

The reason why TiAl has great Debye temperature can be explained by its valence electron structures. The results of valence electronstructures calculated by BLD analysis show that the covalent electrons n_c and lattice electron η belonging to each atom of TiAl are 3.104,4 and 0.395,6 respectively, which indicate that the fraction of covalent bond in TiAl is greater as compared with the other alloys. Table 2 lists the valence electron structures and Debye temperature of TiAl, Ti_3Al and Ti (α). It was shown in ref. [4] that the ratio of covalent electrons and valence electrons , η, indicates the fraction of covalent bond in a solid. As shown in Table 2, the covalent electrons and η of TiAl are higher than that of any other alloy. The above results show that the great Debye Temperature of TiAl corresponds to its valence electron structures.

Table 2 The valence electron structures and θ_D of TiAl, Ti_3Al and Ti(α)

Alloy	n_c	n_l	$\eta = n_c / n_c + n_l$	θ_D,K
TiAl[1]	3.1044	0.3956	88.7%	515
TiAl[4]	2.8743	0.8757	76.6%	480
TiAl[4]	2.7536	1.2464	68.8%	380

According to the Debye theory, the Debye temperature in a solid can be expressed as[5]

$$\theta_D = \hbar\gamma_{max} / K_B \tag{4}$$

where $\hbar = \eta / 2\pi$; γ_{max} is the frequency cooresponding to a total of oscillators being operative. Since the peierls stress depends on the short range stress field of dislocation core, it is sensitive to thermal energy in lattice. To some crystallines with greater peierls stress, the thermal enchantment is needed to make the dislocations move. As intermetallic compound TiAl has high Debye temperature θ_D and γ_{max}, it needs high temperrature to get enough thermal activity to move the glissle dislocation. The above results show that the high brittleductile transition temperature in alloy TiAl corresponds to its Debye temperature and valence electron structures.

5 CONCLUSIONS

(1) The Debye temperature of TiAl at

room temperature measured by X-ray diffraction is 515 K.

(2) The Debye temperature of TiAl is obviously higher than that of pure Ti or Al, indicating that interatomic force of TiAl is strong . This result corresponds to its valence structures.

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