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Electrical Resistivity of $Ti_{0.862}Al_{0.102}V_{0.036}$ Alloy between 4 and 1000 K

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We have measured the electrical resistivity ρ of a $Ti_{0.862}Al_{0.102}V_{0.036}$ alloy in the temperature range 4–1000 K. At temperatures above about 500 K, a saturation behavior of ρ is observed and is ascribed to the breakdown of the Ioffe-Regel criterion. In addition, we observe a considerably weakened temperature dependence of the electron-phonon coupling in the range $\approx$100–1000 K, compared with that in good metals.

[electrical resistivity, resistivity saturation, Ioffe-Regel criterion, electron-phonon coupling, titanium alloys]

§1. Introduction

The electrical conduction in alloy metals has long been of great interest and importance. In particular, in many alloy metals with a room-temperature resistivity of order 100 $\mu\Omega$cm, a saturation of the resistivity, ρ, is observed at high temperatures.[1-3] Despite of the efforts of several studies that attempted to understand this phenomenon,[3-6] the origins of this saturation behavior however remain to be quantitatively studied. Qualitatively, it is currently believed that a saturation of ρ can occur when the electronic mean free path, l, is reaching the interatomic spacing of the material. This issue was first studied by Ioffe and Regel[4] and Mooij,[5] and more recently by Allen.[6] Typical materials that reveal this sort of behavior are, *e.g.*, Nb_3Sn, Nb_3Sb (refs. 1 and 2), and Nb_3Ge (ref. 3). In this paper, we report our investigations of the electrical resistivity of a $Ti_{0.862}Al_{0.102}V_{0.036}$ alloy as a function of temperature T in the range 4–1000 K. The mechanical properties and fracture topography[7-9] and the low-temperature electrical resistivity and superconductivity[10,11] of this alloy has previously been extensively studied. On the other hand, the variation of ρ with T of this alloy, especially at T above 300 K, has not yet been investigated. Since Ti–Al–V, as many other titanium alloys,[12-14] will very likely be of great technological importance, it is therefore a good idea to understand its electrical transport properties above room temperatures.

Physically, presuming that the electronic scattering rates are additive, the resistivity ρ of a metal can be written as

$$\rho(T)=\rho_0+\rho_{ph}(T), \tag{1}$$

where ρ_0 is due to the *elastic* scattering of the conduction electrons by impurities and imperfections in the material, and $\rho_{ph}(T)$ is due to electron-phonon coupling. It is well known that the residual resistivity ρ_0 is temperature-independent, while $\rho_{ph}(T)$ follows the Bloch-Grüneisen law in good metals.[15] At temperatures above, say, 50–100 K or $(1/4\text{–}1/2)\vartheta_D$ (where ϑ_D is the Debye temperature), $\rho_{ph}(T)$ is approximately linear in temperature for most good metals. In (extremely) disordered metals, the behavior of $\rho_{ph}(T)$ has yet to be studied. In the following, our results are compared with eq. (1), and in particular are accounted for in terms of a short electronic mean free path l resulting from strong lattice disorder in

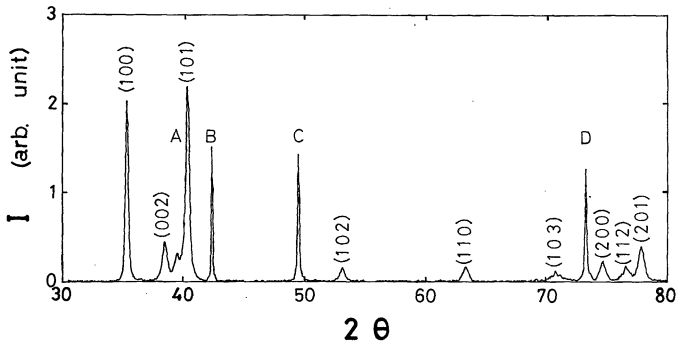

Fig. 1. X-ray diffraction patterns of $Ti_{0.862}Al_{0.102}V_{0.036}$. The sample has a hexagonal structure with lattice parameters $a=2.933\pm0.062$ Å and $c=4.677\pm0.146$ Å.

the atomic level in the alloy. As a consequence of the extremely short $l(<5$ Å), we observe a saturation of ρ at high temperatures (>500 K).

§2. Experimental Method

The ternary $Ti_{0.862}Al_{0.102}V_{0.036}$ (hereafter referred to as Ti-Al-V) alloy was prepared by standard arc melt method. Appropriate amounts of high-purity Ti, Al, and V elements were first arc melted and the melted ingot were annealed at 1200 K for one week. The structure of the specimen was studied by X-ray diffraction method performed on an MXP[18] system obtained from Mac Science Co; Ltd. A least-squares refinement program Crystal System Determination was also utilized. The diffraction patterns of the specimen are shown in Fig. 1, which indicate a dominant hexagonal structure with lattice parameters $a=2.933\pm0.062$ Å and $c=4.677\pm0.146$ Å. Unfortunately, secondary phases are also present which result in the four lines marked as A, B, C and D in Fig. 1. Efforts have been made to study the origin of these impurity lines and are only partly successful. We find the line B can be identified as resulting from V (which has a strongest diffraction peak occurring at $2\vartheta=42.16$). This suggests that V is not fully incorporated into the Ti-Al-V alloy phase. (Therefore, the atomic percents Ti:Al:V=0.862:0.102:0.036 are only meant to be nominal percents.) The three remaining lines A, C and D can be assigned in terms of a secondary hexagonal structure with lattice parameters $a=5.621\pm0.672$ Å and $c=4.568\pm0.415$ Å. However, the exact (say, Ti-Al-V or Ti-Al) phase which possesses such diffraction lines cannot be identified, although we are positive that these three lines are not due to the Ti_3Al phase. Chemical analysis performed on the specimen revealed an Fe impurity level of ≈240 ppm. No other metal impurities were detected. In addition, Meissner effect measurements in specimens cut from this ingot indicated a *single* superconducting transition occurring at 3.8 K. This amount of critical temperature is in agreement with that found in previous study.[10] In the following discussion of the electrical conduction in the specimen, we presume that the overall behavior is dominated by the Ti-Al-V alloy phase.*

Rectangular samples, typically of size $1\times2\times10$ mm^3, were sliced from this ingot by a low speed diamond saw for resistance measurements. Molybdenum electrodes were carefully spot-welded to the samples. DC resistances were measured by standard four-probe technique, using a North Hills Model CS-12 current source and a Keithley Model 181 nanovoltmeter for signal detection. Resistance measurements between 4 and 300 K

* The secondary phase which is characterized by the diffraction peaks A, C and D is not likely to play a crucial role in causing the resistivity saturation at high temperatures. (See below.) This can be understood in terms of the Ti-Al-V alloy phase forming the main body or conduction matrix of the specimen which embeds the secondary phases. The observed behavior or resistivity saturation is a characteristic of the conduction matrix.

were performed on a standard liquid helium dewar, with a silicon diode and a platinum thermometer as temperature sensors; while measurements between 300 and 1000 K were performed on a Marshall Model 1207 furnace, with two K-type thermometers as temperature sensors. The furnace was filled with helium gas during measurements.

§3. Results and Discussion

Figure 2 shows the resistivity ρ as a function of temperature T for the Ti-Al-V alloy (●). The resistivities of the starting elements Ti (○), Al (□), and V (△), respectively, are also shown for comparison. As is expected and is clearly seen in Fig. 2, the temperature dependences of ρ for Al and V, respectively, are typical for metals, i.e., the behavior of ρ is Bloch-Grüneisen-like.[15] The behavior of ρ for Ti is a little more complicated, which we will discuss below. The magnitudes of ρ_0 or ρ(6 K) are 2.93, 0.15, and 5.8 $\mu\Omega$cm for Ti, Al, and V, respectively, while it is about 2 orders of magnitude ($\approx 162\,\mu\Omega$cm) higher in the alloy. The large ρ_0 in Ti-Al-V comprises a dominating part of the total resistivity and results in a small resistivity ratio of $\rho(300\text{ K})/\rho(6\text{ K})=1.16$, compared to those (19.5, 20.9, and 5.0 for Ti, Al, and V, respectively) in the starting elements. More significantly, a deviation from a linear T-dependence of ρ in Ti-Al-V becomes very noticeable at temperatures above about 300 K. At even higher temperatures (>500 K), a "saturation" of ρ is observed, i.e., ρ becomes independent of T. The saturation value of ρ is $\approx 210\,\mu\Omega$cm. This phenomenon of resistivity saturation has been previously seen in other materials such as Nb_3Sb, Nb_3Sn (refs. 1 and 2), and Nb_3Ge (ref. 3). There is however no good theory to explain this phenomenon, although it is generally believed that this behavior is connected with the breakdown of the Joffe-Regel criterion in very disordered metals.[4,5]

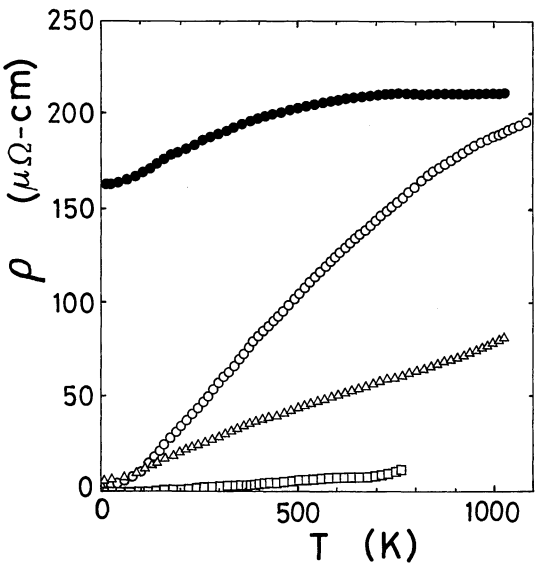

Fig. 2. The resistivities ρ as a function of temperature for Ti-Al-V (●), Ti (○), V (△), and Al (□), respectively.

The Joffe-Regel criterion[4,5] states that a metallic state of a material can exist only when $k_F l$ is larger than unity, where k_F is the Fermi wave number of the material. In good metals, $k_F l \gg 1$; while in disordered metals $k_F l$ can be as small as of order unity, depending on the degree of disorder. Combining with the Drude formula for conductivity, $\sigma=1/\rho=ne^2\tau/m$ (where n, e, τ, and m have the usual meaning), a value of $k_F l \approx 2\pi$ implies a limiting resistivity of $\rho \approx h/(\kappa_F e^2)$ (where h is the Planck's constant). With a typical value ($\approx 1\times 10^8$ cm^{-1}) of k_F in usual metals, this in turn suggests a $\rho \approx 200\,\mu\Omega$cm. Physically, this observation implies that when the resistivity in a metal is of order 100–200 $\mu\Omega$cm, the magnitude of l is reaching the interatomic spacing of the material and hence can no longer be reduced any further, say, by increasing T or the electron-phonon coupling. (Note that k_F is no longer well defined if l is extremely short.) As a consequence, ρ approaches a constant or saturates. Indeed, this is the case for our Ti-Al-V alloy which has a $\rho(300\text{ K})=189\,\mu\Omega$cm. Therefore, the present observation, Fig. 2, supports the validity of the Ioffe-Regel criterion (as a criterion for a metal-insulator transition). Similar but less evident behavior can be seen in the T-dependence of ρ in Ti. In this case a deviation from linearity is observed at T above about 600 K where $\rho \approx 125\,\mu\Omega$cm. Figure 2 shows clearly that the deviation increases with increasing T or decreasing l, although a saturation is not fully developed up to 1100 K. No visible deviation from the

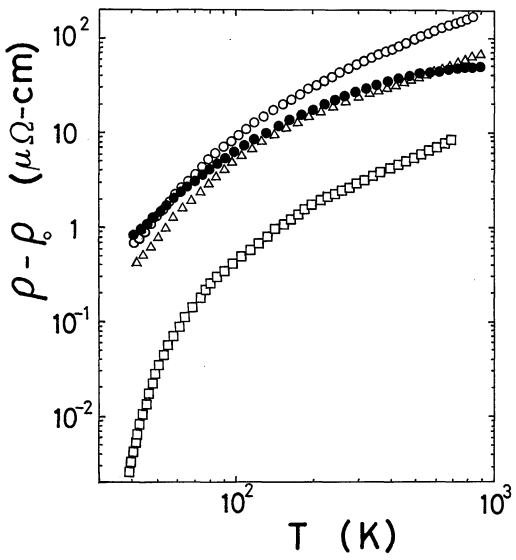

Fig. 3. The variations of ρ-ρ_0 or ρ_{ph} with temperature for the alloy Ti–Al–V (●), and the elements Ti (○), V (△), and Al (□), respectively.

Bloch-Grüneisen law is observed in either Al or V, both having values of ρ well below 200 $\mu\Omega$cm at $T < 1000$ K.

In the above discussion of the Ioffe-Regel criterion, the relevant scattering mechanisms which dominate and hence result in a short l are not explicitly specified. More specifically, it is not clear whether the saturation of ρ at high T is due to a large ρ_0, to some intriguing T-dependent behavior of ρ_{ph} in disordered or alloy metals, or to some combination of both. Efforts to distinguish the relative importance of the factors which determine the saturation behavior of ρ will be of fundamental interest and importance. In crystals or ordered systems, the behavior of ρ_{ph} is well understood and is described by the Bloch-Grüneisen law[15] as mentioned above. To the best of our knowledge, the behavior of $\rho_{ph}(T)$ in (very) disordered metals however has not yet been investigated. Whether or not $\rho_{ph}(T)$ still follows the Bloch-Grüneisen law is not known at present. This problem of course is not trivial, considering that, say, the translational invariance of the lattice is no longer preserved. If the nature of the electron-phonon coupling in disordered or alloy metals is significantly changed from that in crystals, a saturation of ρ at high T might not be inconceivable. For example, if the T-dependence of ρ_{ph} in disordered metals is somehow weakened or diminished, ρ might become independent of T. To explore this idea, we have subtracted the *T-independent* part, i.e., ρ_0, from ρ and plotted the variation of ρ-ρ_0, or $\rho_{ph}(T)$ with T logarithmically in Fig. 3. Figure 3 shows that the magnitudes of $\rho_{ph}(T)$ in the alloy Ti–Al–V (●) and the elements Ti (○) and V (□) are compatible (to within a factor of 2–3) between 40 and 1000 K, being about 2 orders of magnitude higher than that in Al (△). This result suggests that the strength of the electron-phonon coupling is about the same (presumably within a factor of 2–3) in the three materials. The alloying of Ti, Al, and V to form Ti–Al–V does *not* seem to change the contribution of the electron-phonon coupling to resistivity. This is quite surprising in the sense that lattice disorder in the atomic level is significant in alloys. Since the observed amount of ρ_{ph} ($\approx 27\,\mu\Omega$cm at 300 K) is *not* large enough to produce a saturation of ρ, we thus conclude that it is the large ρ_0 which is most responsible for the resistivity saturation in Ti–Al–V. This point can also simply be justified by the fact that the ρ_{ph} in Ti is larger than that in Ti–Al–V between 40–1000 K, Fig. 3, but a saturation behavior of ρ is much *less* evident in Ti than in Ti–Al–V, Fig. 2.

A closer look at Fig. 3 indicates that the temperature dependence of $\rho_{ph}(T)$ in Ti–Al–V is weaker than those in Ti and V, and particularly at T above about 300 K the ρ_{ph} in Ti–Al–V is *barely* T-dependent. This temperature (≈ 300 K) is the temperature where a deviation from a linear T-dependence of ρ first becomes noticeable in the alloy, Fig. 2. The magnitude of ρ_{ph} in Ti–Al–V at 300 K is $\approx 27\,\mu\Omega$cm. This value of resistivity suggests a corresponding mean free path l_{ph} of ≈ 40 Å. This value of l_{ph} is sufficiently larger than the interatomic spacing (< 5 Å), and hence a linear T-dependent resistivity would be expected at least up to 1000 K if the Bloch-Grüneisen law were obeyed. This of course is not what is observed in Fig. 3. The *weakened* temperature dependence of ρ_{ph} in Ti–Al–V compared with that in Ti and V therefore strongly suggests that the nature of the electron-phonon coupling in very disordered metals or alloys might be quite different

from that in crystals. Obviously, it is the Ioffe-Regel criterion which poses constraints on the temperature dependence of the electron-phonon coupling. Microscopically how this weakening behavior occurs is not clear.

The behavior of ρ in Ti shown in Fig. 2 is somewhat similar to that in Nb_3Sb (ref. 1) in which ρ_0 is negligible ($\approx 1\,\mu\Omega$cm at 4 K) and ρ_{ph} ($\approx 70\,\mu\Omega$cm at 300 K) dominates the total resistivity. In the latter material a saturation (at $\approx 130\,\mu\Omega$cm) of ρ occurs at above about 600 K. Thus, the two observations in Nb_3Sb and in Ti suggest that the electron-phonon coupling alone, provided strong enough, can result in a resistivity saturation. Together with the present observation in Ti–Al–V, these results indicate that both the electron-phonon coupling and the elastic scattering of conduction electrons by lattice imperfections can contribute *equally importantly* in determining the Ioffe-Regel criterion. Similar conclusion has previously been drawn in α-particle-damaged Nb_3Ge by Wiesmann *et al.*[3]

Finally, to simplify matters, we have presumed in this work that the interatomic spacings, Debye temperatures, Fermi wave numbers, etc., in Ti, V, and Ti–Al–V are not much different. We have also confined to the temperature region where no structure transition occurs in any of the materials.

§4. Conclusion

We have studied the electrical resistivity ρ of a $Ti_{0.862}Al_{0.102}V_{0.036}$ alloy in the temperature range 4–1000 K. We observe a noticeable deviation of ρ from a linear temperature dependence above about 300 K, and in particular a saturation of ρ above about 500 K is observed. The saturation behavior is ascribed to the electron-phonon coupling and mainly to the elastic scattering of conduction electrons by lattice imperfections in the alloy. In addition, we observe that the temperature dependence of the electron-phonon coupling deviates significantly from the Bloch-Grüneisen-like behavior, showing a considerably weakened dependence on temperature.

Acknowledgments

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