Electrical and thermal conductivity of the Ti_3AlC_2 MAX phase at low temperatures

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SHORT NOTES

Electrical and thermal conductivity of the Ti_3AlC_2 MAX phase at low temperatures

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Electrical and thermal conductivities of a sample containing 96% of MAX-phase Ti_3AlC_2 and 4% of TiC were experimentally studied in the temperature range of 15–300 K. The maximum thermal conductivity is observed at approximately 75 K. As the temperature increases, the fraction of phonon heat transfer decreases from ~90% at low temperatures to ~40% at the room temperature. *Published by AIP Publishing.* https://doi.org/10.1063/1.5034158

The development of novel multifunctional materials with specific processing characteristics[1–5] is one of the most important goals of modern solid state physics.

The so-called MAX phases with a general formula of $M_{n+1}AX_n$, where M is the transition metal, A is the element of the III-A or IV-A subgroup of the periodic system, and X is carbon or nitrogen, represent a highly promising class of such modern materials.[1,6–8] These compounds possess a unique combination of properties of metals and ceramics, such as high hardness, refractoriness and elasticity, as well as good thermal and electrical conductivity.

Elucidation of the electrical and heat transfer mechanisms in these compounds is of great interest, as this provides an important tool for testing the adequacy of numerous theoretical models and identification of empirical ways to improve their processing characteristics.

In the present work, the thermal and electrical conductivity of a Ti_3AlC_2 MAX phase sample was studied.

The sample was made by sintering the original powder using a hot-pressing unit with simultaneous passage of alternating current of the order of several kA along the pressing axis through the graphite mold and the powder itself, which resulted in both heating and cleaning of the surface of powder particles from oxides due to microdischarges. The obtained sample contained 96% of Ti_3AlC_2 and 4% of TiC.

The electrical resistivity of the obtained sample was measured according to the standard four-probe method; the thermal conductivity according to the monoaxial continuous heat flux method, and the temperature decrease along the sample by a copper/constantan thermocouple.

The experimentally determined results for the electrical resistivity and thermal conductivity of the Ti_3AlC_2 sample in the temperature range of 15–320 K are presented in Fig. 1.

The results for electrical resistivity at the studied temperature range may be very accurately approximated using the equation,[9] which describes the electron-phonon and electron-defect scattering

$$\rho(T) = \rho_0 + \rho_{ph}^{s-d}(T) = \rho_0 + C_3\left(\frac{T}{\theta}\right)^3 \int_0^{\theta/T} \frac{x^3 e^x}{(e^x-1)^2}dx. \quad (1)$$

Here ρ_0 is the residual resistance; θ is the Debye temperature; C_3 is the adjustable coefficient.

Minimum approximation error $\Delta\rho/\rho \approx 0.5\%$ was achieved at the values of parameters $\rho_0 = 36.7\ \mu\Omega\,\text{cm}$, $\theta = 611.5\,\text{K}$, $C_3 = 161\ \mu\Omega\,\text{cm}$.

The calculated value of the Debye temperature is consistent with previously reported data.[10]

We note that the temperature dependence of the resistance of the sample is characterized by a small value $RRR \approx 2$ [$RRR = \rho_{ph}/\rho_0 \approx \rho(300\,\text{K})/\rho_0(4.2\,\text{K})$], which indicates a high concentration of defects.

The temperature dependence of the thermal conductivity of the sample was maximal at $Tm \approx 75\,\text{K}$.

The Wiedemann-Franz law applies in the region of elastic scattering of electrons[11]

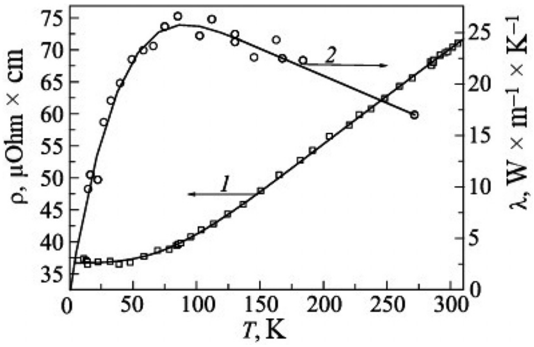

Fig. 1. Electrical resistivity (*1*) and thermal conductivity (*2*) of the Ti_3AlC_2 MAX phase. The symbols represent experimentally obtained values, the lines are drawn for $\rho(T)$ in accordance with (1) and for $\lambda(T)$ by eye.

$$\lambda_e \approx L_0 T/\rho. \qquad (2)$$

Here λ_e is the electronic thermal conductivity, $L_0 = 2.45 \times 10^{-8}$ WΩ K^{-2} is the Sommerfeld value of the Lorentz number.

The conditions for elastic scattering of electrons are satisfied at low temperatures, where elastic electron-defect scattering is predominant. Therefore, $\rho(T) \approx \rho_0$, $\lambda_e \approx L_0 T/\rho_0$, which results in $\lambda_e \approx 1$ W m^{-1} K^{-1} at $T \approx 15$ K. The comparison of this value with the experimentally obtained value of the low-temperature thermal conductivity (≈ 10 W m^{-1} K^{-1}) shows that 90% of heat is transferred by phonons at low temperatures.

Elastic electron-phonon scattering predominates to the right side of the thermal conductivity maximum at sufficiently high temperatures.[11] Here, $\rho(T) \approx \rho_0(1 + \alpha T)$ and $\lambda_e = L_0 T/\rho(T) \approx$ const. Estimation according to (2) results in $\lambda_e = 10$ W m^{-1} K^{-1} at $T \approx 300$ K, which is approximately 60% of the experimental value of thermal conductivity experimental at this temperature. Thus, approximately 40% of the transferred heat is accounted for by phonons.

Consequently, the fraction of heat transferred by phonons in the Ti_3AlC_2 MAX phase decreases with the increase in temperature. This result is consistent with the conclusions of the theory,[11] since the electronic thermal conductivity is constant at high temperatures and the phonon conductivity decreases as $1/T$.

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