Z. Kristallogr. **224** (2009) 56–58 / **DOI** 10.1524/zkri.2009.1051
© by Oldenbourg Wissenschaftsverlag, München

Anisotropic electrical and thermal conductivities of the $Al_{76}Co_{22}Ni_2$ decagonal approximant

Ana Smontara*, [I], Denis Stanić[I], Igor Smiljanic[I], Janez Dolinšek[II] and Peter Gille[III]

[I] Institute of Physics, Laboratory for the Study of Transport Problems, Bijenička 46, POB 304, 10001 Zagreb, Croatia
[II] J. Stefan Institute, University of Ljubljana, Jamova 39, 1000 Ljubljana, Slovenia
[III] Ludwig-Maximilians-Universität München, Department of Earth and Environmental Sciences, Crystallography Section, Theresienstrasse 41, 80333 München, Germany

Received June 13, 2008; accepted August 22, 2008

Thermal conductivity / Quasicrystals / Decagonal approximants / Y–Al–Ni–Co phase

Abstract. The electrical (σ) and thermal conductivity (λ) of $Al_{76}Co_{22}Ni_2$ decagonal approximant has been measured along three orthogonal directions a^*, b and c of the $Al_{76}Co_{22}Ni_2$ unit cell, where (a, c) monoclinic atomic planes are stacked along the perpendicular b direction. Electrical conductivity is relatively high in all crystalline directions, appearing in the order $\sigma^b \gg \sigma^c > \sigma^{a^*}$. Thermal conductivity appears in the same order $\lambda^b > \lambda^c > \lambda^{a^*}$, so that b is the most conducting direction for both electricity and heat. The results are compared to the reported anisotropic electrical and thermal conductivity of the *d*-Al–Ni–Co decagonal quasicrystal.

Introduction

Decagonal quasicrystals can be structurally viewed as a periodic stack of quasiperiodic atomic planes, whereas decagonal quasicrystals are two-dimensional quasicrystals. This makes decagonal quasicrystal especially suitable to study the effect of quasiperiodicity on the electrical and thermal conductivity of the material, as a given property can be investigated on the same sample along the quasiperiodic and periodic directions. Decagonal quasicrystals exhibit anisotropy in their electrical and thermal conductivities, which is related to the structural details of a particular decagonal phase, depending on the number of quasiperiodic layers in one periodic unit [1]. The basic question is whether the observed anisotropy is a consequence of the quasiperiodic structural order within the atomic layers versus the periodic order in the perpendicular direction or the anisotropy is rather a consequence of complex local atomic order on the scale of near-neighbor atoms with no direct relationship to the quasiperiodicity. While this question has so far not been answered satisfactorily for the decagonal quasicrystals, the situation is clearer for approximants of the decagonal phase. Here, we report an experimental study of the electrical and thermal conductivities of a complex metallic alloy $Al_{76}Co_{22}Ni_2$ which is the member of family $Al_{13-x}(Co_{1-y}Ni_y)_4$, known also as the Y–Al–Ni–Co phase. This compound is a monoclinic approximant of the decagonal phase with two atomic layers within one periodic unit along the stacking direction and a relatively small unit cell, comprising 32 atoms. Therefore the structure of $Al_{13-x}(Co_{1-y}Ni_y)_4$ is relatively simple as compared to the much higher complexity of the $Al_4(Cr, Fe)$ phase with 306 atoms/unit cell [2]. The measurements of the $Al_{76}Co_{22}Ni_2$ thus allow comparison of this simple decagonal approximant to the closely related *d*-Al–Ni–Co quasicrystal. We show that the $Al_{76}Co_{22}Ni_2$ is the is best conducting, both electrical and thermal, along the direction perpendicular to the (a, c) atomic planes, whereas both conductivities are smaller in this atomic plane, as also observed in the related *d*-Al–Ni–Co quasicrystal [3–6].

Experimental

The single crystal used in our study was grown from an incongruent Al-rich melt of initial composition $Al_{81.9}Co_{14.5}Ni_{3.6}$ by the Czochralski method using a native seed. The composition of the crystal was $Al_{76}Co_{22}Ni_2$ and its structure matched well to the monoclinic unit cell of the $Al_{75}Co_{22}Ni_3$ [7]. In order to perform crystalline-direction-dependent studies, we have cut from the ingot three bar-shaped samples of dimensions $1 \times 1 \times 7\ mm^3$, with their long axes along three orthogonal directions. The long axis of the first sample was along [010] direction (designated in the following as (b), which corresponds to the periodic direction in the related *d*-Al–Ni–Co quasicrystal. The (a, c) monoclinic plane corresponds to the quasiperiodic plane in decagonal quasicrystal and the second sample was cut with its long axis along [001] (c) direction, whereas the third one was cut along the direction perpendicular to the (b, c) plane. This direction is designated as a^* (it lies in the monoclinic plane at an angle 26° with respect to a and perpendicular to (c). The other two short axes of the samples were along two other orthogonal axes

* Correspondence author (e-mail: ana@ifs.hr)

Bereitgestellt von | provisional account
Unangemeldet
Heruntergeladen am | 28.08.17 17:14

as well. The so-prepared samples enabled us to determine the anisotropic electrical and thermal conductivities along the three orthogonal directions of the investigated monoclinic $Al_{76}Co_{22}Ni_2$ compound. Electrical conductivity was measured along the a^*, b and c directions between 300 and 1.5 K using the standard four-terminal technique, while thermal conductivity was measured on the same specimens using an absolute steady-state heat-flow method in the temperature range 2–300 K. The thermal flux through the samples was generated by a 1 kΩ RuO_2 chip-resistor, glued to one end of the sample, while the other end was attached to a copper heat sink. The temperature gradient across the sample was monitored by a chromel-constantan differential thermocouple.

Electrical and thermal conductivities

Electrical conductivity $\sigma(T)$ data for the three crystalline directions are displayed in Fig. 1. The conductivity is the highest along the b direction perpendicular to the monoclinic planes, where its room temperature value amounts $\sigma^b{}_{300\,K} = 4$ $(\mu\Omega\,m)^{-1}$. The two in-plane conductivities are lower, amounting $\sigma^c{}_{300\,K} = 1.7$ $(\mu\Omega\,m)^{-1}$ for the c direction and $\sigma^{a^*}{}_{300\,K} = 1.3$ $(\mu\Omega\,m)^{-1}$ for the $a*$ direction. While σ^b is considerably higher than σ^{a^*} and σ^c by a factor of about 3, the two in-plane conductivities are much closer, $\sigma^c\sigma^{a^*} \sim 1.3$. The above conductivity values, appearing in the order $\sigma^a < \sigma^c \ll \sigma^b$, reveal that $Al_{76}Co_{22}Ni_2$ is good electrical conductor along all three crystalline directions.

It is interesting to note that the ratios of the conductivities along different crystalline directions vary little over the whole investigated temperature range 300–1.5 K (inset in Fig. 1), amounting at room temperature $\sigma^b\sigma^{a^*} \sim 3.2$, $\sigma^b/\sigma^c \approx 2.4e$ and $\sigma^c/\sigma^{a^*} \sim 1.3$. Comparing the anisotropic conductivity of $Al_{76}Co_{22}Ni_2$ to that of the d-Al–Ni–Co quasicrystal [2, 5, 8] we find that the conductivities of both compounds are about the same along the "periodic" direction with metallic behavior. Conductivity in monoclinic plane is somewhat higher than in quasicrystalline plane, but the overall ratio of in plane to out of plane resistivity is similar. The only significant difference is in the small negative temperature coefficient of the resistivity in quasicrystalline plane of decagonal AlCoNi alloys.

Measured thermal conductivity $\lambda(T)$ along the three crystalline directions is displayed in Fig. 2. The lattice (phonon) contribution $\lambda_{lat} = \lambda - \lambda_e$ was estimated by subtracting the electronic contribution λ_e from the total thermal conductivity using the Wiedemann-Franz law ($\lambda_e = L(T) \cdot \sigma(T) \cdot T$) with temperature-dependent effective Lorentz number $L(T)$ (Eq. (11) from Ref. 9) and the measured electrical conductivity data $\sigma(T)$ from Fig. 1. The temperature dependent Lorentz number $L(T)$ in the limit $T \to 0$, goes towards the empirical Wiedemann-Franz law value $L_o = 2.45 \times 10^{-8}\,WK^{-2}$ [9]. Note, the empirical Wiedemann-Franz law $\lambda_e = L_o \cdot s(T) \cdot T$ is valid at very low temperatures ($T \leq 10$ K) and at high (room) temperatures. This is because in these regions the electrons are scattered elastically. Therefore, at $T \sim 10$–100 K deviations from the law are observed which imply that $\lambda_e/\sigma(T) \cdot T$ depends on T [9]. In this way estimated lattice thermal conductivity λ_{lat} gives an indication of the anisotropy of the phonon spectrum.

At room temperature, we get the following anisotropy: $\lambda^{a^*} = 12.5$ W/mK, $\lambda^{a^*}{}_e = 9.1$ W/mK with their ratio $(\lambda^{a^*}{}_e/\lambda^{a^*})_{300\,K} = 0.7$, $\lambda^b = 46.3$ W/mK, $\lambda^b{}_e = 29.2$ W/mK with $(\lambda^b{}_e/\lambda^b)_{300\,K} = 0.6$ and $\lambda^c = 17.4$ W/mK, $\lambda^c{}_e = 12.2$ W/mK with $(\lambda^c{}_e/\lambda^c)_{300\,K} = 0.7$. Electrons are thus majority heat carriers at room temperature for all three directions. The anisotropic total thermal conductivities appear in the order $\lambda^b > \lambda^c > \lambda^a$ and similarly $\lambda^b{}_e > \lambda^c{}_e > \lambda^{a^*}{}_e$ which is identical to the order in which the anisotropic electrical conductivities appear (Fig. 1): $\sigma^b > \sigma^c > \sigma^a$ The lattice thermal

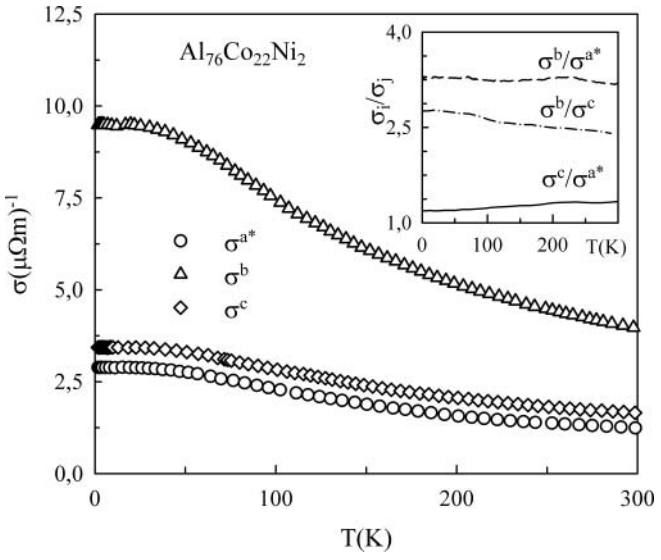

Fig. 1. Temperature-dependent electrical conductivity of $Al_{76}Co_{22}Ni_2$ along three orthogonal crystalline directions a^*, b and c. The inset shows the conductivity ratios σ_i/σ_j ($i, j = a^*, b, c$).

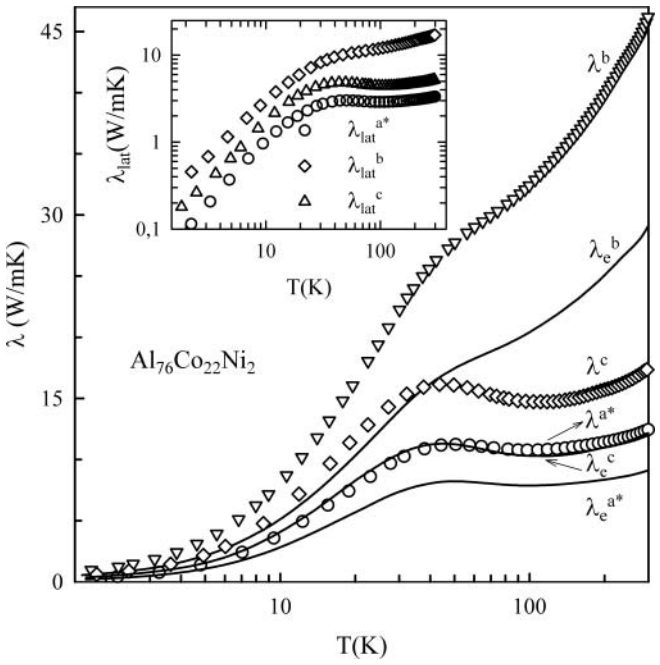

Fig. 2. Temperature-dependent thermal conductivity of $Al_{76}Co_{22}Ni_2$ along three orthogonal crystalline directions a^*, b and c. Solid curves are the electronic contribution λ_e to the total thermal conductivity. Inset: lattice thermal conductivity $\lambda_{lat} = \lambda - \lambda_e$. along three orthogonal crystalline directions a^*, b and c.

Bereitgestellt von | provisional account
Unangemeldet
Heruntergeladen am | 28.08.17 17:14

conductivity is shown in the inset of Fig. 2. We observe that anisotropic λ_{lat} again appear in the same order, $\lambda^b{}_{lat} > \lambda^c{}_{lat} > \lambda^{a^*}{}_{lat}$ so that the lattice conductivity is the highest along the b direction perpendicular to the (a, c) atomic layers, whereas the two in-plane conductivities are lower and show smaller anisotropy. Comparing the anisotropic lattice thermal conductivity of $Al_{76}Co_{22}Ni_2$ to that of the d-Al−Ni−Co quasicrystal [5] we find that the conductivities of both compounds at temperature above 50 K show are about the same.

While it is expected that the anisotropic electronic thermal conductivities should appear in the same order as the anisotropic electrical conductivities (both are related to the electronic density of states), it is not *a priori* obvious that the anisotropic lattice thermal conductivities should also appear in this order, as λ_{latt} is related to the vibrational density of states. Nevertheless, our results show that $Al_{76}Co_{22}Ni_2$ best conducts, both charge and heat, along the b direction, whereas both conductivities are smaller in the (a, c) plane.

Conclusion

We have investigated anisotropic electrical and thermal conductivities of the $Al_{76}Co_{22}Ni_2$ decagonal approximant. Electrical conductivity is high in all three crystalline directions, with the room temperature values in the range 4–12.4 $(\mu\Omega\,m)^{-1}$. There exists appreciable anisotropy between the in-plane electrical conductivity and the conductivity along the perpendicular b direction, whereas the anisotropy between the two in-plane directions a^* and c is much smaller. The anisotropic conductivities appears in the order $\sigma^b \gg \sigma^c > \sigma^{a^*}$, so that b direction is the most electrically conducting one. Anisotropic thermal conductivities appear in the order $\lambda^b > \lambda^c > \lambda^{a^*}$ and the same order applies to their electronic part, $\lambda^b{}_e > \lambda^c{}_e > \lambda^{a^*}{}_e$, estimated from the Wiedemann-Franz law using temperature-dependent effective Lorentz number $L(T)$. This order is identical to the order in which the anisotropic electrical conductivities appear. The anisotropic lattice thermal conductivity appears in the same order, $\lambda^b{}_{lat} > \lambda^c{}_{lat} > \lambda^{a^*}{}_{lat}$. Thus, $Al_{76}Co_{22}Ni_2$ is the is best conducting, both electrically and thermally, along the b direction perpendicular to the atomic planes, whereas both conductivities are smaller in the (a, c) atomic plane. The above results show good analogy between the anisotropic thermal and electrical conductivities of the quasiperiodic d-Al−Ni−Co quasicrystal on one hand and the periodic $Al_{76}Co_{22}Ni_2$ (Y−Al−Ni−Co) decagonal approximant on the other hand. This suggests that long-range quasiperiodicity of the structure is of marginal importance for the anisotropy, which originate the from the complex local atomic order on the scale of nearest-neighbor atoms.

Acknowledgments. This work was done within the activities of the 6th Framework EU Network of Excellence "Complex Metallic Alloys" (Contract No. NMP3-CT-2005-500140) and has been supported in part by the Ministry of Science, Education and Sports of Republic Croatia through the Research Project No. 035-0352826-2848.

References

[1] Krajčí, M.; Hafner, J.: Highly anisotropic electronic structure in decagonal quasicrystals and approximants. Phys. Rev. B **58** (1998) 5378–5383.

[2] Dolinšek, J.; Jeglič, P.; Komelj, M.; Vrtnik, S.; Smontara, A.; Smiljanic, I.; Bilušic, A.; Ivkov, J.; Stanić, D.; Zijlstra, E. S.; Bauer, B.; Gille, P.: Origin of anisotropic nonmetallic transport in the $Al_{80}Cr_{15}Fe_5$ decagonal approximant. Phys. Rev. B **76** (2007) 174207-13, and references therein.

[3] Martin, S.; Hebard, A. F.; Kortan, A. R.; Thiel, F. A.: Transport properties of $Al_{65}Cu_{15}Co_{20}$ and $Al_{70}Ni_{15}Co_{15}$ decagonal quasicrystals. Phys. Rev. Lett. **67** (1991) 719–723.

[4] Shu-yuan, L.; Xue-mei, W.; Lu L.; Dian-lin, Z.; He, L.X.; Kuo, K. X.: Anisotropic transport properties of a stable two-dimensional quasicrystal $Al_{62}Si_3Cu_{20}Co_{15}$. Phys. Rev. B **41** (1990) 9625–9627.

[5] Dian-in, Z.; Shao-chun, C.; Yun-ping, W.; Li, L.; Xue-mei, W.: Anisotropic Thermal conductivity of the 2D single Quasicrystals: $Al_{65}Ni_{20}Co_{15}$ and $Al_{62}Si_3Cu_{20}Co_{15}$. Phys. Rev. Lett. **66** (1991) 2778–2781.

[6] Edagawa, K.; Chernikov, M. A.; Bianchi, A. D.; Felder, E.; Gubler, U.; Ott, H. R.: Low-Temperature Thermodynamic and Thermal-transport Properties of Decagonal $Al_{65}Cu_{20}Co_{15}$. Phys. Rev. Lett. **77** (1996) 1071–1074.

[7] Zhang, B.; Gramlich, V.; Steurer, W.: $Al_{13-x}(Co_{1-y}Ni_y)_4$, a new approximant of the decagonal quasicrystal in the Al–Co–Ni system. Z. Kristallogr. **210** (1995) 498–503.

[8] Yun-pin, W.; Dian-lin Z.: Universality in the resistivity-temperature relationship for decagonal quasicrystals. Phys. Rev.B. **49** (1994) 13204–13207.

[9] Dolinšek, J.; Vrtnik, S.; Klanjšek, M.; Jagličić, Z.; Smontara, A.; Smiljanić., I.; Bilušić, A.; Yokoyama, Y.; Inoue, A.; Landauro, C. V.: Intrinsic electrical, magnetic, and thermal properties of single-crystalline $Al_{64}Cu_{23}Fe_{13}$ icosahedral quasicrystal: Experiment and modeling. Phy. Rev. B **76** (2007) 054201-9.

Bereitgestellt von | provisional account
Unangemeldet
Heruntergeladen am | 28.08.17 17:14