Influence of spins on the electronic transport coefficients of the icosahedral $Al_{64}Cu_{23}Fe_{13}$ quasicrystal

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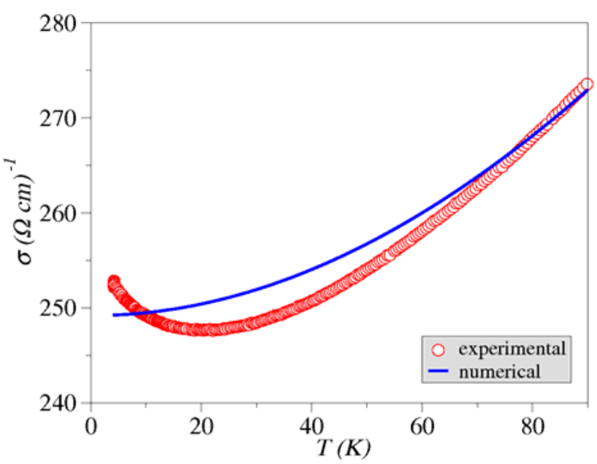
Abstract – In the present work we propose a model for the spectral conductivity which can explain the experimentally obtained transport coefficients of the i-$Al_{64}Cu_{23}Fe_{13}$ quasicrystal. Besides the contributions due to the Hume-Rothery effect and *sp-d* hybridization, this model also considers the contribution of the spins which is important in the low temperature regime.

In a recently published paper by Dolinšek and co-workers[1], a model for the spectral conductivity (SC), originally proposed by Landauro and Solbrig [2], was applied to determine the temperature dependent transport coefficients of a new class of material, called quasicrystal, which is relevant for its potential industrial applications [3]. In such work SC was modeled by means of Lorentzian functions in agreement with ab-initio results (linear muffin-tin orbital basis and Kubo-Greenwood formula). According to the reference [1] the results are in good agreement with experimental values for a broad range of temperature (from 4 K to 315 K). However, for the case of the electrical conductivity, there is a noticeable disagreement with the experiments at low temperatures (<90 K) (see figure 1) which is associated to magnetic effects that are not considered in such model. For the others transport coefficients the disagreement with the experiments is practically negligible.

In this work the influence of the spins on the transport coefficients is modeled including in the SC a Gaussian function. Then, employing the inverse Matthiessen rule, valid for QCs, we add this contribution to the contributions obtained from the original model. The analytical and numerical calculations are in good agreement with the experiments in the whole range of temperatures, even at low temperatures (<90 K). Moreover, for the case of the electrical conductivity, the analytical results allow us to predict a conductivity minimum around of ~19.4 K, also in good agreement with the experimental value of 21 K (see figure 2).



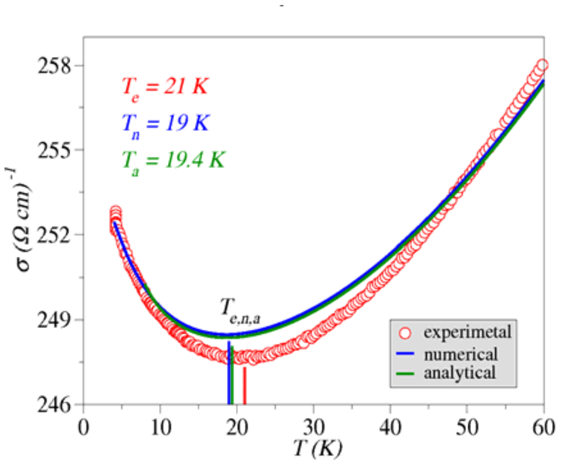


Fig. 1: electrical conductivity of the QC i-$Al_{64}Cu_{23}Fe_{13}$. It is shown noticeable disagreement withe the experimental values at low temperatures (<90K) with the model applied by Dolinsek and co-workers [1]

Fig. 2: electrical conductivity of the QC i-$Al_{64}Cu_{23}Fe_{13}$. The proposed model for the contribution of the spins allow us to reproduce the experiments in the whole range of temperatures, specially at very low temperatures.

References

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