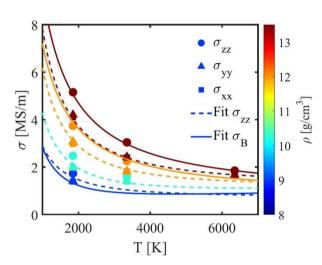
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28th April 2022, 3:00 pm Uwe Kleinschmidt Statistical Physics

Electrical and Thermal Conductivity of Solid Iron under Earth Core Conditions

We used ab initio simulations based on density functional theory to calculate the electrical and thermal conductivity of solid iron in face centered cubic and hexagonal phase - with three different c/a-ratios - up to earth core conditions. In particular, we evaluated Onsager coefficients in linear response theory. The conductivity results show big differences by comparing the two different structures. We found an anisotropic behavior of the conductivity tensor in the hexagonal phase. Our calculated thermal conductivity values



are up to two times larger than results from experimental measurements. The calculated electrical conductivity in our work is much lower in high pressure and temperature regions compared to experimental measurements.



Talk: English Slides: English

Location: Great Lecture Hall, HS1, Institute for Physics, Albert-Einstein Str. 24

Hybrid-Meeting: https://uni-rostock-de.zoom.us/j/67191822515?pwd=UTVJSXVPaDVLV0ZSZW9LR3NRVWF2UT09