Electrical resistivity of liquid iron with high concentration of light element impurities

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Abstract

The Earth's outer core mainly consists of liquid iron, enriched with several weight percent of lighter elements, such as silicon, oxygen, sulfur or carbon. Electrical resistivities of alloys of this type determine the stability of the geodynamo. Both computational and experimental results show that resistivites of Fe-based alloys deviate significantly from values of pure Fe. Using optical conductivity values computed with the Kubo-Greenwood formalism for DFT-based molecular dynamics results, we analyze the high-P and T behavior of resitivities for Fe-alloys containing various concentrations of sulfur, oxygen and silicon. As the electron mean free path length in amorphous and liquid material becomes comparable to interatomic distances at high P and T, electron scattering is expected to be dominated by the short-range order, rather than T-dependent vibrational contributions, and we describe such correlations in our results. In analogy to macroscopic porous media, we further show that resistivity of a liquid metal-nonmetal alloy is determined to first order by the resistivity of the metallic matrix and the volume fraction of non-metallic impurities.

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