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Theoretical prediction of the electronic transport properties of the Al-Cu alloys based on the first-principle calculation and Boltzmann transport equation[1] GARAM CHOI, WON BO LEE, Seoul Natl Univ — Metal alloys, especially Al-based, are commonly-used materials for various industrial applications. In this paper, the Al-Cu alloys with varying the Al-Cu ratio were investigated based on the first-principle calculation using density functional theory. And the electronic transport properties of the Al-Cu alloys were carried out using Boltzmann transport theory. From the results, the transport properties decrease with Cu-containing ratio at the temperature from moderate to high, but with non-linearity. It is inferred by various scattering effects from the calculation results with relaxation time approximation. For the Al-Cu alloy system, where it is hard to find the reliable experimental data for various alloys, it supports understanding and expectation for the thermal electrical properties from the theoretical prediction.

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