

Analysis of Thermal Transport in Graphite Intercalated Compounds

The University of Tokyo, School of Engineering [Wu Yijia]

Purpose Uncover the mechanisms observed in GICs experiments.

Outline NEMD Simulation of FeCl₃-GIC system

Result Suppression and Control of Thermal Transport

Computing system:
node-hour
Software
parallelize

SQUID General Purpose CPU nodes
35 node-hour
LAMMPS
152 nodes

