Electrical conductivity of warm expanded aluminum

GERALD FAUSSURIER, CHRISTOPHE BLANCARD, PATRICK RENAUDIN, CEA,
PIER-LUIGI SILVESTRELLI, Università di Padova, CEA COLLABORATION,
UNIVERSITÀ DI PADOVA COLLABORATION

The electronic and ionic structures of warm expanded aluminum are determined self-consistently using an average-atom formalism based on density-functional theory and Gibbs-Bogolyubov inequality. Ion configurations are generated using a least-square fit of the pair distribution function deduced from the average-atom model calculations. The electrical conductivity is computed from the Kubo-Greenwood formula implemented in a molecular dynamics scheme based on density-functional theory. This method goes beyond the Ziman approach used in the average-atom formalism. Moreover, it is faster than performing quantum molecular dynamics simulations to obtain ion configurations for the conductivity calculation. Numerical results and comparisons with experiments are presented and discussed.