Abstract Submitted
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Calculation of transmission in low symmetry lattices and its application[1] MANOJ SRIVASTAVA, University of Florida, X.-G. ZHANG, Oak Ridge National Laboratory, H.-P. CHENG, University of Florida — Conductance calculations using first-principles plane-wave method have been performed to study scattering in high symmetry lattices [1]. The Original implementation of above method in the code Quantum Espresso [2] has limitation that it only allows the transport direction along a lattice vector perpendicular to the basal plane formed by two other lattice vectors, e.g., the c-axis of a tetragonal lattice. We have generalized this method to non-orthogonal lattices with transport direction not necessarily aligned with any lattice vector. With the generalization, we have calculated transmission, reflection coefficients in transport direction and velocity of Bloch's states along various directions in the lattice. With first-principles results as input for Boltzmann's transport equations, we have obtained resistance of grain boundaries in Cu such as twin(111), $\Sigma 5(100)$ and $\Sigma 7(111)$.

[1] Hyoung Joon Choi and Jisoon Ihm, Phys. Rev. B 59, 2267 (1999)
[2] http://www.quantum-espresso.org/

[1]US/DOE/BES/DE-FG02-02ER45995, Portion of This research was conducted at the CNMS , which is sponsored at ORNL by the Division of Scientific User Facilities, U.S. Department of Energy.

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