Ab initio calculations of electronic transport properties and of the thermoelectric phonon drag effect in semiconductors

Raja Sen∗1, Jelena Sjakste1, and Nathalie Vast1

1Laboratoire des Solides Irradiés – CEA-DRF-IRAMIS, Centre National de la Recherche Scientifique - CNRS, Institut Polytechnique de Paris, Polytechnique - X – LSI - UMR 7642, 28 route de Saclay, F-91128 Palaiseau Cedex, France

Résumé

In the present work, we first consider the state-of-the-art computational techniques to accurately calculate the electronic transport properties of n-doped silicon. The calculations, performed with the EPW code [1], are based on the iterative solution of the linearized Boltzmann transport equation (BTE) coupled to the data obtained using density functional theory and density functional perturbation theory. Concurrently, a special focus is made on understanding the enhancement of the Seebeck coefficient by electron-phonon coupling, known as the ”phonon-drag” effect [2]. To take this effect into account, we modified the standard EPW code so that it allows us to solve the BTE for electronic transport in presence of non-equilibrium phonon populations introduced by a temperature gradient. We will present our recent results related to electron-phonon scattering times, phonon and/or impurity limited carrier mobility, as well as the Seebeck coefficient of silicon. Our results for n-doped silicon not only show a good agreement with the experimental data [3] but also pave the way to further understand the contribution of phonon-drag in semiconductor nanostructures, which still remains largely unexplored. References


Mots-Clés: Density functional theory, electronic transport, Seebeck, Phonon, drag

∗Intervenant